

IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 33(10) 1981-2184 (2009)



Cover

See André Vioux *et al.*, pp. 2015–2021. Ionogels are able to keep ionic liquids confined in silica matrices cast as pellets. Chemical reactions were shown to take place within the confined ionic liquid phase encapsulating a metal catalyst without leaching. Image reproduced by permission of Serge Bertrand (ICG Montpellier) from Sabrina Volland, Marina Gruit, Thomas Régner, Lydie Viau, Olivier Lavastre and André Vioux *New J. Chem.*, 2009, **33**, 2015.



Inside cover

See Pauline M. Schwartz *et al.*, pp. 2022–2027. Models of some chemical systems predict non-obvious and paradoxical behavior under thermal cycling conditions. These models may inspire interesting new chemistry. Image copyright Daniel C. Osipovitch from Daniel C. Osipovitch, Carl Barratt and Pauline M. Schwartz, *New J. Chem.*, 2009, **33**, 2022.

HIGHLIGHTS IN CHEMICAL SCIENCE

C73

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Highlights in Chemical Science

October 2009/Volume 6/Issue 10

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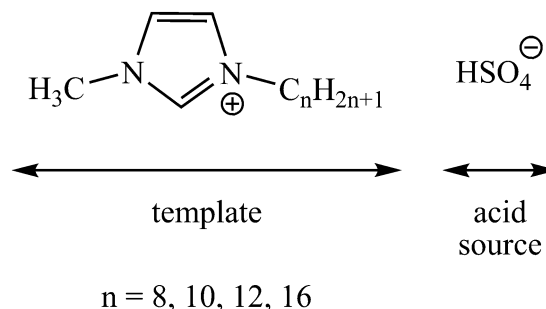
LETTERS

1997

The use of acidic task-specific ionic liquids in the formation of high surface area mesoporous silica

Ajit A. Pujari, Jessica J. Chadbourne, Antony J. Ward, Lorenzo Costanzo, Anthony F. Masters and Thomas Maschmeyer*

The convenient synthesis of a series of acidic task-specific ionic liquids and their subsequent use as templates for high surface area mesoporous silicas is introduced.



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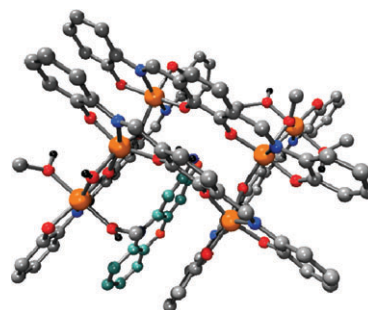
LETTERS

2001

A hexanuclear iron(III) complex of a hexadentate fully conjugated diimine ligand derived from 1,4-diformyl-2,3-dihydroxybenzene

Humphrey L. C. Feltham, David S. Larsen and Sally Brooker*

The first iron complex of any ligand derived from 1,4-diformyl-2,3-dihydroxybenzene was synthesized and revealed to be a hexanuclear iron(III) complex.

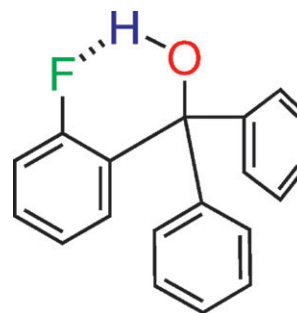


2004

The intramolecular C–F...HO hydrogen bond of 2-fluorophenyldiphenylmethanol

Hiroyuki Takemura,* Megumi Kaneko, Katsuya Sako and Tetsuo Iwanaga

The intramolecular C–F...HO hydrogen bond of 2-fluorophenyldiphenylmethanol was clarified by X-ray crystallographic analysis and ^1H NMR spectroscopy.



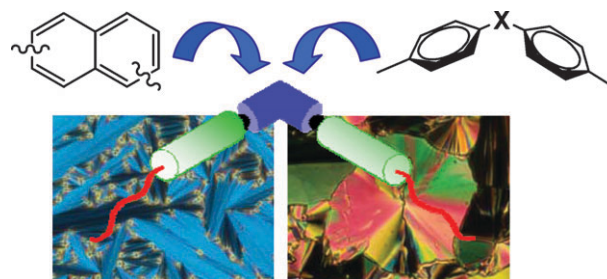
PAPERS

2007

On the supramolecular packing of bent-shaped molecules: the influence of the central bent-core on the liquid crystalline behaviour

Nélide Gimeno, María José Clemente, Patricia Forcén, José Luis Serrano and Maria Blanca Ros*

The supramolecular self-organization of bent-compounds derived from naphthalene or bis-4,4'-disubstituted phenylenes at variable temperature results in polar tilted lamellar (SmCaPA) or orthogonal lamellar arrangement (SmA) depending on the bent-angle of the central core.

