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See Gang Wu *et al.*, page 682.
First ^{43}Ca NMR characterization of Ca^{2+} ion binding to G-quartets.
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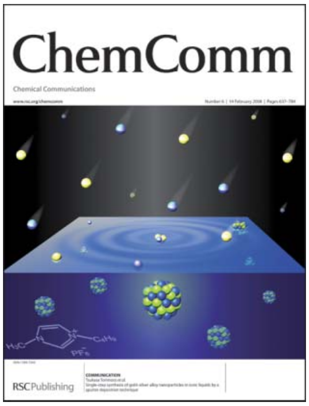

Inside cover
See Tsukasa Torimoto *et al.*, page 691.
The simultaneous sputter deposition of gold and silver onto ionic liquid formed bimetallic alloy nanoparticles.
Image reproduced by permission of Ken-ichi Okazaki, Tomonori Kiyama, Kaori Hirahara, Nobuo Tanaka, Susumu Kuwabata and Tsukasa Torimoto from *Chem. Commun.*, 2008, 691.

CHEMICAL TECHNOLOGY

T9

Chemical Technology highlights the latest applications and technological aspects of research across the chemical sciences.

Chemical Technology
February 2008/Volume 5/issue 2
www.rsc.org/chemicaltechnology

FEATURE ARTICLES

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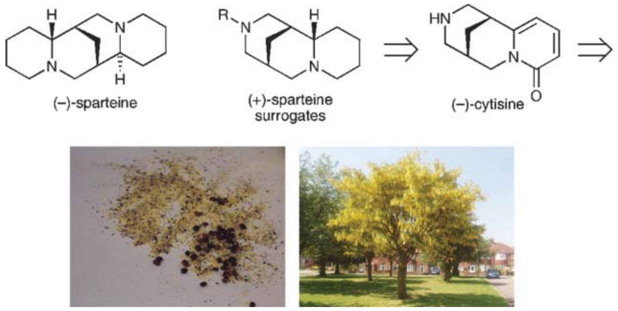
Basic instinct: design, synthesis and evaluation of (+)-sparteine surrogates for asymmetric synthesis

Peter O'Brien*

An overview of synthetic routes to the (+)-sparteine surrogates and a detailed comparison with (−)-sparteine in a range of asymmetric reactions is presented.



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FEATURE ARTICLES

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Materials for hydrogen storage: current research trends and perspectives

Annemieke W. C. van den Berg and Carlos Otero Areán*

Widespread use of hydrogen as a fuel for vehicles requires development of efficient means for on-board storage. Several kinds of material hold potential for that purpose but, can their performance be improved on?

COMMUNICATIONS

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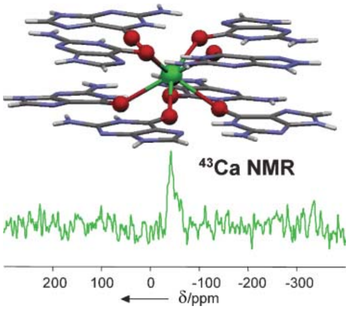
Direct NMR evidence for Ca^{2+} ion binding to G-quartets

Irene C. M. Kwan, Alan Wong, Yi-Min She,
Mark E. Smith and Gang Wu*

The first ^{43}Ca NMR characterization of Ca^{2+} binding to G-quartets is described.



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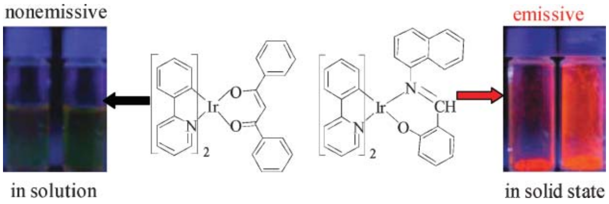
Aggregation-induced phosphorescent emission (AIPE) of iridium(III) complexes

Qiang Zhao, Lei Li, Fuyou Li,* Mengxiao Yu,
Zhipan Liu,* Tao Yi and Chunhui Huang*

Intermolecular packing switches the non-emissive ^3LX excited state to the emissive ^3MLLCT transition, resulting in a novel aggregation-induced phosphorescent emission of iridium(III) complexes, which is confirmed by X-ray diffraction studies as well as theoretical calculations.



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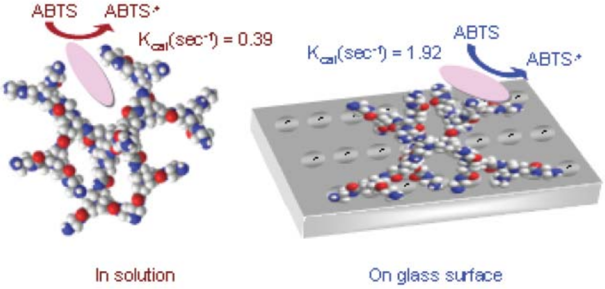
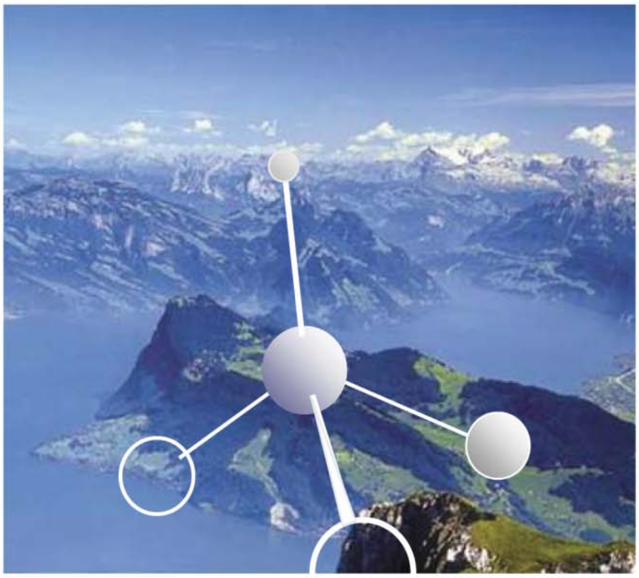
Supramolecular mimetic peroxidase based on hemin and PAMAM dendrimers

Maria Angela Castriciano, Andrea Romeo,
Maria Camilla Baratto, Rebecca Pogni and
Luigi Monsù Scolaro*

Supramolecular non-covalent adducts between hemin and PAMAM dendrimers adsorb onto solid surfaces, where they exhibit enhanced peroxidase activity with respect to the solution phase.



EUCHEM Conference on Stereochemistry



Known as the '**Bürgenstock Conference**', this annual meeting has become famous as an outstanding international chemistry conference because of its high scientific quality, an optimal setting for intense interdisciplinary discussion, and a magnificent location above the lake of Lucerne in Switzerland. Stereochemistry is the underlying principle by which we understand the processes of life and the properties of matter at the molecular level. It is a key element not only in all chemical disciplines, but also in molecular biology, molecular medicine, biophysics, and material design. The 'Bürgenstock Conference' has grown over the years into a multidisciplinary conference where frontier science is discussed. For accounts of the 2007-conference see: a) J. Gardiner, H. W. Lam, *Chimia* **2007**, *61*, 378. b) M. L. Maddess, A. F. M. Kilbinger, *Chem. Commun.* **2007**, 3231. (**DOI:** 10.1039/b707067p)

The 43rd EUCHEM Conference on Stereochemistry (Bürgenstock-Conference 2008)

will be held under the presidency of **Prof. Don Hilvert**, ETH Zurich, Switzerland, from the

12th to the 18th April 2008 at Fürigen on the Bürgenstock, Switzerland

Attendance will be limited to ca.120 participants. The organisers (the president: Don Hilvert and the members of the committee: François Diederich, Peter Kündig, Klaus Müller, Philippe Renaud, and Jay Siegel) will aim at a good balance of younger and more experienced participants from academic and industrial laboratories. Following its long tradition the detailed program (names of speakers and lecture titles) is not announced prior to the conference and both lecturers and participants are requested to stay for the entire conference.

As previous Bürgenstock Conferences, the 2008 edition will again be highly interdisciplinary, covering many areas of chemistry in its main body, but allowing also for relevant highlights from neighboring disciplines, with due focus on structural and mechanistic aspects in all contributions. Specifically, lectures will cover organic and metal-organic chemistry: new reactions, new reagents, novel synthetic strategies; asymmetric catalysis, advances in enantioselective control, evolutionary methods and technologies in organic chemistry, as well as complex natural product synthesis; frontier chemistry at the interfaces to biology and material science: structural and mechanistic biology, carbohydrate and protein chemical biology, novel molecular probes of biological functions, advances in fragrance chemistry, non-ribosomal peptide synthesis, functional and structural design of biomolecules and polymers.

