

# Chem Soc Rev

Chemical Society Reviews  
[www.rsc.org/chemsocrev](http://www.rsc.org/chemsocrev)

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from [www.rsc.org](http://www.rsc.org)

## IN THIS ISSUE

ISSN 0306-0012 CODEN CSRVR 37(2) 237–432 (2008)



### Cover

Fluorinated organic compounds have long fascinated chemists and are finding uses in a wide selection of applications. This review highlights how fluorine substitution serves medicinal chemistry using a case study approach.

The cover picture was produced by Dr Karl Harrison [University of Oxford].

Image reproduced by permission of Sophie Purser, Peter R. Moore, Steve Swallow and Véronique Gouverneur from *Chem. Soc. Rev.*, 2008, 37, 320.



### Inside cover

See Tehila S. Koblenz, Jeroen Wassenaar and Joost N. H. Reek, page 247. Nanospace-molecular reactivity as not observed before.

This cover illustrates a self-assembled nanocapsule which acts a catalyst for a bimolecular reaction. Image reproduced by permission of Tehila S. Koblenz, Jeroen Wassenaar and Joost N. H. Reek from *Chem. Soc. Rev.*, 2008, 37, 247.

## CHEMICAL SCIENCE

C9

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

## Chemical Science

February 2008/Volume 5/Issue 2

[www.rsc.org/chemicalscience](http://www.rsc.org/chemicalscience)

## TUTORIAL REVIEWS

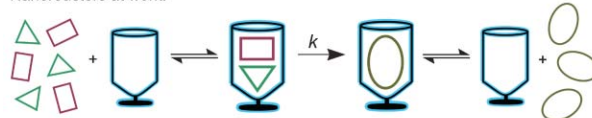
247

### Reactivity within a confined self-assembled nanospace

Tehila S. Koblenz, Jeroen Wassenaar and Joost N. H. Reek\*

Imprisoned molecules go wild. This review explains why reactions carried out within nanocapsules can give different rates and selectivities compared to the bulk phase.

Nanoreactors at work:



Self-assembled nanocapsules:



## EDITORIAL STAFF

### Editor

Robert Eagling

### Publishing assistant

Natalie Ford

### Team leader, serials production

Helen Saxton

### Technical editors

Celia Clarke, Nicola Convine, Alan Holder,  
Laura Howes, Sandra Jones, David Parker,  
Ken Wilkinson

### Production administration coordinator

Sonya Spring

### Administration assistants

Clare Davies, Donna Fordham, Kirsty Lunnon,  
Julie Thompson

### Publisher

Janet Dean

Chemical Society Reviews (print: ISSN 0306-0012; electronic: ISSN 1460-4744) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK CO2 8HP. Tel +44 (0) 1206 226050; Email [sales@rscdistribution.org](mailto:sales@rscdistribution.org)

2008 Annual (print + electronic) subscription price: £514; US\$995. 2008 Annual (electronic) subscription price: £463; US\$896. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any RSC journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at [www.rsc.org/ip](http://www.rsc.org/ip). Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank. Periodicals postage paid at Rahway, NJ, USA and at additional mailing offices. Airfreight and mailing in the USA by Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001, USA.

US Postmaster: send address changes to: Chemical Society Reviews, c/o Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001. All dispatches outside the UK by Consolidated Airfreight.

PRINTED IN THE UK

Advertisement sales: Tel +44 (0) 1223 432243;  
Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

# Chem Soc Rev

## Chemical Society Reviews

[www.rsc.org/chemsocrev](http://www.rsc.org/chemsocrev)

Chemical Society Reviews publishes accessible, succinct and reader-friendly articles on topics of current interest in the chemical sciences. The promotion of international and multidisciplinary awareness and cooperation is particularly encouraged. Chemical Society Reviews publishes two article types: tutorial reviews, which present an accessible introduction to the topic, and critical reviews, which provide a deeper evaluation of the current literature.

## EDITORIAL BOARD

### Chair

Wilhelm Huck, Cambridge, UK  
[wtsh2@cam.ac.uk](mailto:wtsh2@cam.ac.uk)

Fabio Biscarini, Bologna, Italy  
[f.biscarini@ism.bo.cnr.it](mailto:f.biscarini@ism.bo.cnr.it)

Carsten Bolm, Aachen, Germany  
[carsten.bolm@oc.rwth-Aachen.de](mailto:carsten.bolm@oc.rwth-Aachen.de)

Joseph Caruso, Cincinnati, USA  
[joseph.caruso@uc.edu](mailto:joseph.caruso@uc.edu)

Huw Davies, Buffalo, USA  
[hdavies@acsu.buffalo.edu](mailto:hdavies@acsu.buffalo.edu)

Philip Gale, Southampton, UK  
[philip.gale@soton.ac.uk](mailto:philip.gale@soton.ac.uk)

Dirk Guldi, Erlangen, Germany  
[dirk.guldi@chemie.uni-erlangen.de](mailto:dirk.guldi@chemie.uni-erlangen.de)

Jeffrey R. Long, Berkeley, USA  
[jrlong@berkeley.edu](mailto:jrlong@berkeley.edu)

Jon Preece, Birmingham, UK  
[j.a.preece@bham.ac.uk](mailto:j.a.preece@bham.ac.uk)

David Spring, Cambridge, UK  
[drspring@ch.cam.ac.uk](mailto:drspring@ch.cam.ac.uk)

Claudio Zannoni, Bologna, Italy  
[claudio.zannoni@unibo.it](mailto:claudio.zannoni@unibo.it)

Adriano Zecchina, Turin, Italy  
[adriano.zecchina@unito.it](mailto:adriano.zecchina@unito.it)