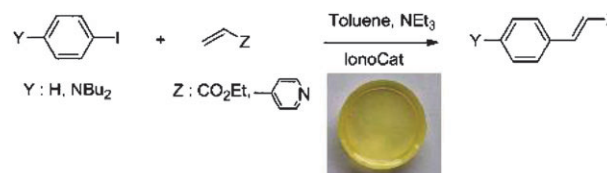


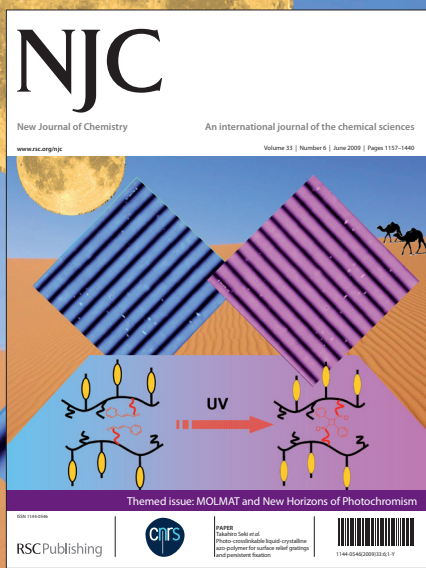
2015

Encapsulation of Pd(OAc)₂ catalyst in an ionic liquid phase confined in silica gels. Application to Heck–Mizoroki reaction

Sabrina Volland, Marina Gruit, Thomas Régnier, Lydie Viau, Olivier Lavastre* and André Vioux*

Ionic liquids confined into silica matrices (*i.e.* ionogels) encapsulating Pd(OAc)₂ were successfully used as catalysts in Heck–Mizoroki coupling reactions with reaction rates analogous to homogeneous conditions and without leaching.





Themed Issue: MOLMAT and New Horizons of Photochromism

This themed issue comprises articles from two key meetings. Firstly, the 3rd International Symposium on Molecular Materials (MOLMAT) covering topical research within chemical synthesis to solid-state physics, nanotechnology and the theory of molecular materials based on inorganic and organometallic chemistry. This section of the issue is guest edited by Azzedine Bousseksou, Andreas Hauser and Jean-Paul Malrieu.

Secondly, the New Horizons of Photochromism meeting. Guest edited by Kenji Matsuda and Keitaro Nakatani, the 21 articles, (including 6 Letters and a Perspective) are largely written by attendants of the seminar, but also by other researchers involved in this topic.

MOLMAT articles include:

Perspective:

Cyano-bridged coordination polymer nanoparticles

Joulia Larionova, Yannick Guari, Claudio Sangregorio and Christian Guérin

Papers:

Molecular engineering to improve the charge carrier balance in single-layer silole-based OLEDs

Laurent Aubouy, Nolwenn Huby, Lionel Hirsch, Arie van der Lee and Philippe Gerbier

Chemical disorder and spin crossover in a mixed ethanol–2-propanol solvate of Fe^{II} tris(2-picolyamine) dichloride

Dmitry Chernyshov, Brita Vangdal, Karl Wilhelm Törnroos and Hans-Beat Bürgi

Photochromism articles include:

Letter:

The photochromic and self-assembling properties of diarylethenes having chiral amphiphilic chains at the reactive carbon atoms

Takashi Hirose, Masahiro Irie and Kenji Matsuda

Papers:

Photoswitching in diarylethene nanoparticles, a trade-off between bulk solid and solution: towards balanced photochromic and fluorescent properties

Jonathan Piard, Rémi Métyvier, Marion Giraud, Anne Léaustic, Pei Yu and Keitaro Nakatani

Photo-crosslinkable liquid-crystalline azo-polymer for surface relief gratings and persistent fixation

Wenhan Li, Shusaku Nagano and Takahiro Seki

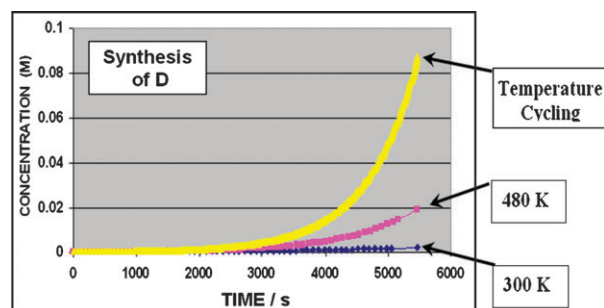
PAPERS

2022

Systems chemistry and Parrondo's paradox: computational models of thermal cycling

Daniel C. Osipovitch, Carl Barratt and Pauline M. Schwartz*

Parrondo's paradox motivated development of several novel computational models of chemical systems. The models predicted a greater concentration of product under thermal cycling than under fixed temperature conditions. We show that even simple chemical systems may behave paradoxically.