The program consists of 14 plenary lectures with ample time for discussions so that each topic can be presented fully and be examined from different angles and perspectives. Lectures and discussions are held in the mornings and the evenings. The afternoons are free for recreation, informal discussions, and poster sessions.

Please check the conference web-page for more details and registration procedures.

http://www.stereochemistry-buergenstock.ch/

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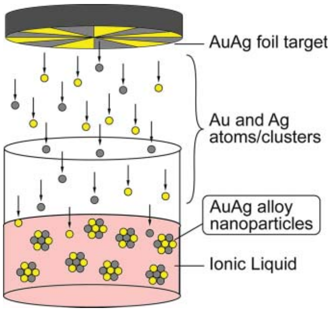
Single-step synthesis of gold–silver alloy nanoparticles in ionic liquids by a sputter deposition technique

Ken-ichi Okazaki, Tomonori Kiyama, Kaori Hirahara, Nobuo Tanaka, Susumu Kuwabata and Tsukasa Torimoto*

Simultaneous sputter deposition of gold and silver onto ionic liquids resulted in the formation of bimetallic alloy nanoparticles that exhibited composition-sensitive surface plasmon resonance, the peak wavelength being red-shifted with an increase in the surface area of the gold foil targets sputtered.



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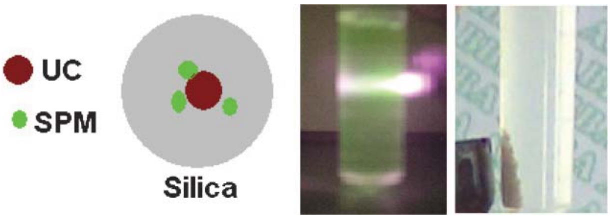
Monodisperse silica nanoparticles encapsulating upconversion fluorescent and superparamagnetic nanocrystals

Zhaoyang Liu,* Guangshun Yi, Haitao Zhang, Jun Ding, Yongwei Zhang and Junmin Xue*

By encapsulating upconversion fluorescent nanocrystals (UC) and superparamagnetic nanocrystals (SPM) in silica shells, a novel type of nanocomposites, detectable by their upconversion fluorescence and addressable by a magnetic field, was synthesized.



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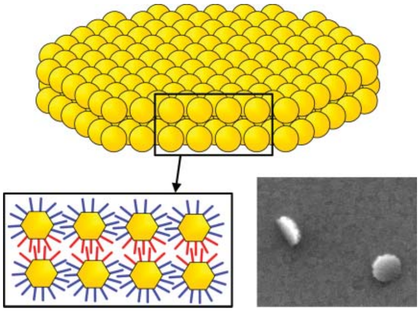
Disk micelles from amphiphilic Janus gold nanoparticles

Jeroen van Herrikhuyzen, Giuseppe Portale, Jeroen C. Gielen, Peter C. M. Christianen, Nico A. J. M. Sommerdijk, Stefan C. J. Meskers* and Albertus P. H. J. Schenning*

Janus gold nanoparticles are synthesised *via* a simple preparation method and behave as amphiphiles self-assembling in water into disk-shaped micelles.

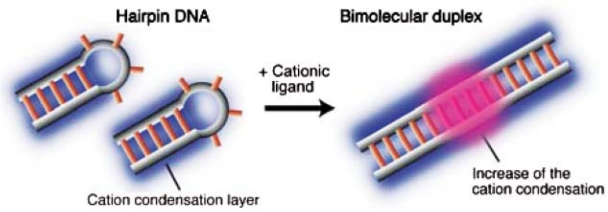


700

Capture of cationic ligands bound diffusely to base pairs during DNA refolding

Shu-ichi Nakano, Toshimasa Kirihata and Naoki Sugimoto*

The intrinsic binding affinities for metal ions, polyamines, and oligolysine peptides diffusely bound to base-paired sites in DNA were obtained by monitoring the shift of the hairpin–duplex equilibrium of the self-complementary DNA sequences.



RESEARCH CONFERENCES

ESF-COST High-Level Research Conference

Natural Products Chemistry, Biology and Medicine

Hotel Villa del Mare, Acquafredda di Maratea • Italy
18-23 May 2008

The conference will gather together some of the current and future leaders in the field of natural products and related areas to discuss the latest developments in the field and exchange ideas, foster collaborations, and promote education and training of young students. Although the majority of the speakers and attendees will be from the EU, representatives from the US, Japan, Singapore and Australia will also be present. About 120 participants are expected to attend.

It will primarily focus on the synthesis, biology and medicine of naturally occurring substances and their designed analogues as well as related areas, such as chemical synthesis technologies and isolation.

The meeting will serve to bring together researchers from several parts of the EU and from around the world to discuss the latest developments in the field and to provide opportunities for young students to advance their education and training. Time will be alloted to poster presentations.

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M. Léon Ghosez, UCL Louvain, BE
Athanassios Giannis, Leipzig U., DE
Veronique Gouverneur, Oxford U., UK
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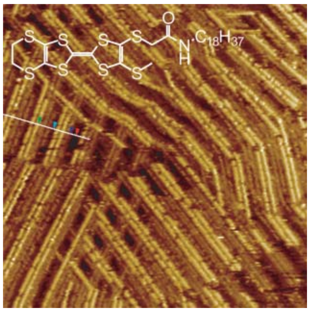
Bottom-up assembly of high density molecular nanowire cross junctions at a solid/liquid interface

Shengbin Lei, Josep Puigmartí-Luis, Andrea Minoia, Mark Van der Auweraer, Concepció Rovira, Roberto Lazzaroni,* David B. Amabilino* and Steven De Feyter*

A monoalkylated tetrathiafulvalene derivative forms multilayer structures at the solid–liquid interface, with high density of cross junctions, which are interesting for molecular electronic circuit self-assembly.



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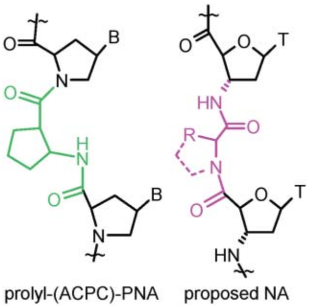
Chimeric (α-amino acid + nucleoside-β-amino acid)$_n$ peptide oligomers show sequence specific DNA/RNA recognition

Khirud Gogoi* and Vaijayanti A. Kumar*

An α/β-peptide backbone oligonucleotide comprising natural α-amino acids alternating with a β-amino acid component derived from thymidine sequence specifically recognizes and binds to deoxy- and ribo-oligoadenylates in triplex mode.



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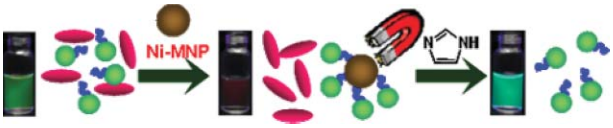
Decoration of superparamagnetic iron oxide nanoparticles with Ni^{2+}: agent to bind and separate histidine-tagged proteins

Kyung Sig Lee and In Su Lee*

The decoration of iron oxide nanoparticles with Ni^{2+} ions provided the superparamagnetic nanoparticles with a binding site for His-tagged proteins, allowing their selective binding and convenient separation from a multi-component solution with an appropriately applied magnetic field.



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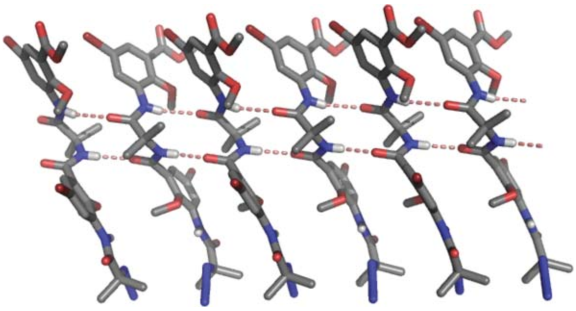
Sheet-forming abiotic hetero foldamers

Pranjal K. Baruah, Naduthottiyil K. Sreedevi, Baisakhi Majumdar, Renu Pasricha, Pankaj Poddar, Rajesh Gonnade, Sapna Ravindranathan and Gangadhar J. Sanjayan*

Abiotic hetero foldamers that adopt a well-defined, compact structure governed by combined conformational restriction imposed by the individual amino acids are described. The striking feature is their extended self-assembled sheet-like structure.