## ADVISORY BOARD

David Amabilino, Bellaterra, Spain

Carlos Barbas III, La Jolla, USA

Bertrand Castro, Sanofi, France

George Christou, Gainesville, USA

Li-Xin Dai, Shanghai, China

Anne Dell, London, UK

Odile Eisenstein, Montpellier, France

Shunichi Fukuzumi, Osaka, Japan

Hiroyuki Furuta, Fukuoka, Japan

Song Gao, Beijing, China

Sam Gellman, Madison, USA

Kenneth D. M. Harris, Cardiff, UK

Ari Koskinen, Helsinki, Finland

Peter K Ho, Singapore

Kai Johnsson, Lausanne, Switzerland

Cameron Kepert, Sydney, Australia

Sunggak Kim, Daejeon, Korea

Stephen Loeb, Windsor, Canada

Uday Maitra, Bangalore, India

George Marston, Reading, UK

Johannes Messinger, Mülheim, Germany

Chris Orvig, Vancouver, Canada

Albert Philipse, Utrecht, The Netherlands

Peter Roesky, Berlin, Germany

Rint Sijbesma, Eindhoven, The Netherlands

Ulrich Wiesner, Cornell, USA

## INFORMATION FOR AUTHORS

The Editorial Board commissions articles that encourage international, interdisciplinary progress in chemical research. The Board welcomes proposals for new tutorial reviews or critical reviews and the appropriate synopsis pro forma should be requested from the Editorial Office ([csr@rsc.org](mailto:csr@rsc.org)). Full details of how to submit material for publication in Chemical Society Reviews are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be sent via ReSource: <http://www.rsc.org/resource>

Authors may reproduce/republish portions of their published contribution without seeking permission from the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation) – Reproduced by permission of The Royal Society of Chemistry.

© The Royal Society of Chemistry 2008. Apart from fair dealing for the purposes of research

or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

♻️ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

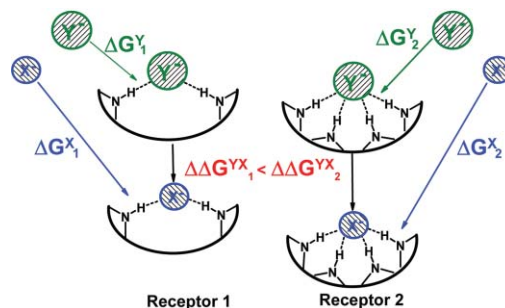
Royal Society of Chemistry: Registered Charity No. 207890.

263

### Selectivity in supramolecular host–guest complexes

Hans-Jörg Schneider\* and Anatoly K. Yatsimirsky\*

Stronger binding should theoretically lead to a stronger discrimination between guests for certain types of host–guest systems, but there are important limitations of the affinity–selectivity principle.

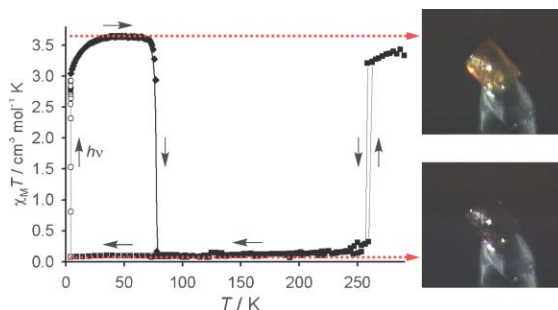


278

### Trapping and manipulating excited spin states of transition metal compounds

Malcolm A. Halcrow\*

Different types of spin-transition material can be trapped in excited spin states, by irradiation or thermal quenching. This involves a change in magnetic moment and (often) in colour, and the metastable products may be stable to thermal relaxation below temperatures as high as 130 K.

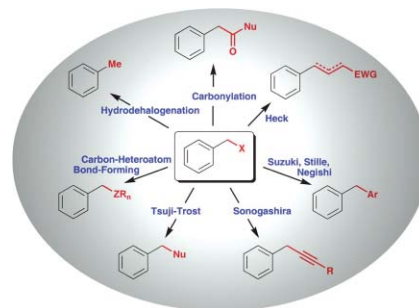


290

### Activation and functionalization of benzylic derivatives by palladium catalysts

Benoît Liégault, Jean-Luc Renaud\* and Christian Bruneau\*

This review highlights the potential and efficiency of palladium catalysts to perform selective transformations of reactive benzylic derivatives. It focuses on palladium-catalyzed transformations of benzylic halides, and pseudo-halides such as acetates, carbonates, phosphonates. It includes selected examples of carbonylation, carbon–carbon and carbon–heteroatom bond-forming reactions, hydrodehalogenation, and some more specific transformations.

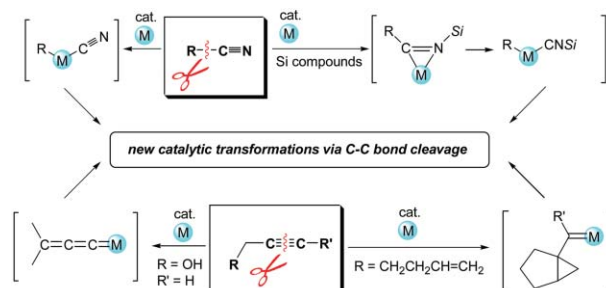


300

### Catalytic reactions involving the cleavage of carbon–cyano and carbon–carbon triple bonds

Mamoru Tobisu and Naoto Chatani\*

The catalytic cleavage of a C–CN bond can proceed by two different mechanisms: oxidative addition and deinsertion of silyl isocyanide. A carbon–carbon triple bond can be cleaved in the absence of an organic promoter *via* the formation of unique organometallic species, such as allenylidene and cyclopropyl carbenoid complexes.



# Physically demanding



*PCCP* publishes its tenth volume in 2008. A challenging decade has seen the journal successfully establish its place on the physical chemistry leaderboard; a reflection of its physical endurance, speed of publication, quality and high impact.

Acknowledged as the journal of choice for fast publication of cutting-edge research in physical chemistry, chemical physics and biophysical chemistry, *PCCP* is committed to publishing research of only the highest quality. At **0.866**, *PCCP* has the highest official ISI immediacy index of any general physical chemistry journal and an impressive impact factor of **2.892**.\*

## Enduring quality

\* 2006 Thomson Scientific (ISI) Journal Citation Reports®

RSC Publishing

[www.rsc.org/pccp](http://www.rsc.org/pccp)

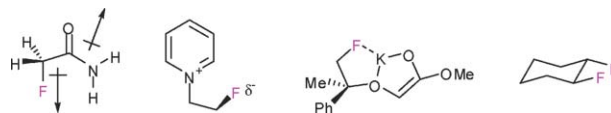
Registered Charity Number 207890

308

### Understanding organofluorine chemistry. An introduction to the C–F bond

David O'Hagan

The C–F bond is the fundamental unit of organic chemistry. This *tutorial review* takes a close look at the C–F bond and describes its influence on the reactivity and behaviour of selectively fluorinated compounds, highlighting in particular the polar nature of the bond and the consequences that emerge from that.