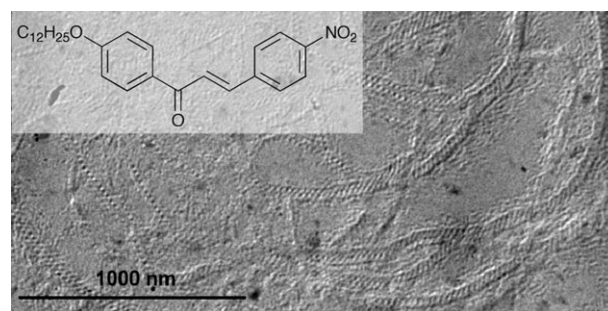


2028

Nitrochalcones as organogelators: evidence of the involvement of nitro groups and solvent in gel formation

François-Xavier Simon, Thi-Thanh-Tam Nguyen, Marc Schmutz, Gero Decher, Jean-François Nicoud* and Philippe J. Mésini*

New organogels based on 4-alkoxynitrochalcones are synthesized and described; their self-assembly proceeds by strong interaction of the nitro groups and co-assembly with the solvent.

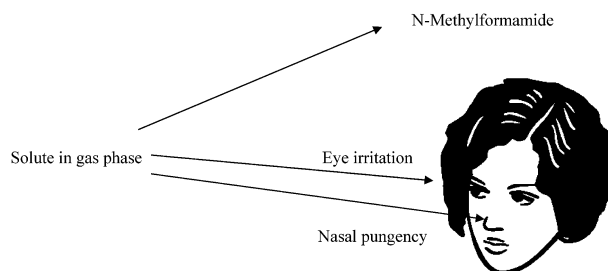


2034

Partition of compounds from water and from air into amides

Michael H. Abraham,* William E. Acree, Jr and J. Enrique Cometto-Muñiz

Equations for gas to amide partition coefficients are reported for 12 amides; the equations can be used to predict further partition coefficients. Transfer of solutes from the gas phase to *N*-methylformamide is a good model for eye irritation and nasal pungency thresholds. Primary and tertiary amides are poor models.

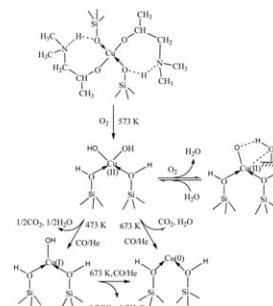


2044

Controlled synthesis of pure and highly dispersive Cu(II), Cu(I), and Cu(0)/MCM-41 with Cu[OCHMeCH₂NMe₂]₂/MCM-41 as precursor

Guoying Zhang, Jinlin Long, Xuxu Wang,* Wenxin Dai, Zhaohui Li, Ling Wu and Xianzhi Fu*

Pure Cu(II), Cu(I) and Cu(0) isolated sites highly dispersed on a MCM-41 surface were synthesized by a surface organometallic chemistry procedure under controlled conditions.



5.340*

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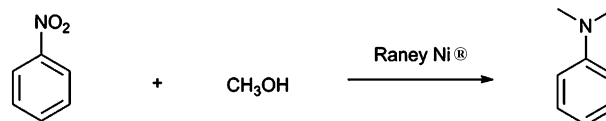
PAPERS

2051

One-pot synthesis of *N,N*-dimethylaniline from nitrobenzene and methanol

Long Xu, Xiaonian Li,* Yifeng Zhu and Yizhi Xiang

Direct synthesis of *N,N*-dimethylaniline from nitrobenzene and methanol over Raney-Ni[®] through the sequential coupling of hydrogen produced from methanol, hydrogenation of nitrobenzene for aniline, and *N*-methylation of aniline for *N,N*-dimethylaniline.

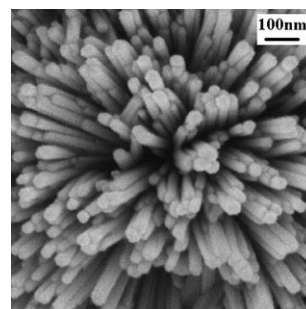


2055

Co₂P nanostructures constructed by nanorods: hydrothermal synthesis and applications in the removal of heavy metal ions

Yonghong Ni,* Jun Li, Lina Jin, Jun Xia, Jianming Hong and Kaiming Liao

Co₂P nanostructures built up of nanorods show excellent capacities to remove heavy metal Pb²⁺ and Cd²⁺ ions, and have potential applications in waste water treatment.