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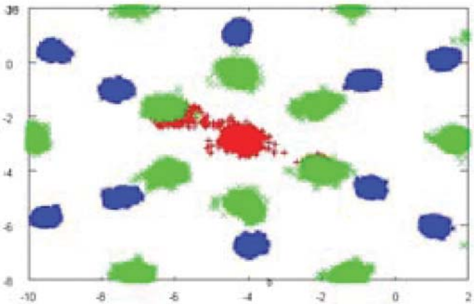

Atomic-scale mechanistic features of oxide ion conduction in apatite-type germanates

Emma Kendrick, M. Saiful Islam and Peter R. Slater*

Atomistic modelling studies of the oxide ion conductor $La_{9.33}(GeO_4)_6O_2$ show the formation of interstitial oxide ion defects, and their migration *via* the GeO_4 tetrahedra.

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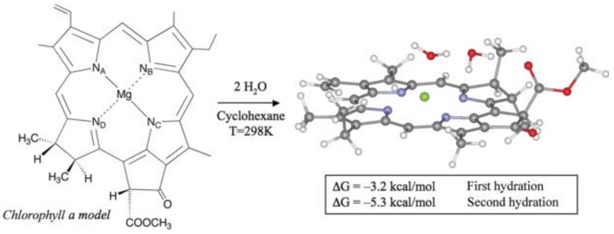

The structure of chlorophyll a–water complexes: insights from quantum chemistry calculations

A. Ben Fredj, Z. Ben Lakhdar and M. F. Ruiz-López*

Computations show that chlorophyll a is able to coordinate a maximum of two water molecules in hydrophobic media that form a bridge between the Mg atom and the methyl ester carbonyl group.

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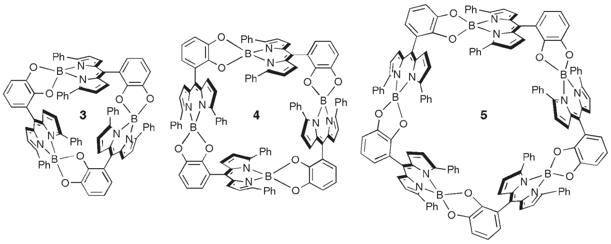

Self-assembled cyclic boron-dipyrrin oligomers

Chusaku Ikeda and Tatsuya Nabeshima*

Self-assembled cyclic boron–dipyrrin oligomers **3–5** obtained by the reaction of catecholyldipyrrin with boron trichloride were characterized by ^{1}H NMR, MALDI-TOF MS, and X-ray measurements and the interaction between **3** and alkali metal ions was examined.

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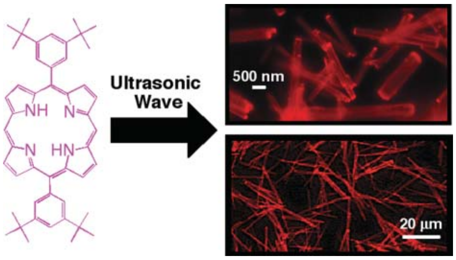

Sonication-assisted supramolecular nanorods of *meso*-diaryl-substituted porphyrins

Taku Hasobe,* Hideaki Oki, Atula S. D. Sandanayaka and Hideyuki Murata*

Supramolecular nanorods of 5,15-diaryl-substituted porphyrins prepared by sonication method exhibit a broad absorption property, which is confirmed by photocurrent generation measurement in a photoelectrochemical cell.

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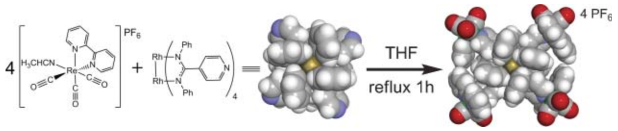
Facile synthesis of multinuclear complexes based on a tetra(4-pyridyl)amidinate dirhodium(II) dimer

Daniel Chartrand and Garry S. Hanan*

A metal dimer readily directs the assembly of a light-harvesting complex in a divergent synthetic approach.



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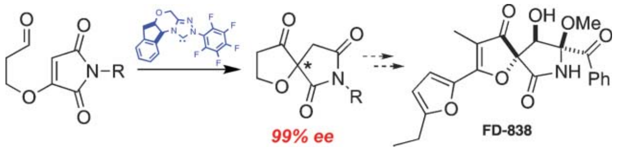
Towards the total synthesis of FD-838: modular enantioselective assembly of the core

Arturo Orellana and Tomislav Rovis*

A rapid assembly of the tetracyclic core of FD-838, featuring a catalytic asymmetric Stetter reaction, is described.



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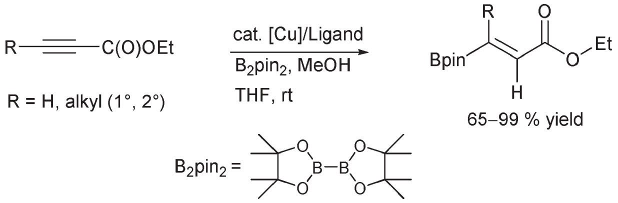
Copper-catalyzed addition of diboron reagents to α,β-acetylenic esters: efficient synthesis of β-boryl-α,β-ethylenic esters

Ji-Eon Lee, Jisook Kwon and Jaesook Yun*

The efficient copper-catalyzed addition reaction of bis(pinacolato)diboron to α,β-acetylenic esters has been developed. This new method provides a one-step preparation method for β-borylated-α,β-ethylenic esters from the corresponding alkyno esters with high levels of stereoselectivity.



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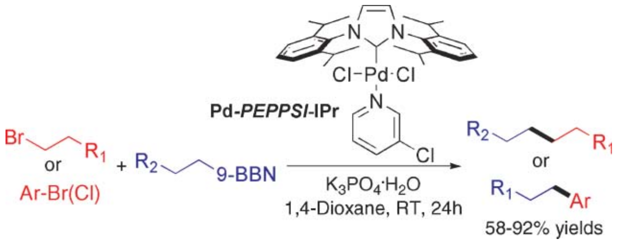
High yielding alkylations of unactivated sp^3 and sp^2 centres with alkyl-9-BBN reagents using an NHC-based catalyst: Pd-PEPPSI-IPr

Cory Valente, Sylvia Baglione, David Candito, Christopher J. O'Brien and Michael G. Organ*

A general protocol is described for the cross coupling of unactivated alkyl bromides and aryl bromides/chlorides with alkyl-9-BBN reagents *via* the well-defined precatalyst Pd-PEPPSI-IPr.



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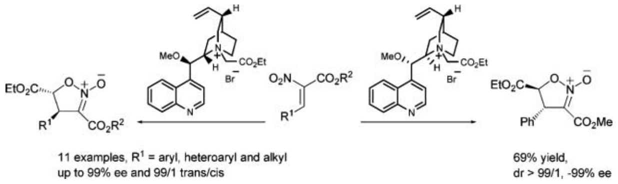
Highly enantioselective synthesis of isoxazoline *N*-oxides

Chun-Yin Zhu, Xian-Ming Deng, Xiu-Li Sun,
Jun-Cheng Zheng and Yong Tang*

The reaction of cinchonidine (cinchonine)-derived ammonium salts with nitroolefins in the presence of Cs_2CO_3 to afford optically active isoxazoline *N*-oxides with excellent ee and high de values has been developed.



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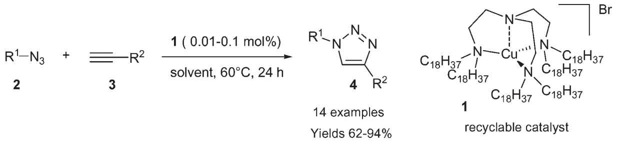
A highly active and reusable copper(I)-tren catalyst for the ‘‘click’’ 1,3-dipolar cycloaddition of azides and alkynes

Nicolas Candelon, Dominique Lastécouères,
Abdou Khadri Diallo, Jaime Ruiz Aranzaes, Didier Astruc
and Jean-Marc Vincent*

The copper(I)-tren complex **1** is a highly active and reusable catalyst for the ‘‘click’’ 1,3-dipolar cycloaddition of azides and alkynes.

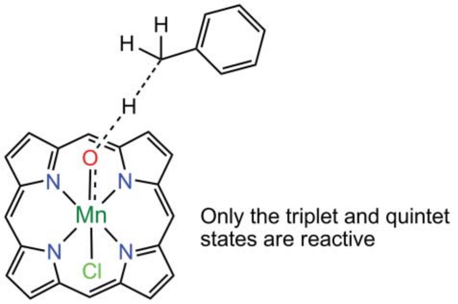


744

The rebound mechanism in catalytic C–H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species

David Balcells, Christophe Raynaud, Robert H. Crabtree
and Odile Eisenstein*

DFT studies show that the rebound mechanism for MnO(tpp)(Cl)-catalyzed C–H hydroxylation is favored for spin states with oxyl character.