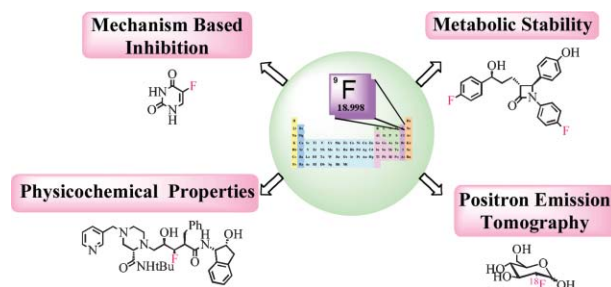


320

### Fluorine in medicinal chemistry

Sophie Purser, Peter R. Moore, Steve Swallow and Véronique Gouverneur\*

This *tutorial review* uses a case study approach explaining how fluorine substitution improves drug potency.

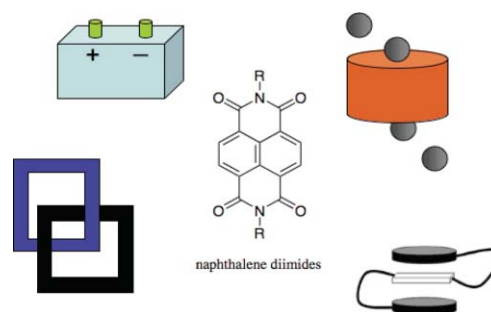


331

### Chemistry of naphthalene diimides

Sheshanath V. Bhosale, Chintan H. Jani and Steven J. Langford\*

As a versatile, electronically and optically addressable building block, naphthalene diimides have found a special importance in supramolecular and materials chemistry. Examples from mechanically interlocked molecules to molecular batteries, conducting wires and self-assembling channels are discussed.

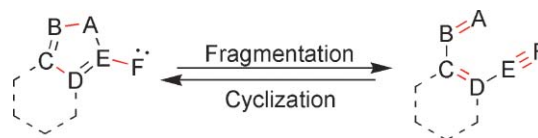


343

### Reactions in the conjugated 'ene–ene–yne' manifold: five-membered ring fragmentation and ring formation via coarctate/pseudocoarctate mechanisms

Laura D. Shirtcliff, Sean P. McClintock and Michael M. Haley\*

Reversible reactivity, the hallmark of molecules in the conjugated 'ene–ene–yne' manifold, can be harnessed to generate unique classes of heterocyclic compounds or highly unsaturated acyclic systems.



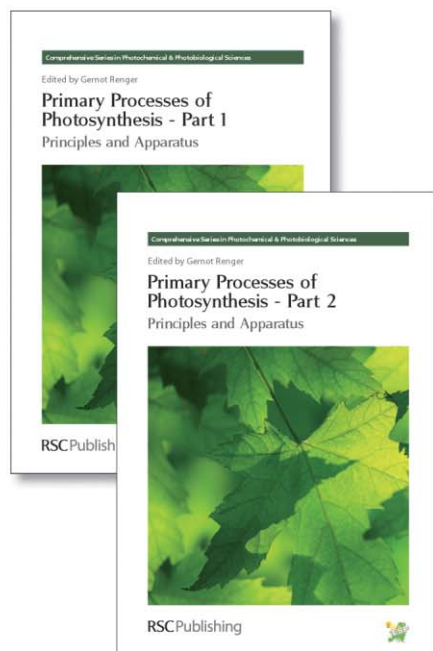
# RSC Comprehensive Series in Photochemical & Photobiological Sciences

Initiated by the European Society for Photobiology, this series provides comprehensive overviews on specific areas of photoscience. It gives in-depth coverage of the very different fields related to light effects and embraces both well-established and emerging areas.

## New Reference Work

# Primary Processes of Photosynthesis

Edited by Gernot Renger



In this comprehensive two part set, the Editor has brought together contributions from numerous leading scientific experts from across the globe to provide a compendium of information.

- The most up-to-date understanding of the primary processes of photosynthesis.
- A summary of current knowledge on the mechanisms of light harvesting, charge separation, electron transport, water cleavage and ATP synthesis.
- High quality structure information at atomic resolution.

Well suited for all those working in the fields of Photochemistry, Bio-organic Chemistry, Bio-inorganic Chemistry, Crystallography, Biological Sciences, Biochemistry and related disciplines.

BB Hardback | 996 pages | ISBN 9780854043644 | 2007 | £339.00

110751

RSC Publishing

[www.rsc.org/books](http://www.rsc.org/books)

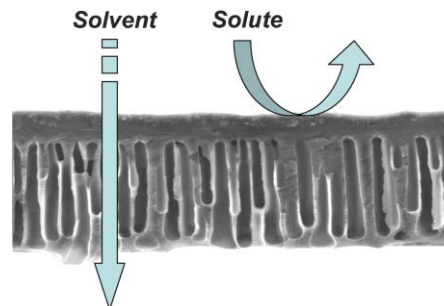
Registered Charity Number 207890

365

**Solvent resistant nanofiltration: separating on a molecular level**

Pieter Vandezande, Lieven E. M. Gevers and Ivo F. J. Vankelecom\*

New membranes allow energy and waste efficient solvent resistant nanofiltration to be used to separate molecules from their organic solvents.

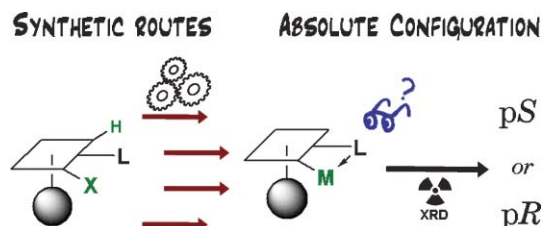


406

**Non-racemic (scalemic) planar-chiral five-membered metallacycles: routes, means, and pitfalls in their synthesis and characterization**


Jean-Pierre Djukic,\* Akram Hijazi, Howard D. Flack and Gérald Bernardinelli

A critical review of the synthetic routes to planar-chiral five-membered metallacycles and their absolute-configuration determination is presented.