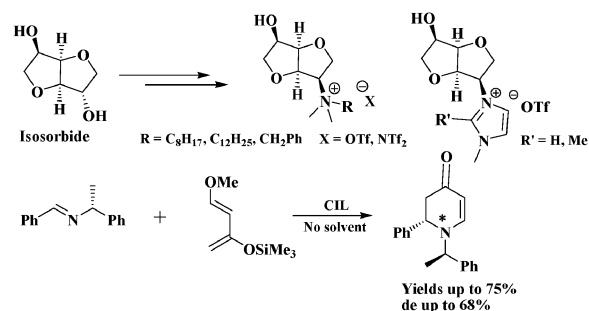


2060

Chiral ionic liquids derived from isosorbide: synthesis, properties and applications in asymmetric synthesis

Olivier Nguyen Van Buu, Audrey Aupoix, Nhung Doan Thi Hong and Giang Vo-Thanh*

A novel class of chiral ammonium and imidazolium-based ionic liquids has been designed and synthesized using isosorbide as a biorenewable substrate. These chiral ionic liquids were found to catalyze the aza Diels–Alder reaction to give good yields and moderate diastereoselectivities.

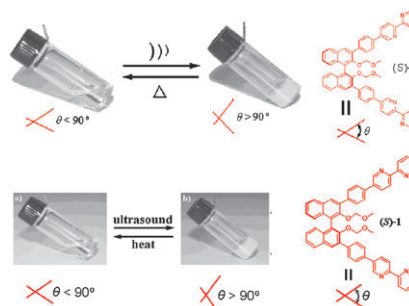


2073

Ultrasound-promoted chiral fluorescent organogel

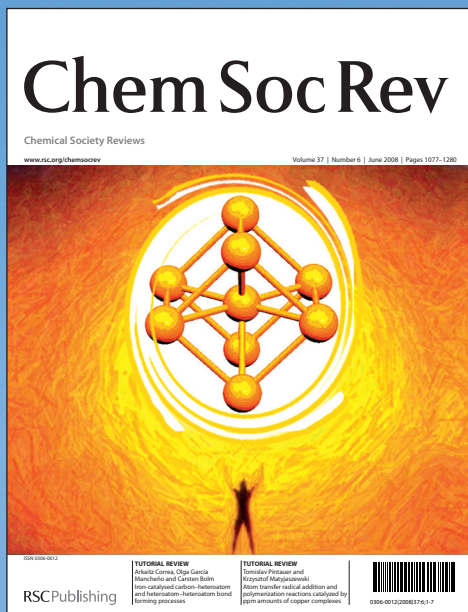
Yabing He, Zheng Bian,* Chuanqing Kang, Rizhe Jin and Lianxun Gao*

The observed ultrasound-induced gelation is a rapid crystallisation behavior similar to sonocrystallisation of organics, and the dihedral angle between the two naphthyl rings of the 1,1'-binaphthyl unit in (*S*)-1 will increase upon gelation.



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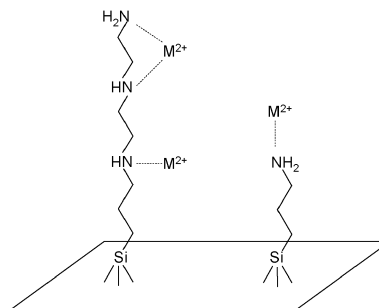
PAPERS

2081

New inorganic–organic lamellar derivatives synthesized from H-RUB-18 and thermodynamics of cation sorption

Thaís R. Macedo and Claudio Airoidi*

Amine and diethylenetriamine functionalized nanostructured inorganic–organic hybrids were synthesized from crystalline layered H-RUB-18. The hybrids show ability to remove divalent cations (M^{2+}) from aqueous solutions and favorable thermodynamic data were determined from calorimetric titration corresponding to binding of nitrogen basic atoms attached to the pendant chain to cations.