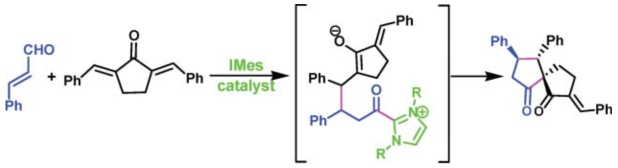


747

Stereoselective synthesis of spirocyclopentanones *via* *N*-heterocyclic carbene-catalyzed reactions of enals and dienones

Vijay Nair,* Beneesh Pattoorpadi Babu,
Sreekumar Vellalath and Eringathodi Suresh

Homoenolate generated from enals, by nucleophilic heterocyclic carbene (NHC) catalysis, undergoes conjugate addition/cyclization sequence with cyclic dienones and culminates in the efficient synthesis of spirocyclopentanones. The stereoselective construction of quaternary carbon center is noteworthy.



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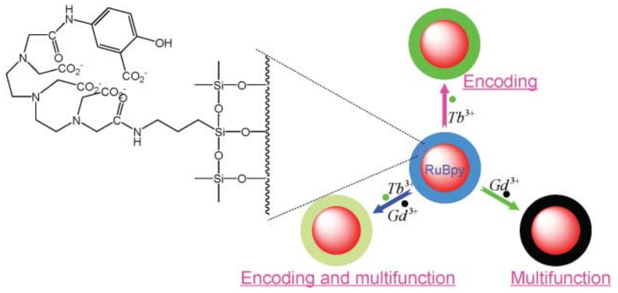
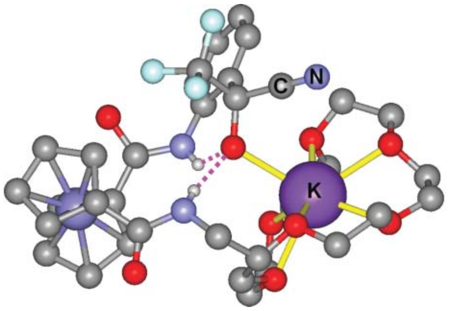


Fluorescent core-shell silica nanoparticles as tunable precursors: towards encoding and multifunctional nano-probes

Chuanliu Wu, Jinqing Hong, Xiangqun Guo, Chaobiao Huang, Jinping Lai, Jinsheng Zheng, Jianbin Chen, Xue Mu and Yibing Zhao*

Core-shell silica nanoparticles comprised of a RuBpy doped silica core and a Pas-DTPA doped silica shell were synthesized and post-functionalized with an encoding fluorescence combination and a multiplex imaging function.

753

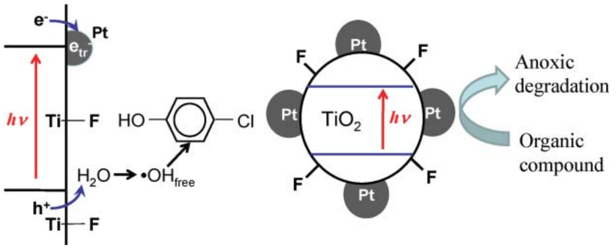


Highly cooperative ion-pair recognition of potassium cyanide using a heteroditopic ferrocene-based crown ether–trifluoroacetylcarboxanilide receptor

Hidekazu Miyaji,* Dae-Sik Kim, Byoung-Yong Chang, Eunju Park, Su-Moon Park* and Kyo Han Ahn*

A heteroditopic ferrocene-based crown ether–trifluoroacetylcarboxanilide receptor selectively recognizes both potassium and cyanide ions in acetonitrile with an association constant of as high as $K_a = 1.9 \times 10^7$ M^{-1}.

756

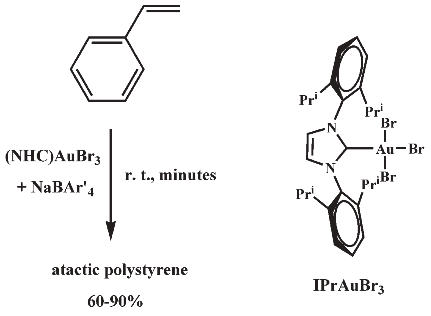


Synergic effect of simultaneous fluorination and platinization of TiO_2 surface on anoxic photocatalytic degradation of organic compounds

Jungwon Kim, Jaesang Lee and Wonyong Choi*

Simultaneously surface fluorinated and platinized TiO_2 (F–TiO_2/Pt) exhibits a novel photocatalytic activity for the anoxic degradation of organic compounds, which is attributed to the unique synergic effect of surface fluorination and platinization on the photo-induced charge transfer process.

759



Gold-promoted styrene polymerization

Juan Urbano, A. Jesús Hormigo, Pierre de Frémont, Steven P. Nolan, M. Mar Díaz-Requejo* and Pedro J. Pérez*

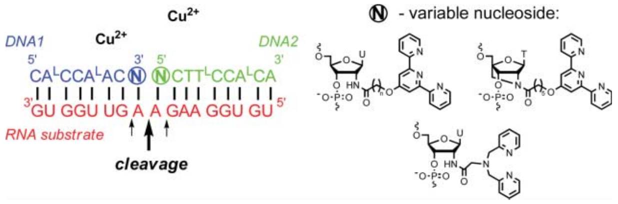
Styrene can be polymerized at room temperature in the presence of equimolar mixtures of the gold(III) complexes $(NHC)AuBr_3$ (NHC = *N*-heterocyclic carbene ligand) and NaBAr$'_4$, in the first example of a gold-induced olefin polymerization reaction.

762

Identification of efficient and sequence specific bimolecular artificial ribonucleases by a combinatorial approach

Marcin Kalek, Peter Benediktson, Birte Vester and Jesper Wengel*

A novel principle for identifying efficient dinuclear artificial ribonuclease constructs by parallel screening is introduced, allowing convenient identification of a sequence specific artificial nuclease that is comparable to the best so far reported.



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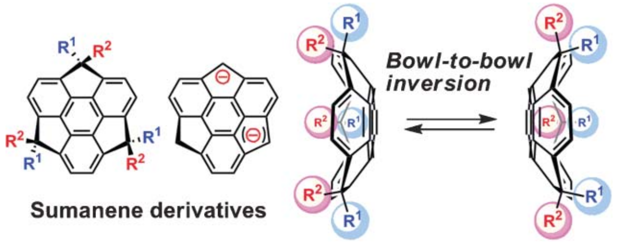
Bowl-to-bowl inversion of sumanene derivatives

Toru Amaya, Hiroyuki Sakane, Toshiko Muneishi and Toshikazu Hirao*

The bowl-to-bowl inversion of the non-planar bowl-shaped compounds derived from sumanene as a fullerene C_{3v} fragment was found to be slow and tuned by a solvent, and the benzylic mono- and di-anions inverted even more slowly.



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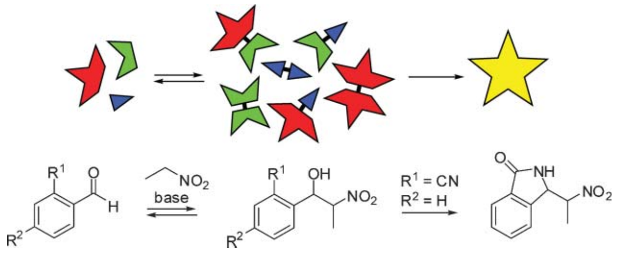
Tandem driven dynamic combinatorial resolution *via* Henry–iminolactone rearrangement

Marcus Angelin, Pornrapee Vongvilai, Andreas Fischer and Olof Ramström*

The concept of tandem driven dynamic libraries is demonstrated. In a dynamic nitroaldol library, internal selection pressure from an unexplored intramolecular tandem cyclization caused quantitative amplification of an interesting 3-substituted isoindolinone.



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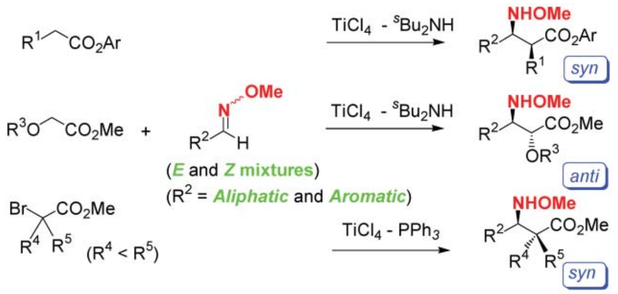
Ti-mediated direct and highly stereoselective Mannich reactions between esters and oxime ethers

Takashi Funatomi, Shogo Nakazawa, Kunshi Matsumoto, Ryohei Nagase and Yoo Tanabe*

The first general method of direct and highly stereoselective Ti-mediated Mannich reaction between three types of simple esters and *E* and *Z* mixtures of oxime ethers (aliphatic and aromatic) is accomplished.