## FREE E-MAIL ALERTS AND RSS FEEDS


Contents lists in advance of publication are available on the web *via* [www.rsc.org/csr](http://www.rsc.org/csr) – or take advantage of our free e-mail alerting service ([www.rsc.org/ej\\_alert](http://www.rsc.org/ej_alert)) to receive notification each time a new list becomes available.

 Try our RSS feeds for up-to-the-minute news of the latest research. By setting up RSS feeds, preferably using feed reader software, you can be alerted to the latest Advance Articles published on the RSC web site. Visit [www.rsc.org/publishing/technology/rss.asp](http://www.rsc.org/publishing/technology/rss.asp) for details.

## ADVANCE ARTICLES AND ELECTRONIC JOURNAL

Free site-wide access to Advance Articles and electronic form of this journal is provided with a full-rate institutional subscription. See [www.rsc.org/ejs](http://www.rsc.org/ejs) for more information.

\* Indicates the author for correspondence: see article for details.

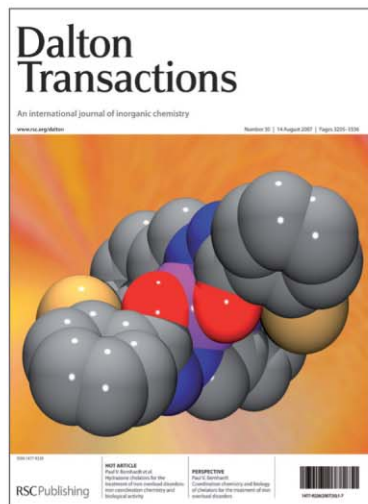
 Electronic supplementary information (ESI) is available *via* the online article (see <http://www.rsc.org/esi> for general information about ESI).

# A step ahead

Publishing  
the most topical  
organometallic and  
inorganic chemistry  
research.  
Faster!

"We are all VERY impressed with the rapidity with which this communication has been processed and typeset – six days!"

Professor Michael I Bruce,  
University of Adelaide, Australia



*Dalton Transactions*, the leading European and one of the world's most respected international organometallic and inorganic chemistry journals, embraces all aspects of the chemistry of inorganic and organometallic compounds including bioinorganic chemistry and materials chemistry.

The first general inorganic chemistry journal to publish weekly issues, *Dalton Transactions* prides itself on making the best organometallic and inorganic chemistry research available, fast! With typical online publication times of only 75 days from receipt for full papers and 35 days for communications, *Dalton Transactions* is the fastest in the field. What's more, an immediacy index of 0.89\* ranks the journal as the most topical in general inorganic chemistry.

An impact factor of 3.012\*, a variety of article types, no page charges, and additional innovative features such as html enhancement with our new award-winning *Project Prospect* ([www.projectprospect.org](http://www.projectprospect.org)), mean the benefits to authors and readers just go on and on. Find out more online now!

\*2006 Thomson Scientific (ISI) Journal Citation Reports®

RSC Publishing

[www.rsc.org/dalton](http://www.rsc.org/dalton)

Registered Charity Number 207890



# Chemical Science

New technology could lead to widely available antibacterial coatings

## Bacteria drop dead on killer surfaces

Surfaces that kill bacteria on contact could soon be a reality in our homes and hospitals, thanks to researchers from the Curie Institute in Paris. The French group has developed a method for making surfaces bactericidal that it says is straightforward and versatile enough to be widely used.

Vincent Semetey and colleagues have devised a simple way to attach polymers containing quaternary ammonium groups to surfaces. Surfaces modified in this way kill any bacteria that come into contact with them.

'The strategies developed so far for attaching the polymers use organic solvents and require multiple steps, limiting their implementation in industry,' said Semetey. 'Our method requires just a single reaction step in water.' He added that because the polymer is bound covalently, the antibacterial activity is permanent, which is an advantage over techniques with surfaces impregnated with biocides such as silver ions.

Past experiments with similar



surfaces have shown that the ammonium groups do not induce resistance in bacteria, said Semetey, a great advantage in these days of multiresistant superbugs.

The researchers say that their method can be used to modify any

surfaces that have free hydroxyl groups, including glass, ceramics and some plastics. According to Semetey the technology is particularly suited to treating textiles, for example bandages.

'There is an urgent need for easy-to-apply coatings to make materials permanently bactericidal,' said Alexander Klibanov of the Massachusetts Institute of Technology, USA. Himself a pioneer in the field, he said Semetey's work was timely and that the method was straightforward and could help control the spread of infections.

Semetey said that his group are considering several applications of their method in hospitals, and are working together on this with colleagues based at the hospital run by the Curie Institute. Furthermore, the technology has received interest from several companies.

*Danièle Gibney*

**Any surfaces with free hydroxyl groups can be made permanently bactericidal**

### Reference

O Bouloussa, F Rondelez and V Semetey, *Chem. Commun.*, 2008, DOI: 10.1039/b716026g

## In this issue

### Genetic testing in a shoe-box

Cost of on-the-spot genetic tests slashed

### Molecular daisy chains

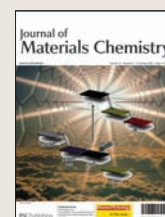
Rotaxane molecules that link together could be used in molecular electronics

### Interview: A time for transition

Peter Kündig discusses his chemistry career and new editorial role with Joanne Thomson

### Instant insight: The light touch

Kishan Dholakia examines how light can move and sort biological objects at the microscopic scale



A snapshot of the latest developments from across the chemical sciences

# Research highlights

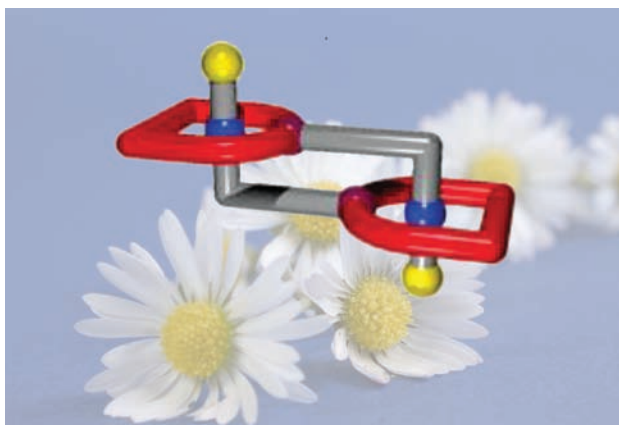
Rotaxane molecules that link together could be used in molecular electronics

## Molecular daisy chains

A molecular daisy chain that threads itself together could have future uses in molecular electronic devices, say scientists in Taiwan.