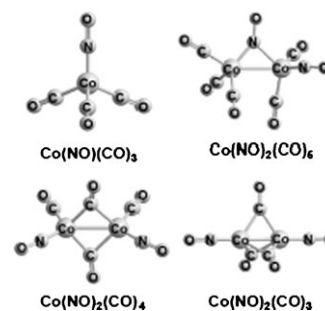


2090

Mononuclear and binuclear cobalt carbonyl nitrosyls: comparison with isoelectronic nickel carbonyls

Xiaoli Gong, Qian-Shu Li,* Yaoming Xie, R. Bruce King* and Henry F. Schaefer III

The lowest energy structures for $\text{Co}(\text{NO})(\text{CO})_n$ ($n = 3, 2, 1$) predicted by density functional theory parallel those of the corresponding isoelectronic $\text{Ni}(\text{CO})_{n+1}$ derivatives. The lowest energy structures of $\text{Co}_2(\text{NO})_2(\text{CO})_5$, $\text{Co}_2(\text{NO})_2(\text{CO})_4$, and $\text{Co}_2(\text{NO})_2(\text{CO})_3$ have one, two, and three bridging groups, respectively, just like the isoelectronic $\text{Ni}_2(\text{CO})_{n+2}$.

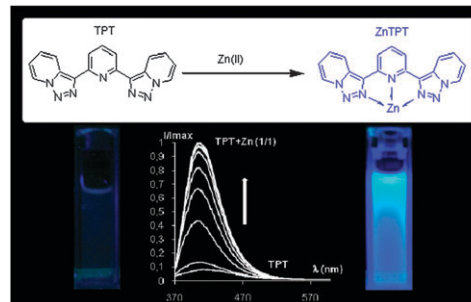


2102

[1,2,3]Triazolo[1,5-a]pyridine derivatives as molecular chemosensors for zinc(II), nitrite and cyanide anions

Rafael Ballesteros-Garrido, Belén Abarca,* Rafael Ballesteros, Carmen Ramírez de Arellano, Frédéric R. Leroux,* Françoise Colobert* and Enrique García-España*

The ligands TPF, TPS and TPT, based on the triazolopyridine–pyridine nucleus, have been tested as chemosensors for metal ions. The Zn^{2+} TPT 1 : 1 complex has proved to be an efficient fluorescent chemosensor for nitrite and cyanide anions.

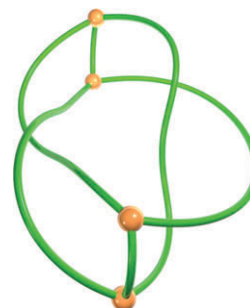


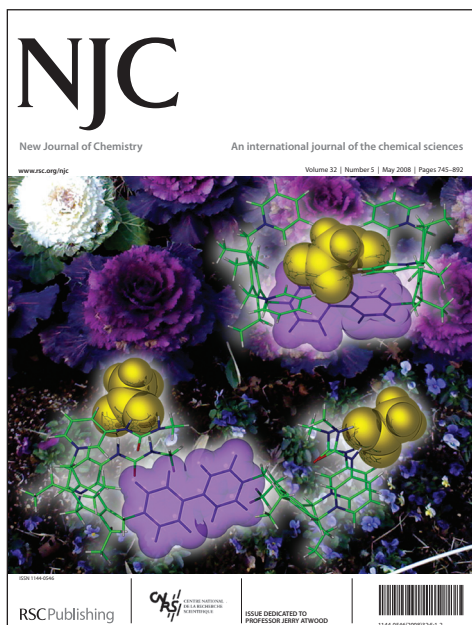
2107

All toroidal embeddings of polyhedral graphs in 3-space are chiral

T. Castle, Myfanwy E. Evans and S. T. Hyde*

The simplest tangled embeddings of polyhedral graphs (such as the network of edges of a tetrahedron) lie on a torus rather than a sphere. These tangled patterns – such as the knotted tetrahedron shown here – are always chiral, regardless of the chirality of the original graph.





Drawing disciplines together

Introducing Professor Peter Junk

Associate Editor

Peter Junk graduated from the University of Western Australia in 1984 obtaining a Bachelor of Science with first class honours in physical and inorganic chemistry, and completed his PhD in organometallic chemistry under the supervision of Professor Colin Raston in 1988. He currently holds a position of Professor of Chemistry and is the Head of the School of Chemistry at Monash University, Australia.

His main research interests are in rare earth and main group organometallic, organoamido and aryloxo chemistry, but has applied interests in X-ray imaging and corrosion inhibition. To date, he has published more than of 250 publications and reviews.