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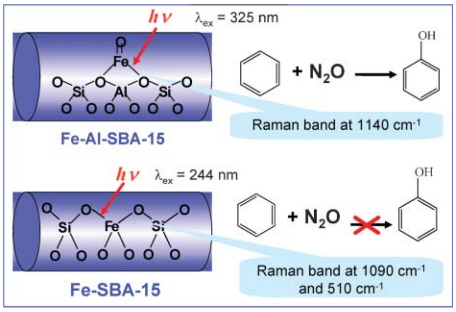
Iron-functionalized Al-SBA-15 for benzene hydroxylation

Ying Li, Haian Xia, Fengtao Fan, Zhaochi Feng, Rutger A. van Santen, Emiel J. M. Hensen* and Can Li*

For the first time an ordered mesoporous silica (Fe–Al-SBA-15) with catalytically active isolated Fe surface species for the hydroxylation of benzene with nitrous oxide is prepared by introduction of Fe^{3+} in the synthesis gel of Al-SBA-15.



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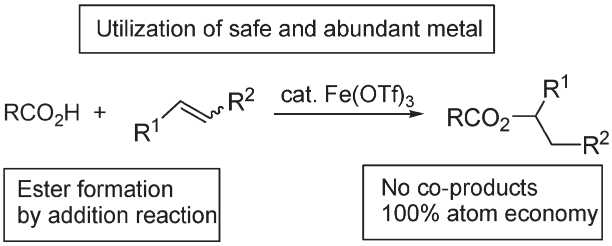
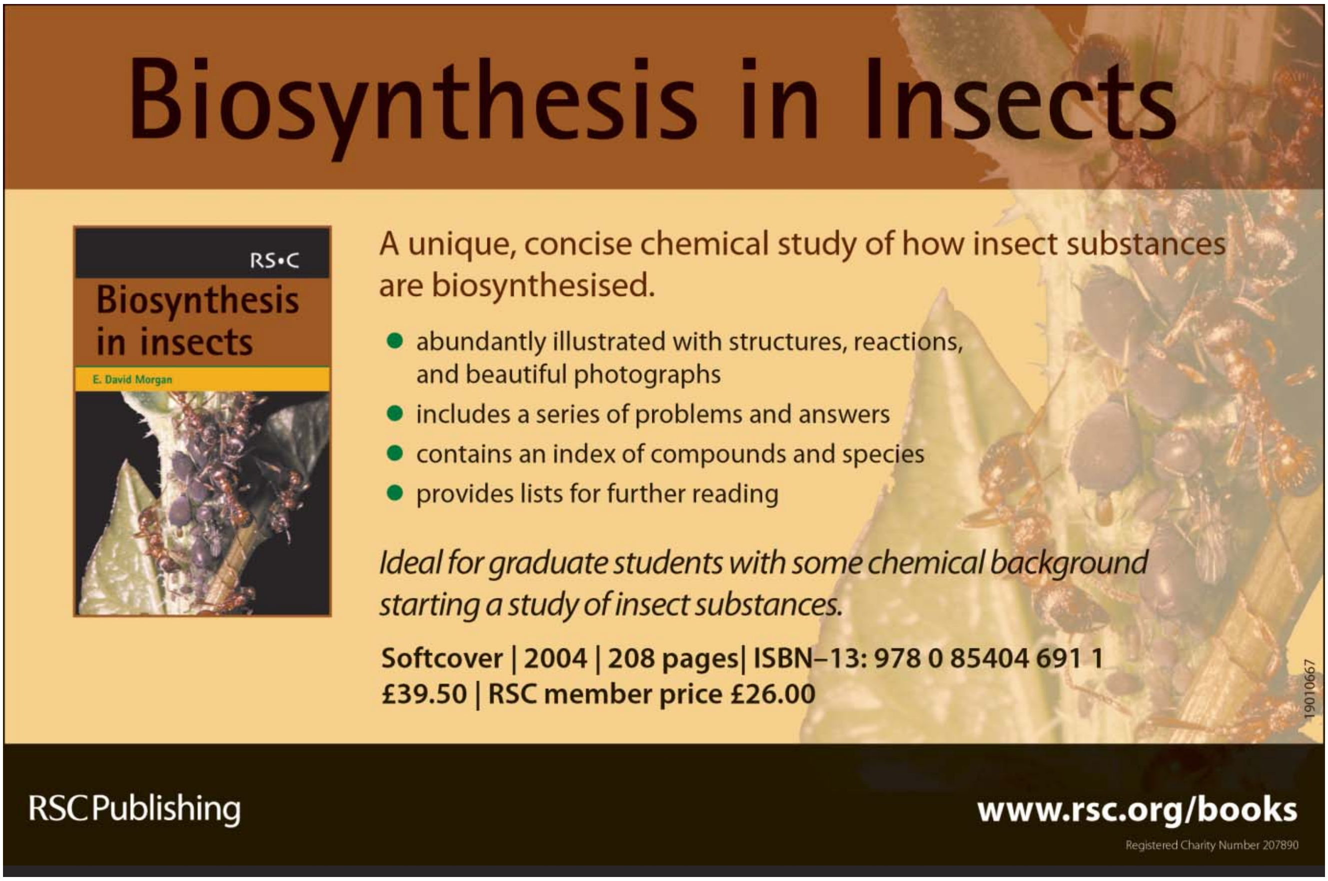
Iron-catalysed green synthesis of carboxylic esters by the intermolecular addition of carboxylic acids to alkenes

Jun-Chul Choi,* Kazufumi Kohno, Daisuke Masuda, Hiroyuki Yasuda and Toshiyasu Sakakura*

Iron(III) triflate efficiently catalyzes the intermolecular addition of carboxylic acids to various alkenes to yield carboxylic esters. This procedure is green and attractive because there are no co-products. Iron triflate, *in situ*-formed from $FeCl_3$ and triflic acid, or $FeCl_3$ and silver triflate exhibit similar catalytic activities to the isolated iron triflate.





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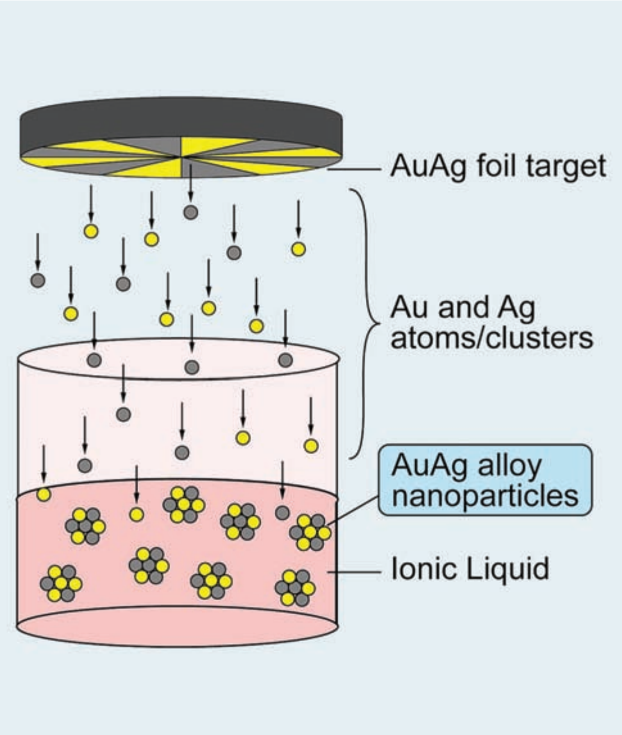
Chemical Technology

Nanoparticle make up can be controlled by varying the foil's composition

Bimetallic particles from sputter deposition



Ionic liquids can withstand the high vacuum conditions required

Gold and silver alloy particles have been made using a simple technique involving ionic liquids.

The team, led by Tsukasa Torimoto at Nagoya University and Susumu Kuwabata at Osaka University in Japan, have used a process called sputter deposition to form bimetallic particles. The particles, which have applications in biosensors and as catalysts, are formed in an ionic liquid from atoms sputtered from a metal foil.

Torimoto explained that the team investigated ionic liquids because of their very low vapour pressures. This means they can be used under the high vacuum conditions required for sputter deposition used here, without their physical and chemical properties changing.

The technique involves bombarding a gold and silver metal foil with high energy gaseous ions. Metal atoms are ejected from the surface of the foil into an ionic liquid, where they coalesce to form the bimetallic nanoparticles.