Sheng-Hsien Chiu and his colleagues at the National Taiwan University, Taipei, and National Chung Hsing University, Taichung, have found a way to interlock pseudorotaxanes and rotaxanes, creating chains that could prove useful as molecular actuators and switches for molecular electronic devices.

Daisy chains are typically made by making a hole in the stalk and passing another daisy stalk through this hole, where the flower head acts as a stopper. Chiu's method is akin to passing the flower head through the hole in the stalk. Here the flower head is a dialkenyl cyclopropane unit that rearranges to a cycloheptadiene unit at elevated temperatures, which then acts as a stopper.



The daisy monomer used in this study is a hydrogen-bond-donating thread-like unit (a stalk), a hydrogen-bond-accepting macrocycle (the hole in stalk) and a dialkenyl cyclopropane terminal group (a flower head). These components are allowed to self-assemble in solution into

**The interlocked rotaxane molecules resemble daisy chains**

### Reference

Shau-Hua Ueng *et al*, *Chem. Commun.*, 2007, DOI:10.1039/b716331b

daisy-chain-like complexes, before heating the system to rearrange the terminal groups and trap the units in place.

Chiu and co-workers isolated the daisy chain by chromatography and confirmed its structure using X-ray crystallography. They found a cyclic dimeric daisy chain was formed. This two-daisy ring is the entropically favoured product, Chiu explained.

'The challenge remains to overcome entropy and assemble larger cyclic and acyclic molecular daisy chains,' Chiu said.

He believes the solution to this problem is to use a more structurally rigid monomer that would disfavour dimerisation and form longer chains.

In the future Chiu hopes to use this approach to isolate other types of molecular daisy chains and functional interlocked polymers. *Emma Shiells*

Enclosing nutraceuticals in silica particles enables their use as oral drugs

## East meets west

Curcumin is a major component of the spice turmeric, which has been used in Eastern medicine for thousands of years. Curcumin and  $\beta$ -carotene, another bioactive compound, both have limited use in Western medicine due to poor bioavailability, but all this could change thanks to mesoporous silica particles.

Curcumin and  $\beta$ -carotene are nutraceuticals – dietary supplements with a medicinal effect on human health – that show anti-inflammatory, anti-carcinogenic, anti-tumour and anti-cancer capabilities. Tests have found that neither compound remains in the bloodstream long after consumption, because of poor water solubility. This means they are unsuitable as oral drugs.

To overcome this hurdle, Colin Raston and colleagues, from the University of Western Australia, Perth, have encapsulated both



curcumin and  $\beta$ -carotene, respectively inside mesoporous silica capsules. These capsules can be used for the delivery and controlled release of the compounds.

The silica capsules have well-defined nanochannels that ensure the drugs controlled release. They are also highly fluorescent, so can act as trackers for monitoring drug dose.

The nanosized capsules are

**Curcumin and  $\beta$ -carotene could now be used in Western medicine**

### Reference

N W Clifford, K Swaminathanlyer and C L Raston, *J. Mater. Chem.*, 2008, **18**, 162 (DOI: 10.1039/b715100d)

made in a continuous flow reactor called a spinning disc processor. This rapid approach uniquely makes nanoparticles of a uniform size. Raston said he believes the reactor can be used to make a wide range of other nanomaterials. 'The technology is not only scalable but also offers precise control over the particle size, shape and surface properties,' he said.

An advantage of spinning disc processing is that nanotoxicology issues, scalability, effluent treatment and hazardous work environments are dealt with at the conception stage rather than attempting to make a new process or product scalable and non-toxic after its development, explained Raston.

Challenges facing the future of this system are, according to Raston, adapting the technology to a wide range of therapeutics and turning it into a commercial product.

*Elinor Richards*

## Cost of on-the-spot genetic tests slashed

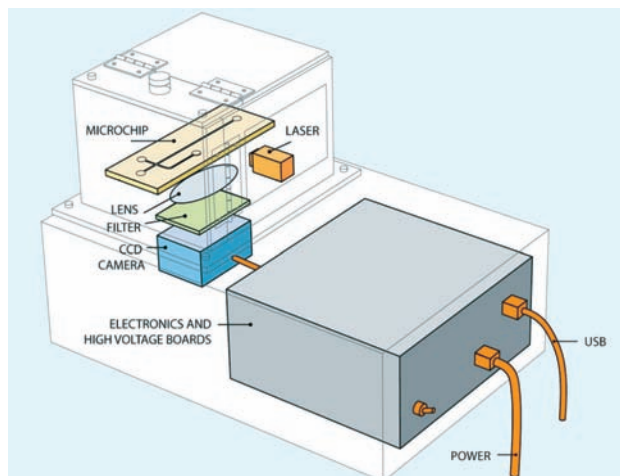
# Genetic testing in a shoe-box

Canadian scientists have lowered the cost of portable devices for rapid genetic testing.

The cost of carrying out a single genetic test currently varies from hundreds to thousands of pounds, and the wait for results can be weeks. Now a group led by Christopher Backhouse, University of Alberta, Edmonton, have developed a reusable microchip-based system that is small enough to be portable, can be used for point-of-care medical testing and costs just £500 to build. This is the least expensive device made so far.

The well-known techniques reverse transcription, polymerase chain reaction and capillary electrophoresis have been developed over recent decades to take tiny amounts of genetic material, grow and amplify them. These handling techniques make detecting genes possible, and have previously been miniaturised so they fit on a microchip that uses small channels, valves and reaction chambers.

The team have redesigned



the gene handling microchip, and used a different detection method, to develop a system that is 'comparable in performance to much bigger and more expensive machines', explained Backhouse. The size of the device is reduced to that of a shoe-box with optics instrumentation and supporting electronics filling the space around the microchip.

**The £500 device could be used to test a person's predisposition to cancer**

**Reference**  
G V Kaigala *et al*, *Analyst*, 2008, DOI: 10.1039/b714308g

To keep costs down, 'instead of using the very expensive confocal optics systems currently used in these types of devices we used a consumer-grade digital camera', Backhouse explained.