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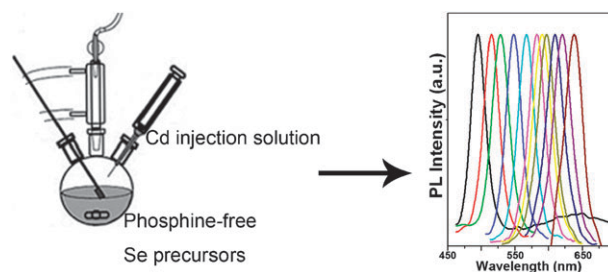
PAPERS

2114

Investigation on the phosphine-free synthesis of CdSe nanocrystals by cadmium precursor injection

Jin Zhong Niu, Huaibin Shen, Hongzhe Wang, Weiwei Xu, Shiyun Lou, Zuliang Du and Lin Song Li*

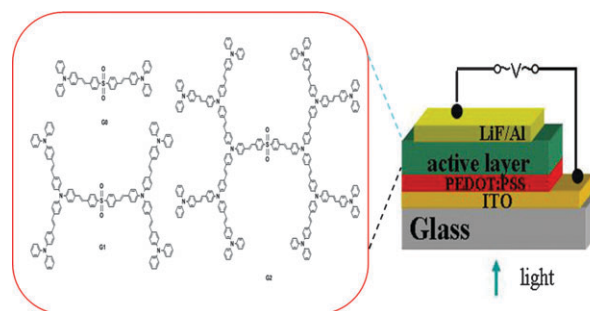
Green Se precursors combined with a Cd inverse injection method for the synthesis of high quality CdSe nanocrystals.



2120

Synthesis and photovoltaic properties of novel solution-processable triphenylamine-based dendrimers with sulfonyldibenzene cores

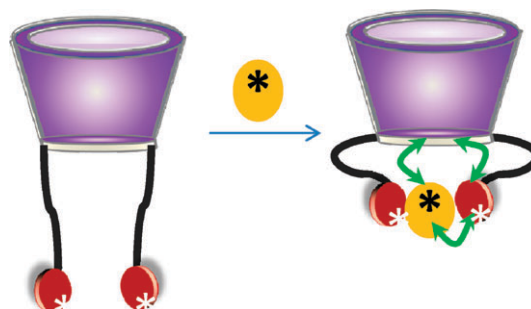
Kunpeng Li, Jiali Qu, Bin Xu, Yinhua Zhou, Leijing Liu, Ping Peng and Wenjing Tian*

A series of novel dendrimers with symmetrical donor- π -bridge-acceptor- π -bridge-donor (D- π -A- π -D) structure and with triphenylamines as dendrons have been synthesized and studied in heterojunction OSCs.

2128

Enantioselective recognition of amino acids by chiral peptido-calix[4]arenes and thiacalix[4]arenes

Joackim Bois, Isabelle Bonnamour, Christian Duchamp, Helene Parrot-Lopez, Ulrich Darbost and Caroline Felix*

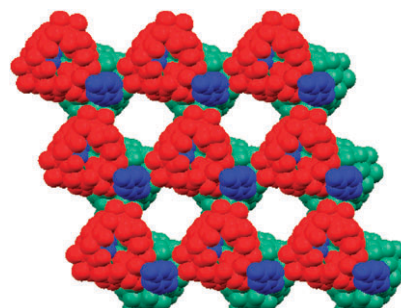
New chiral thiacalix[4]arene derivatives appended with amino-acid units were synthesised. Recognition ability and chiral differentiation towards neutral amino acids were studied by ^1H NMR spectroscopy.

2136

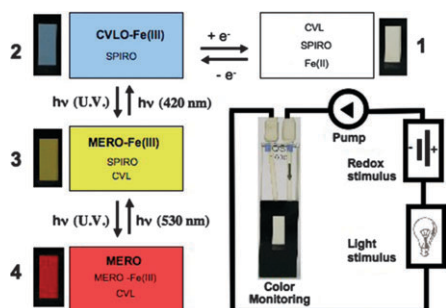
Exclusion complexes of the HCl salts of benzidine and bis(4-aminophenyl) methane with two methyl-substituted cucurbiturils

Ying Yan, Sai-Feng Xue,* Hang Cong, Jian-Xing Zhang, Yun-Qian Zhang, Qian-Jiang Zhu and Zhu Tao

We demonstrate the formation of two host-guest exclusion complexes in which the guest molecules are excluded at the portals of the host cucurbiturils. In the solid state, each guest or host is sandwiched by neighboring hosts or guests leading to the formation of 1D supramolecular chains.



2144



Multiresponsive chromogenic systems operated by light and electrical inputs

Carlos Pinheiro, A. Jorge Parola, César A. T. Laia, António Câmara and Fernando Pina*

A chromogenic multistate system capable of switching between cyan, magenta, yellow and transparent states, independently addressable by light and electric inputs, is presented. The system profits from complexes of Fe(III)/Fe(II) with crystal violet lactone and a spiropyran. Electric stimulus operates the metal.