Up to now, explained Torimoto, it has been difficult to obtain homogeneous alloy nanoparticles using conventional solution methods because of the differing chemical redox potentials of the metals. Using the sputtering technique the composition of the particles and their properties can be tuned by varying the composition ratios of the metal foil.

Frank Endres at Clausthal University of Technology in Germany said the team 'present a simple and therefore elegant process for the large-scale production of metal and alloy nanoparticles'. He suggested a further step could be to combine the sputter technique used by Torimoto with a plasmaelectrochemical deposition method developed by himself and colleagues in Germany. 'This might be a route to making ternary compound nanoparticles,' he explained.

Katherine Davies

Reference

K Okazaki *et al*, *Chem. Commun.*, 2008, 691 (DOI: 10.1039/b714761a)

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Make nanoparticles while the sun shines
Solar ablation less energy intensive than laser or chemical routes

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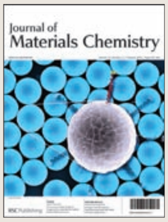
Colour change reveals faulty food packaging

Interview: Analyse this
Joe Caruso talks to May Copsey about warfare agents, proteomics and why elemental mass spectrometry is not just about the metal

Instant insight: Watching the burn
Craig Taatjes of Sandia National Labs, Livermore, US, and colleagues look inside the mysterious chemistry of combustion



The latest applications and technological aspects of research across the chemical sciences

Application highlights

Colour change reveals faulty packaging

Intelligent inks

The ink loses its colour when activated, then regains it when exposed to oxygen

An ink that changes its colour when exposed to oxygen could help shoppers decide if their packaged food is fresh.

Oxygen is the enemy of fresh food because it causes food to degrade and bacteria need it to grow. Hence, much of today's packaged food comes in a protective atmosphere of gases such as nitrogen – with oxygen almost totally removed.

Andrew Mills and David Hazafy at University of Strathclyde, UK, have developed a blue ink that loses all its colour and becomes oxygen sensitive when activated with UV light. It only turns blue again after exposure to oxygen.

The major advantages of the oxygen ink over most of the traditional methods for detecting oxygen is that it is cheap and easy to use, especially as it relies on a colour change detectable by the human eye, said Mills. Solvent-based inks such as these are also easier to print on the common polymers used in food packaging, he added.

'An oxygen-sensitive ink, such as ours, could be used to show if the modified atmosphere remains intact, first at the packaging factory, then at the supermarket, ensuring faulty, damaged or tampered packages are not sold,' said Mills. The customers themselves will be able to pick up the food and tell instantly if it has been spoiled.

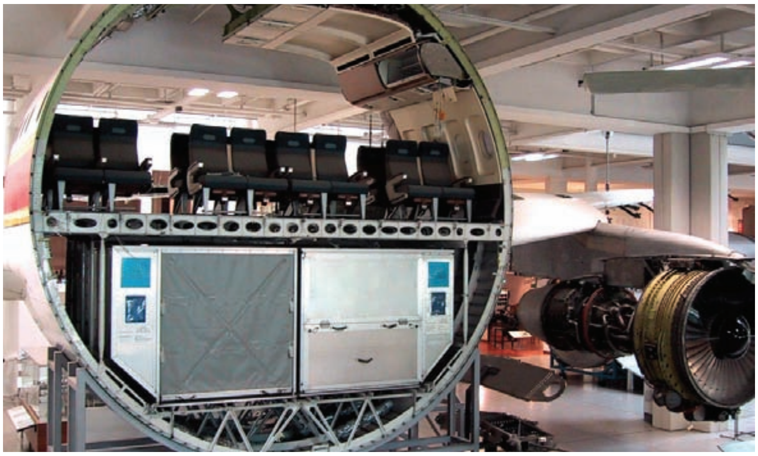
Sarah Corcoran

Reference

A Mills and D Hazafy, *Analyst*, 2008, **133**, 213 (DOI: 10.1039/b713450a)

If you want to detect disease in an airline cabin, where do you put the sensors?

SARS on a plane



Fluid dynamics revealed the best place to find biological agents

It's fairly unlikely that you'll ever worry about snakes on a plane, but what if one of your co-passengers has SARS, or worse, is about to release some anthrax spores? US researchers are working to find the best way to detect such hazards.

Nearly two billion people travel on commercial airliners each year, and it is important to detect these problems as quickly as possible by installing sensors. However, the number of sensors that can be installed is limited by cost, size and weight. The question then remains: Where do you put the sensors to get the fastest response?

Instead of using a full size replica of an airliner cabin, Sagnik Mazumdar and Qingyan Chen from Purdue University, West Lafayette, created a virtual cabin and used computational fluid dynamics to study the effects of the seating arrangement and the number of occupants on the optimum position for these sensors.

'In 2003, one passenger passed on SARS to more than a dozen others,' said Mazumdar. 'It's this kind of tragedy that we hope to help avoid.'

Their research is one part of a larger coordinated research effort called ACER (airliner cabin environment research). 'It is essential to deploy sensors that can provide instantaneous information. New sensors that can provide instantaneous results, particularly for biological agents, is another important area for research,' said Mazumdar.

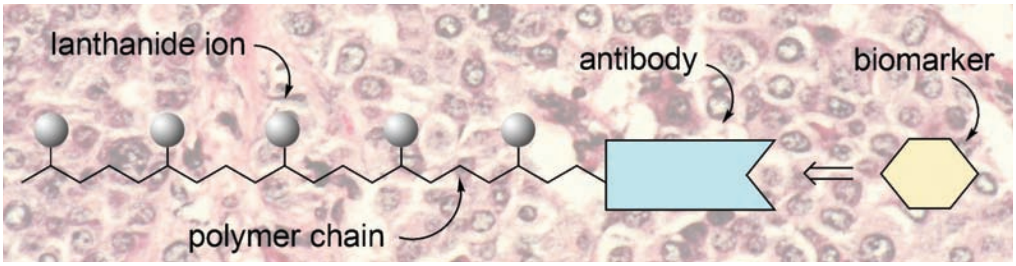
Stephen Davey

Reference

S Mazumdar and Q Chen, *J. Environ. Monit.*, 2008, **10**, 71 (DOI: 10.1039/b713187a)

Simultaneous screening for many disease biomarkers is now on the horizon

Lanthanide ions hold key to disease screening



Different biomarkers can be targeted by different lanthanide isotopes

Canadian researchers have devised a way to assess biological samples for the presence of multiple small molecules, which has profound implications for rapidly identifying diseases.

Being able to distinguish diseased cells from healthy ones is vital in identifying diseases in humans. A rapidly advancing way of doing this is to determine the concentrations of small molecules (biomarkers) present in biological samples, as amounts of these chemicals differ between diseased and healthy cells. Vladimir Baranov and colleagues from the University of Toronto have now developed a sensitive method that, by using lanthanide ions, is able to determine the concentrations of many biomarkers at once. This, they say, will have important applications in clinical diagnostics.

Baranov and colleagues bound ^{151}Eu ions to a polymer chain chemically attached to an antibody, which itself binds to a natural biomarker. Once the unreacted antibody derivative is washed away, the sample is exposed to inductively coupled plasma mass spectrometry. This atomises the entire sample and allows the elemental composition to be determined. In this case, the amount of ^{151}Eu correlates to the amount of biomarker present in the original sample. The number of ^{151}Eu ions within each molecule means that the method is more sensitive to the amount of biomarker than existing techniques, said Baranov.

The power of the team's method is that it can measure many biomarkers simultaneously, simply by using a different one of the 50-plus stable lanthanide isotopes for antibodies against different targets. Baranov's team are now working to apply their technique to the classification of leukaemia samples.

The importance of this research is emphasised by Les Ebdon, Vice-Chancellor of the University of Bedfordshire, UK, who said 'This exciting study ... promises to advance our abilities to understand and diagnose complex diseases such as leukaemia.'

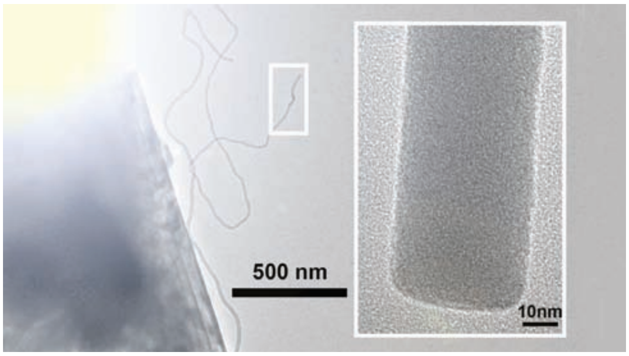
David Barden

Reference

O I Ornatsky *et al*, *J. At. Anal. Spectrosc.*, 2008, DOI: 10.1039/b710510j

Solar ablation less energy intensive than laser or chemical routes

Make nanoparticles while the sun shines



Sunlight is transmitted to the reaction vessel by optical fibres

Concentrated sunlight is all you need to make useful nanomaterials, according to Israeli researchers.