The device can be adapted for use in many different genetic tests. 'By making small changes to the system you could test for a person's predisposition to cancer, carry out pharmacogenetic tests for adverse drug reactions or even test for pathogens in a water supply,' said Backhouse.

The group strives to make genetic testing accessible to everyone in the same way computers are now. 'It's not long ago that computers were inaccessible to most people but now we all carry more than one on our person. This was made possible by integration and cost reductions,' said Backhouse. He said he plans to cut the manufacturing costs of this device to £50 in the very near future by integrating more of the electronics and further miniaturising the microfluidics. *Gavin Armstrong*

## Moving towards using viruses to transport therapeutics to target cells

# Viral cargo delivery

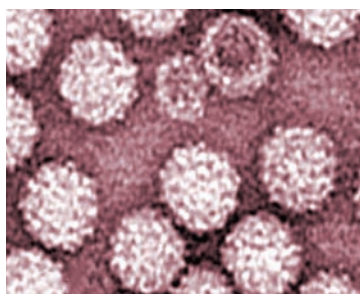
US chemists have used a virus capsule to package and release molecules, which could lead to targeted delivery of therapeutic compounds.

Stefan Franzen and his colleagues at North Carolina State University in Raleigh used the red clover necrotic mosaic virus as a vehicle for dye molecules that can be loaded and unloaded on demand.

Red clover necrotic mosaic virus is a plant virus with a protein shell, or capsid, of multiple subunits that self-assemble to form a cage. Franzen explained that, 'these protein cages offer a rigid structure with an interior cavity that can function as an ideal container for cargo encapsulation'.

To explore its versatility for nanopackaging and delivery,

**Microscopic image of red clover necrotic mosaic viruses carrying dye molecules**



**Reference**  
L Loo *et al*, *Chem. Commun.*, 2008, 88 (DOI: 10.1039/b714748a)

Franzen first worked on capturing dye molecules into the capsid. As divalent ions are integral to the virus structure,  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  depletion in the solution induces significant conformational changes. This leads to surface pores forming, allowing dye molecules to infuse into the interior cavity. Restoring the ion balance closes the pores,

trapping the dye inside the virus. When Franzen lowered the ion concentration, the pores reopened and the dye molecules were released.

Franzen's final aim is to use the capsids for intracellular drug delivery – the next stage is to study their ability to package and deliver cargo into a target cell, he explained. The idea is that loaded viruses should be triggered to open their surface pores and release their package inside a cell where the divalent ion concentrations are low. This concept is 'advantageous because the virus capsid will be able to act as container to protect a cargo until it reaches the targeted cell to be released', explained Franzen. *Michael Spencelayh*

# Natural enantiomer of a grape vine pest's sex pheromone has been identified

## Mealybugs look in the mirror

US researchers have used spectroscopy to identify the absolute configuration of the mealybug sex pheromone, with potential uses in pest control.

An interdisciplinary team worked together to determine the 3D arrangements of the atoms in this molecule. Entomologist Jocelyn Millar and organic chemist Bruno Figadère at the University of California, Riverside, teamed up with an expert in vibrational circular dichroism (VCD) spectroscopy, Philip Stephens from the University of Southern California, Los Angeles.

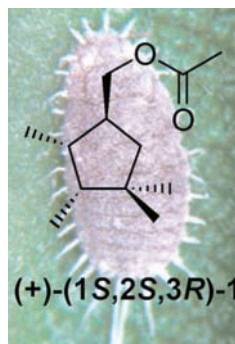
Millar explained the importance of the finding: 'This insect is a worldwide pest of grape vines and numerous other plants. To determine whether the pheromone can be incorporated into pest management, full identification was required.'

The chiral pheromone of the mealybug *Pseudococcus viburni* had been made diastereoselectively by Millar before, and its relative configuration established using

NMR. The absolute configuration could not be confirmed as only a few micrograms of the natural compound are available, preventing measurement of its optical rotation. In the absence of one enantiomer of known configuration, Millar had no way of determining which enantiomer was the natural pheromone.

'To break this impasse we reasoned that if at least one enantiomer could be resolved from the synthetic racemate, it might be possible to determine its absolute configuration by comparing its experimentally-determined VCD spectrum to the theoretical VCD spectra of the two enantiomers, calculated using density functional theory,' explained Figadère. This proved to be the case and enabled unambiguous assignment of the absolute configuration of the pheromone.

'Comparison of experimental and theoretical VCD spectra has again been shown to be a valuable method for determining the absolute



**Knowledge of the absolute stereochemistry of the bug's sex pheromone could be used to stop crop infestations**

**Reference**  
B Figadère *et al.*, *Chem. Commun.*, 2008, DOI: 10.1039/b717440c

configuration of chiral compounds without enantioselective synthesis of one or both enantiomers,' remarked Stephens. 'This method should be particularly useful for newly-identified natural products where the very small amounts of sample may eliminate the use of other methods for determining absolute configuration.'

'There are a number of chemical and enzymatic methods for resolving racemates, and the ability to determine the absolute configurations of the resulting enantiomers without having to do a chiral synthesis will save a lot of time and effort,' Millar added.

Hans-Erik Högberg, a Professor of Organic Chemistry at the Mid Sweden University, Sundsvall, agreed 'Millar presents an elegant solution to this problem and provides researchers in chemical ecology with a powerful new tool for determining absolute stereochemistry. I expect this to greatly impact future research in chemical ecology.'

*Michael Spencelayh*

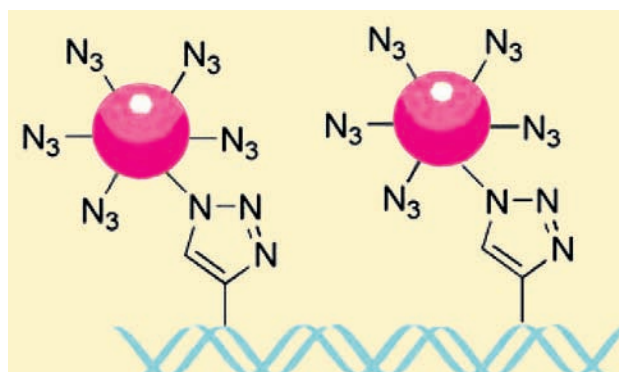
# DNA proves a useful template for nanosized electronic devices

## DNA nanowires

Fastening azide-functionalised gold nanoparticles onto modified DNA holds great promise for nanoscale electrical circuits, say German researchers.