2148

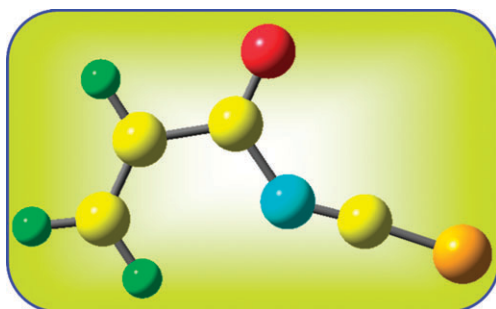


[3]Rotaxanes and [3]pseudorotaxanes with a rigid two-bidentate chelate axle threaded through two coordinating rings

Jean-Paul Collin, Jean-Pierre Sauvage,* Yann Trolez and Kari Rissanen

New [3]rotaxanes and [3]pseudorotaxanes have been synthesised using the “gathering and threading” effect of copper(I).

2155

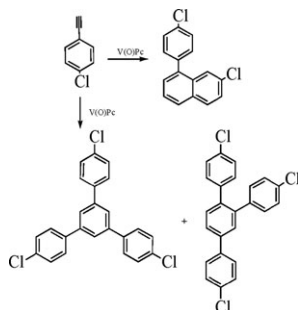


Molecular and electronic structures of acryloyl isothiocyanate, CH₂CHC(O)NCS: a joint experimental and theoretical study

Maofa Ge,* Chunping Ma, Shengrui Tong, Wei Xue, Zhifeng Pu and Dianxun Wang

Molecular and electronic structures of a novel isothiocyanate, CH₂=CHC(O)NCS, were investigated by photoelectron spectroscopy, photoionization mass spectroscopy, FTIR and Raman, combined with theoretical calculations.

2162



The highly selective formation of biaryls by the cyclization of arylethyne catalyzed by vanadyl phthalocyanine

Daniel Cicero, Angelo Lembo, Alessandro Leoni and Pietro Tagliatesta*

Vanadyl phthalocyanine is able to catalyze the cyclooligomerization of arylethyne, giving biaryl derivatives in high yield and selectivity. The mechanism of the reaction has been studied using 2,6-dimethoxyethynylbenzene and deuterated ethynylbenzene as substrates.

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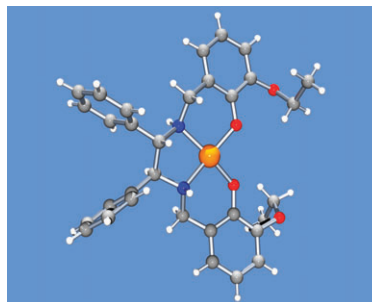


2166

Enantioselective catalysts for the Henry reaction: fine-tuning the catalytic components

Edwin C. Constable,* Guoqi Zhang,
Catherine E. Housecroft,* Markus Neuburger,
Silvia Schaffner, Wolf-D. Woggon and Jennifer A. Zampese

Catalysts for the asymmetric Henry reaction using 1,6-bis(3-ethoxy-2-hydroxyphenyl)-(3*S*,4*S*)-(–)-diphenyl-2,5-diazahexane and copper salts have been screened; optimized conditions have been tested on a range of substrates.

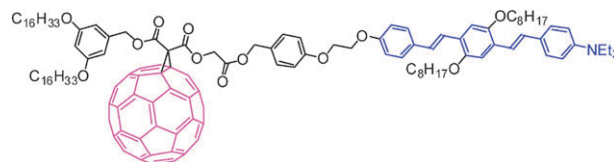


2174

Photoinduced electron transfer in a fullerene–oligophenylenevinylene dyad

Aline Gégout, Juan Luis Delgado,
Jean-François Nierengarten,* Béatrice Delavaux-Nicot,*
Andrea Listorti, Claudio Chiorboli, Abdelhalim Belbakra
and Nicola Armaroli*

A new C₆₀–oligophenylenevinylene (OPV) derivative in which the OPV unit has been functionalized with a dialkylamine electron donor group is described. OPV → C₆₀ photoinduced electron transfer is observed in polar and apolar solvents.



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Highlights in Chemical Science

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Damaged teeth could be repaired in the mouth using a simple technique Enamel regeneration makes scientists smile



Regrowing enamel in the mouth could provide an alternative to crowns and veneers

Chinese researchers are a step closer to being able to regrow tooth enamel in the mouth.