Jeffrey Gordon of Ben-Gurion University in the Negev desert, Reshef Tenne of the Weizmann Institute, Rehovot, and their collaborators collect solar radiation outdoors and transmit it to an indoor laboratory with optical fibres. Here it is focussed on molybdenum sulfide or quartz powders, transforming them into nanotubes and nanocages. This is the first time that silica nanofibres and nanospheres have been produced from pure quartz, they said.

Wolfgang Tremel, who works on inorganic nanoparticles at the University of Mainz in Germany explained 'A particular problem in the synthesis of fullerene-type nanoparticles and nanotubes is that high temperatures are needed to interconnect the edges of fragments in such a way as to provide curvature to otherwise flat slabs.'

Gordon and Tenne believe that the solar route is far less energy intensive than laser ablation or high-temperature chemical reactors, simpler and less costly, with only an 'uncomplicated optical system' required to deliver the light to the reaction vessel.

There are plenty of refinements that can be made: 'We need to find optical and reactor configurations that ensure nanotube and nanoparticle generation in a more uniform and reproducible fashion,' said the researchers. And, they add, it opens up new mechanistic questions: 'Does photochemistry play a role or are the only important factors the temperature and flux gradients?'

Tremel warned that in its current state the technique will be unable to 'yield samples at the gram scale'. More importantly though, he said that it promises new sorts of fullerene-like nanoparticles. These conditions, he said, 'enable the formation and trapping of nanoparticles from metal oxide compounds which, like quartz, have significantly lower vapour pressures than metal chalcogenides'.

Colin Batchelor

Reference

J M Gordon *et al*, *J. Mater. Chem.*, 2008, **18**, 458 (DOI: 10.1039/b714108d)

Banned muscle strength hormone somatotropin detected months after use

Immunoassays put pay to foal play

French scientists have designed tests to catch cheats who use prohibited drugs to dope racehorses.

Somatotropin, a protein hormone, increases muscle strength. Recombinant equine somatotropin is banned in horseracing since it can enhance the performance of the horse, giving it an unfair advantage. Somatotropin can be used legitimately to help repair tendon or bone injuries in horses, or to improve the condition of horses that no longer race.

Ludovic Bailly-Chouriberry, who works at both the Laboratory of Horse Racing in Verrières-le-Buisson and the National Veterinary School in Nantes, and colleagues have developed a method to test for somatotropin based on detection of antibodies raised against the hormone in serum or plasma.

Other tests to screen for somatotropin abuse, the researchers said, include the detection of insulin-like growth factor (IGF-1) whose production is also triggered by somatotropin. They hope that by detecting antibodies instead of IGF-1 a longer period for screening will be possible.

Detecting antibodies enables a longer screening period

They identified the antibodies using two techniques: a biosensor immunoassay (BIA) and an enzyme-linked immunosorbent assay (ELISA). The developed technologies meant it was possible to detect the antibodies 80 days after administering somatotropin with BIA and 200 days after with ELISA.

Bailly-Chouriberry said that this could also provide a cheap and important tool to indirectly detect insulin or recombinant erythropoietin (EPO) misuse through the detection of their antibodies, supposing it can be adapted.

Sarah Corcoran

Reference

L Bailly-Chouriberry *et al*, *Analyst*, 2008, **133**, 270 (DOI: 10.1039/b713712e)

A renewable alternative to crude-oil-based self-curing agents is now possible

Get set with the ene reaction

Researchers from the US have discovered that soy bean oil could be used as a renewable feedstock for gels and resins.

Materials with self-curing, thickening, and self-gelling properties are used in many industrial applications, as caulking agents, cements or coatings. However, many current products are ultimately derived from crude oil. Alongside current developments in the use of biofuels, there is also interest in alternative and renewable sources for such materials.

Now Atanu Biswas from the United States Department of Agriculture and co-workers have discovered that one such renewable raw material can be made to spontaneously form a gel. In the absence of solvent, and without the need for heating or catalyst, soy bean oil undergoes an ene reaction with DEAD (diethylazodicarboxylate).

'We have been interested in combining green chemistry with the use of agricultural raw materials,' said Biswas. 'A particular interest of ours is vegetable oil, because it is relatively low-priced, abundant, and environmentally friendly,' he continued.

Biswas and colleagues hope that this work can be the beginning of a new platform for materials that need self-thickening, self-gelling and self-curing properties. 'Obviously for specific applications, some customization of end-use properties would be needed. Fortunately, there are many types of oils available that we can use to optimize given properties,' he explained.

Soy bean oil spontaneously forms a gel

Surya Prakash from the University of Southern California, Los Angeles,US, said 'Biswas and colleagues have discovered a novel condensation of soybean oil leading to self-curing and thickening. This chemistry will have enormous promise in preparing gels, resins and adhesives using vegetable oil based bio-feedstocks.'

A future challenge will be to find an alternative to the aptly named DEAD, which is known to be toxic. However, Biswas is confident that this will be achievable. 'The key reaction for this new platform is the ene reaction. There are many reactants known to undergo ene reactions. For commercial applications, what is needed in the future is to screen these potential reactants, in view of reaction efficiency, toxicity, and economics, in order to target specific products,' he said.

Stephen Davey

Reference

A Biswas *et al*, *Green Chem.*, 2008, DOI: 10.1039/b712385j

Interview

Analyse this

Joe Caruso talks to May Copsey about warfare agents, proteomics and why elemental mass spectrometry is not just all about the metal

Joe Caruso

Joe Caruso is a professor of analytical chemistry at the University of Cincinnati. His research interests include metal profiling in clinical samples and studies of selenium phytoremediation. Formerly chairman of the *Journal of Analytical Atomic Spectrometry* editorial board, Joe is a member of the *Chemical Society Reviews* editorial board.

What inspired you to become a scientist?

I started out as a high school chemistry teacher but I realised that there was so much exciting chemistry out there and I wanted to teach it at a higher level. I became increasingly interested in the research. In particular, working with graduate students and postdocs is a great plus.

What influenced your decision to study analytical science?

I had a fantastic teacher at university who taught a course in qualitative analysis and he really inspired me. I also think analytical chemistry suits my personality. It is a very practical part of chemistry. For example, if you develop a new method to analyse for lead in somebody's blood, you see a clear application. It is this kind of outcome-based research that drives me.

Can you tell me about the techniques that you use?

Our main-stay is elemental mass spectrometry, known as ICP-MS. It's mainly a metal-based technique, but it does an excellent job at looking at non-metal elements such as bromine, iodine, phosphorus and sulfur. It can be used to analyse for a variety of compounds, such as brominated fire-retardants or phosphorus-based warfare agents. It has a wide range of uses, from small inorganic molecule analysis to proteomics.

What are you working on at the moment?

We are trying to obtain a better molecular understanding of phytoremediation, the use of plants to remove pollutants from soil or water. We study selenium because it is present at high levels in agricultural fields in the western US. There's relatively little difference between the amounts that are toxic and the amounts that are required for life. We look at selenium as it undergoes changes within the plant. You can actually modify certain metabolic changes genetically, taking chemical pathways in different directions and ultimately enhancing the bioremediation qualities of the plant.

We've also been looking at chemical warfare agent hydrolyzates. We aren't certified for handling the actual agents themselves so we study these degradation products. These provide an interesting track to reveal if an agent was present or not. We started this project because our basis for detection is to look at phosphorus as an internal tag by mass spectrometry, rather than looking at the molecule or functional group.

Some of our work focuses on clinical applications of analytical mass spectrometry. We combine elemental mass spectrometry and molecular mass spectrometry to allow metabolite detection at very low levels. We are collaborating with a neuroscientist, Dr Joe Clarke, in the neurology department at Cincinnati. He's very interested in the metabolites associated with certain types of stroke. He believes there may be metabolic markers involving non-metals, such as phosphorus and sulfur, that appear at very low levels in patients with post-stroke complications. If detected early enough, an appropriate intervention might be taken, either through drug therapy or some kind of physical intervention.

What is the next big thing that you would like to tackle in your lab?

Our movement into clinical applications is going to expand. There are particular sets of proteins in the shell, or capsid, of viruses. There's very little known about the metalloprotein aspect of various capsid proteins and this is something we'd like to take a look at. We are interested in seeing how the capsid reacts to either adding metals or removing them.