The trend for miniaturisation in electronics, and size and cost limitations of conventional lithographic techniques, has led researchers to develop alternative routes to nanoelectronic components. DNA is a useful template for nanoscale electronic devices, explained Simon from the Institute for Inorganic Chemistry, Aachen, Germany, due to its well-defined structure and many electrostatic and chemical binding sites which can be modified.

Simon and colleagues have made a new type of gold nanoparticle containing an azide ( $-N_3$ ) functional



**Gold nanoparticles are attached to modified DNA making nanowires**

**Reference**  
M Fischler *et al.*, *Chem. Commun.*, 2008, 169 (DOI: 10.1039/b715602b)

group. They have coupled the nanoparticles to artificial DNA, where thymine bases are replaced by alkyne-modified derivatives, using a copper catalysed cycloaddition reaction. This densely covers the DNA with

nanoparticles at highly regular intervals. As the nanoparticles can conduct electricity, the nanoparticle-modified DNA can potentially be used as a nanowire.

Monika Fischler, who also worked on the project, said that the 'major advantages [of this route] are the programmability of the DNA template through incorporating artificial bases, as well as the high selectivity and yield of the copper catalysed reaction'.

Duncan Graham of the University of Strathclyde, UK, praised the work. He said that the 'formation of chains of nanoparticles is very challenging and this is a good approach to producing nanowires that potentially conduct electricity better'.

*Vikki Chapman*

# A time for transition

*Peter Kündig discusses his chemistry career and new editorial role with Joanne Thomson*



**Peter Kündig**

**Peter Kündig is Professor of Organic Chemistry at the University of Geneva. His research focuses on the use of transition metals for organic synthesis. He is the new chairman of the *Chemical Communications* editorial board.**

**What early influences steered you towards a career as a chemist?**

As a child, I was fascinated by science and technology. Shortwave radios, watching planes, homemade explosives and fireworks were all part of my youth. It was much easier to make explosives at home back then because the ingredients – fuses, weed-killer, sulfur – were more readily available.

**What are you working on at the moment?**

New and more efficient ways to make chiral organic molecules using transition metals is my main concern. We develop new efficient ways to make new and existing catalysts and we carry out mechanistic studies. We have made new chiral bulky ligands, such as *N*-heterocyclic carbenes, phosphoramidates, and perfluoroarylphosphinites.

These modify the reactivity of metals and catalyse highly asymmetric reactions including the arylation of amides, hydrogenolysis, cycloadditions and coupling reactions under mild conditions. These and the application of chromium-mediated dearomatisation reactions to natural product synthesis are all areas where I have current interests and research projects.

**Transition metal catalysed reactions are already recognised as a significant component of the organic chemist's arsenal. How do you see the field progressing?**

Catalysis will continue to see tremendous growth and asymmetric reactions will take a lead in future developments. With the impressive array of reported reactions, it is surprising to see that less than thirty of these processes are used in industrial production. Almost all of them are asymmetric hydrogenations and oxidations. This is bound to change.

Carbon-heteroatom and carbon-carbon bond forming reactions will come to the fore but catalyst access, stability, efficiency and selectivity will need to be improved. New reactions and cascade processes will keep us busy. There are a lot of things still to do.

**What scientific discovery would you like to have been responsible for?**

Alkene metathesis as applied to organic synthesis. It is a reaction that has been around for many years. It has been used widely in polymer science and the petroleum industry but its application to fine chemistry needed the selective catalysts developed by Dick Schrock and Bob Grubbs. For this they received the Nobel Prize, along with Yves Chauvin who provided the mechanism. It was something that was waiting to be discovered and it has had a huge impact on organic chemistry.

**You are the new chairman of the *ChemComm* editorial board. What are your aspirations for the journal?**

I am looking forward to working with an editorial staff that has been doing an outstanding job over the years. I would like to help to further increase the visibility of the journal in all areas of frontier chemistry and strengthen its position as one of the leading communication journals in which everyone wants to publish their best and newest research.

**You won the EuCheMS award for service in recognition of your work for European cooperation in science. Why is cooperation between European chemical societies so important?**

With more than 50 societies, European chemistry is too fragmented. More and more decisions, and a growing part of our research funding, will come from Brussels. There has to be a rallying point for chemists in Europe otherwise chemistry will be neglected by European politicians. EuCheMS provides this umbrella structure and it will be far more effective than the individual societies on their own.

**What do you do in your spare time?**

My wife would tell you that I have no spare time, and that chemistry is my life. However, I like carpentry and motorcycle riding and repairing. I like skiing and mountain walks and travelling to out-of-the-way places in Asia or South America. I have a passion for wines, and keeping the cellar well-stocked is a challenge. Time is, of course, the missing ingredient and chemistry takes up most of it.

Would anyone really put  
a Formula One engine in  
a family saloon?

In the NMR world however,  
it makes perfect sense...

**Our new generation of 5mm  $^{13}\text{C}$ -optimised  
CryoProbe is available at 400MHz and above!**

This makes your 400MHz spectrometer as sensitive as an 800.  
Just think what this could mean to you...

- 16-fold productivity improvement
- Run a  $^{13}\text{C}$  spectrum in minutes, not hours
- Why not a  $^{13}\text{C}$  on every sample?
- And DEPT-135 and  $^{13}\text{C}$  HSQC spectrum as well?

**At last, CryoProbe™ sensitivity for the organic chemist**



Contact us for more details: +44 (0)24 7685 5200 [sales@bruker.co.uk](mailto:sales@bruker.co.uk) [www.bruker-biospin.com](http://www.bruker-biospin.com)

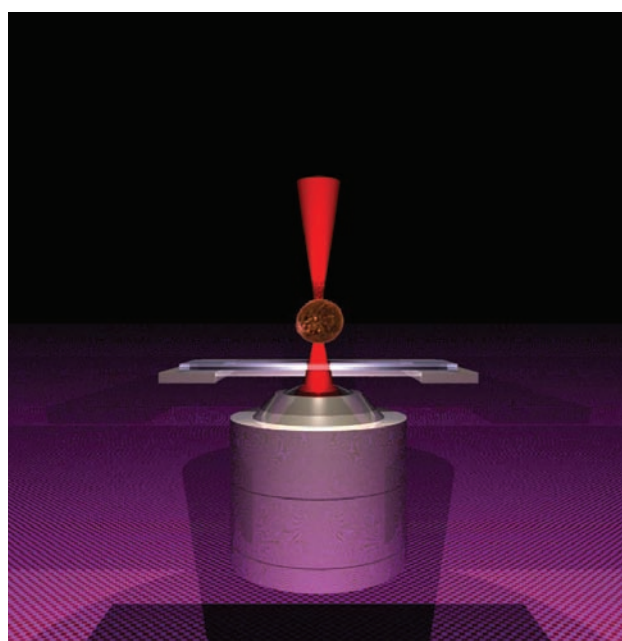
# The light touch

Kishan Dholakia, Peter Reece and Min Gu from the University of St Andrews, UK, examine how light can move and sort biological objects, and be used for studying physics and chemistry at the microscopic scale

Holding and moving objects using light might seem like science fiction, but it is actually science fact – at the microscopic scale. The characteristics of light and light–matter interactions on a small scale have allowed some astounding scientific advances in the last forty years. The invention of the laser opened up many new research fields including optical micromanipulation – where light exerts a force, to hold (trap) and move objects. This force comes from transferring momentum possessed by light to objects. For example if an object refracts the light, the light's momentum will change as it bends. Naturally the momentum of a single quantum of light, the photon, is very small, meaning these forces are barely a million millionth of a Newton.

Such forces cannot hope to move macroscopic objects, but are perfect for holding and moving objects the size of single cells or smaller. A tightly focused beam of light can move objects this size without damage, as carefully choosing the light wavelength avoids absorption and ensures the force transfer is non-invasive.

In the biological world, this technique can measure exceptionally precise and minuscule forces where macromolecules are tethered to microscopic beads. Here we are in the realm of molecular motors that convert chemical energy to mechanical work. Examples include the actin-myosin system which operates using energy from chemical reactions, typically the hydrolysis of adenosine triphosphate (ATP) to adenosine diphosphate (ADP) and phosphate. Trapping allows this process to be observed in real time. The exact positions of



trapped particles are observed to much higher accuracies than the wavelength of light, as detectors can take in to account an object's centre of gravity, meaning the movement of biological molecules can be observed with amazing sensitivity. Transcriptional elongation of *Escherichia coli* RNA polymerase motion can even be monitored on a DNA template with its motion recorded at the Ångström level.

Light can do much more than just make accurate force measurements. It can move single or multiple droplets for subsequent mixing and study chemical reactions – opening up new chemistry including combinatorial chemistry using only picolitres of reagents, studying coagulation dynamics and micro-reactions. Optical forces combined with fluidic forces are also used in

**Light passing through a microscope objective can grab and hold objects in the bright part of the beam**

the area of microfluidics for lab-on-a-chip research.

Novel photonics in the form of arrays of traps or the implementation of new light patterns (rather than the standard circular mode pattern from most lasers) is core to many recent advances. If extended light patterns are created instead of one single beam, an array of light spots (akin to a set of egg-boxes) are generated. These arrays of traps are known as a potential energy landscape. The motion of a particle across this optical array is like a small ball moving along a slanted corrugated roof, where gravity causes the object to move across the roof, but the exact trajectory followed is dependent upon the slant of the corrugation in the roof. Extending this analogy, arrays of traps can be created so that when particles flow over them they deflect objects to a degree based on their affinity to the light. This method allows the separation (sorting) of cells and colloidal particles without adding fluorescent markers. This is just one example of what these landscapes may achieve: their impact should reach a wide range of colloidal and soft matter research, and may even help us better understand superconductivity.

Optical micromanipulation has been around for over 35 years, with its impact significantly expanding recently. These new applications and insights make the field more dynamic and exciting than ever – light has ‘caught’ more than the imaginations of scientists.

Read Kishan Dholakia et al's tutorial review on 'Optical micromanipulation' in issue 1, 2008 of Chemical Society Reviews.

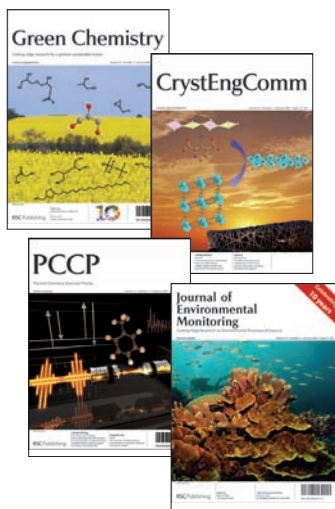
**Reference**  
K Dholakia, P Reece and M Gu, *Chem. Soc. Rev.*, 2008, **37**, 42 (DOI: 10.1039/b512471a)

# 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 Gilmudtinov) 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](http://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...

## 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](http://www.molecularbiosystems.org)

## 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.



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](http://www.rsc.org/books)

*Chemical Science* (ISSN: 1478-6524) is published monthly by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge UK CB24 0WF. It is distributed free with *Chemical Communications*, *Dalton Transactions*, *Organic & Biomolecular Chemistry*, *Journal of Materials Chemistry*, *Physical Chemistry Chemical Physics*, *Chemical Society Reviews*, *New Journal of Chemistry*, and *Journal of Environmental Monitoring*. *Chemical Science* can also be purchased separately. 2008 annual subscription rate: £199; US \$396.

All orders accompanied by payment should be sent to Sales and Customer Services, RSC (address above). Tel +44 (0) 1223 432360, Fax +44 (0) 1223 426017. Email: [sales@rsc.org](mailto:sales@rsc.org)

**Editor:** Nina Notman

**Associate editors:** Neil Withers, Celia Clarke

**Interviews editor:** Joanne Thomson

**Essential elements:** Daniel Bradnam, Rebecca Jeeves and Valerie Simpson

**Publishing assistant:** Ruth Bircham

**Publisher:** Janet Dean

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the copyright and Related Rights Regulations 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission of the Publisher or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

Royal Society of Chemistry: Registered Charity No. 207890.

# RSC Publishing