Do you have any advice for a young researcher keen to develop a successful scientific career?

The important thing is to keep your mind open. Scientists should not limit themselves or their thinking from reaching out into new areas. Collaborations will be even more the way of the future, but this also is consistent with establishing yourself as an independent scientist.

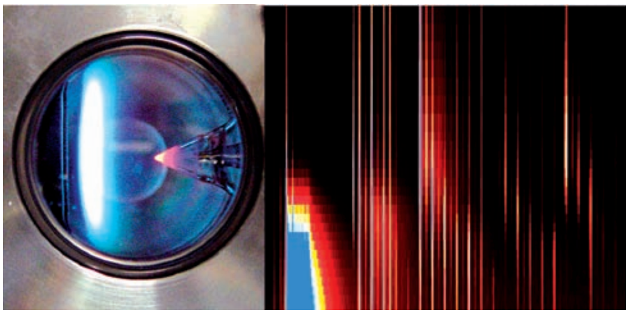
What do you like doing when you're not doing chemistry?

I enjoy boating and my grandchildren. I like to travel with family or friends. I often combine a few days holiday with my scientific commitments.

Instant insight

Watching the burn

Craig Taatjes of Sandia National Labs, Livermore, US, and colleagues look inside the mysterious chemistry of combustion using photoionization mass spectrometry combined with synchrotron radiation



A visual interpretation of multidimensional data can give a glimpse of chemical mechanisms – if you know what to look for

Combustion is an ancient technology, but it remains the dominant means of releasing stored energy in the world today. When Nikolaus Otto invented the four-stroke engine in 1876 and when Rudolf Diesel patented his engine in 1898, scientists did not even have the basic knowledge that combustion was driven by chain-reaction chemistry, an insight that would yield Nikolay Semenov the Nobel Prize decades later. The science of combustion systems, with interacting fluid mechanics and complex chemistry, is a daunting multiscale and multiphase problem that continues to tax state-of-the-art computational and experimental methods. There is an intensifying emphasis on reducing pollutant levels, and new engine technologies are emerging that rely on chemical kinetics for ignition timing. These have made understanding the fundamentals of combustion a key to designing new practical devices and have brought detailed chemistry to the forefront of twenty-first-century combustion research.

Understanding the chemistry behind some of the most stubborn problems in combustion technology relies on knowledge of isomer-specific concentrations of products and intermediates. For example, the efficiency of advanced engines that rely on compression ignition of a premixed fuel–air charge depends on the particulars of alkylperoxy radical isomerizations. The problem of soot formation in hydrocarbon flames hinges on whether reactions of small hydrocarbon species in a flame form aromatic rings or not. Photoionization mass spectrometry is a powerful technique for probing chemical reactions and combustion processes, and the photon-energy dependence of the ionization can distinguish isomers. Recently, photoionization by synchrotron radiation has been combined with simultaneous detection of multiple masses to investigate the chemistry of low-pressure flames. The brightness of the synchrotron source and the multiplexed mass spectrometry permits rapid acquisition of three-dimensional data: signal as a function of the mass, the ionization photon energy, and either reaction time or distance from the burner surface.

'Slices' taken out of such datasets by integrating over two of the dimensions would correspond to more traditional measurements, such as profiles of species as a function of distance from the burner or kinetic concentration against time. However, interpretation of the multidimensional data directly from an image yields great insight into global chemical mechanisms and can highlight previously unknown reactive pathways. For example, an image of the evolving mass spectrum of molecules sampled from a rich ethene flame as a function of the distance from the burner shows soot precursor chemistry at a glance. Moving away from the burner, the fuel is consumed and higher-molecular-weight hydrocarbons begin to be formed; species with three carbon atoms appear very close to the burner, four-carbon species slightly farther away, five-carbon species farther still, and so on. Comparison with an image of a similarly rich flame of the oxygenated fuel dimethyl ether shows immediately that the growth of these soot precursors is almost completely absent in the ether flame, consistent with the soot-reducing effects of oxygenates.

Additionally, possession of the entire three-dimensional data set allows the measurements to be correlated in different ways. As one example, the change in the photon-energy dependence of signal at a given mass can be related to a change in the isomeric populations. Correlating this with time then allows the separation of contributions from different stages of the reactions. Spectra derived from such correlations offer means to detect important ignition-chemistry intermediates.

The investigation of increasingly complex chemical systems not only requires the ability to simultaneously monitor many channels, but demands new strategies to manage and visualize the resulting data. Tunable photoionization and simultaneous multiple-mass detection can effectively depict flame and chemical kinetic processes; continuing development of spectroscopic and visualization technologies will deliver new insights into combustion.

Read more in Craig Taatjes et al's critical review '"Imaging" combustion chemistry via multiplexed synchrotron-photoionization mass spectrometry' in issue 1, 2008 of PCCP.

Reference

Craig A Taatjes *et al*, *Phys. Chem. Chem. Phys.*, 2008, **10**, 20 (DOI: 10.1039/b713460f)

Essential elements

Celebrating a decade of success

2008 is a big year for RSC Publishing as four titles from its successful journal portfolio celebrate their tenth year of publication. *CrystEngComm*, *Green Chemistry*, *Journal of Environmental Monitoring* (*JEM*), and *Physical Chemistry Chemical Physics* (*PCCP*) have all made huge advances in their first decade.

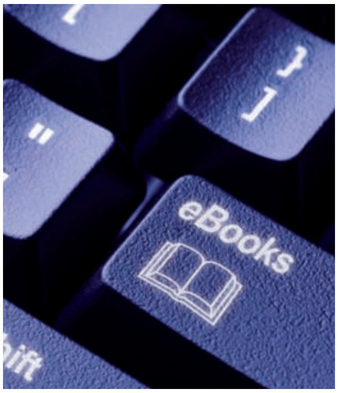
PCCP boasts the highest ISI immediacy index of any general physical chemistry journal and *CrystEngComm*, with an impact factor of 3.729, is *the* journal in which to publish crystal engineering research. *JEM* is packed full of cutting-edge work on environmental processes and impacts and *Green Chemistry*, the most highly cited journal in its field, has an impact factor of 4.192.

A number of celebratory activities are planned this year to mark the anniversaries, including receptions, sponsored lectures, poster prizes and commissioned articles. Look out for specially selected reviews representing the many areas of *Green Chemistry*, and *JEM* sponsored lectures at Airmon 2008 (Albert Gilmutdinov) and DIOXIN 2008 (Kevin Jones). *PCCP* and *CrystEngComm* will also be maintaining a high profile at key conferences across their fields, including sponsoring ten poster prizes.

For further information on these and other anniversary events visit the website (www.rsc.org/journals) or speak to us at one of the many conferences RSC Publishing staff will be attending throughout 2008. Watch out for celebrations at the Spring ACS meeting in New Orleans in April...

RSC Books 2008

2007 witnessed the launch of the RSC eBook Collection, an innovative online product for scientists across the globe. A further highlight was *Elegant Solutions* by Philip Ball being awarded the 2007 Dingle Prize for the best recent book to communicate the history of science, technology and/or medicine to a wide audience of non-specialists. As we begin 2008, RSC Publishing is confident that our exciting 2008 book list will achieve further success, reinforcing our position at the forefront of international chemistry research publishing.



ISTOCKPHOTOS

Looking forward to the year ahead, RSC Books plans to continue providing a first class online publishing service and is aiming to achieve simultaneous eBook and print publication. Our eBook project saw 44 new eBooks go live in 2007 with a further 52 forecast to go live during 2008. Expect to see groundbreaking titles from our exclusive RSC Nanoscience & Nanotechnology, RSC Biomolecular Sciences series and the new RSC Green Chemistry and RSC Energy Series which join the RSC eBook Collection during 2008.

For more information on our prestigious international best sellers visit www.rsc.org/books

And finally...

This month sees the publication of an exciting theme issue of *Molecular BioSystems* on the subject of metabolomic analysis of microorganisms. The issue is introduced by Hirotada Mori and Tadhg Begley of the *Molecular BioSystems* editorial board and features a good mix of review and primary research material.

The investigation of cellular metabolic pathway networks is a remarkably varied field, requiring a wide range of knowledge and theoretical and experimental tools taken from a diversity of scientific disciplines.

Approaches involving time-of-flight mass spectrometry, TOCSY NMR, informatics and computational strategies are described, along with the modelling and reconstruction of metabolic networks. A review of flux analysis, dynamic changes in metabolite profiles, new techniques to identify extracellular components and dynamic changes in gene regulation are all to be found in this issue. Enjoy!

See www. molecularbiosystems.org

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