Haifeng Chen and colleagues at Peking University, Beijing, etched a tooth's surface with phosphoric acid to create nucleation sites and then immersed it in a solution of calcium, phosphate and fluoride ions. The ions reacted at the nucleation sites, with help from a chelating agent called *N*-(2-hydroxyethyl)ethylene-diamine-

N,N,N-triacetic acid (HEDTA), to form a new layer of enamel.

The method could be used to repair damaged teeth or as sealant to prevent cavities, says Chen. Although other methods of making enamel have been developed, none of them can be carried out in dental clinics because they require harsh reaction conditions. The new method is simpler and less expensive than existing methods and can be carried out at body

temperature.

'The beauty of this process is that we are on the way to rebuilding our tooth enamel with exactly the same matter and microstructures as natural enamel,' states Chen.

But HEDTA is not safe for consumption so the team is working on a device to separate the HEDTA solution from the mouth so it can be used in the clinic. 'We are also trying to use some small peptides to mimic the enamel protein structure and replace the HEDTA that directs the organisation of enamel crystals,' Chen explains. 'These peptides will bind to these crystals and make our enamel structure less brittle.'

'This novel procedure offers the possibility of real alternatives to replacement crowns and veneers, which are expensive to place and difficult to maintain,' comments Colin Robinson, an expert in biomineralisation at the Leeds Dental Institute, UK.

Sylvia Pegg

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In this issue

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First aid for electronics

Microcapsules filled with nanotubes could repair batteries

Twist of fate for two-to-one assemblies

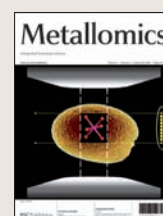
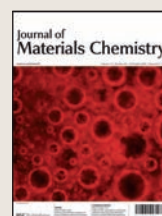
Unique nanospiral structures could be useful for minaturising optoelectronics

Understanding our food

Proteomics can be used to assure the safety of GM food say German scientists in October's Instant Insight

Riding high

Philip Mountford talks about jockeying, bribing techniques and the challenges ahead for chemistry in this month's interview



A snapshot of the latest developments from across the chemical sciences

Research highlights

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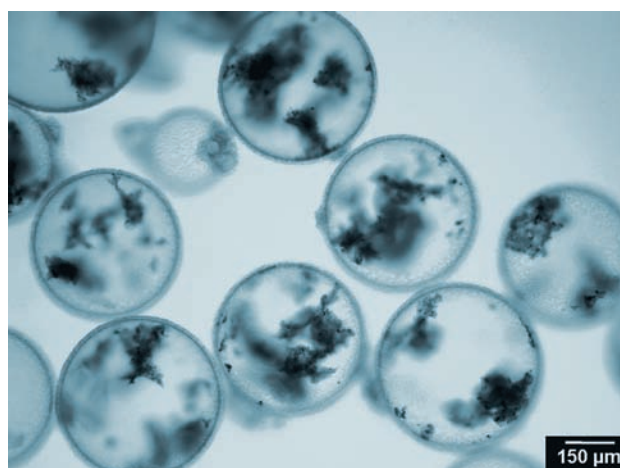
Microcapsules filled with carbon nanotubes could be used to repair batteries

First aid for electronics

US scientists have developed a first aid kit for electrical systems that could stop circuits failing and lead to safer, longer lasting batteries.

Jeffrey Moore, at the University of Illinois at Urbana-Champaign, and colleagues made microcapsules with robust walls and filled them with carbon nanotubes (CNTs). They then ruptured the microcapsules using vigorous stirring and measured the contents' ability to conduct electricity between two electric probes separated by around 100 micrometres. As the team swept the applied voltage from minus to plus 50 volts, the CNTs migrated towards the probe tips. They aligned with the electric field and completed the circuit, enabling the current to flow.

They found the best capsules were between 280 and 350 micrometres – smaller ones were



too difficult to break and larger ones broke too easily.

'Battery safety and lifetime are two problems that may benefit from this approach,' says Moore. 'You may want to restore electrical conductivity of damaged battery

On breaking the microcapsule's contents spill out and complete the circuit

electrodes. On the other hand, if battery electrodes short circuit, the battery becomes dangerous and has the potential to explode. One may thus want to coat the electrodes with a resistive material to shut down a run-away battery. Exploring these ideas are some of our future plans.'

'I think it is a neat approach that can become very useful if taken further,' comments Vsevolod Rostovtsev, a nanotube expert at DuPont, Wilmington, US. 'The capsules need to become smarter so that their precise and accurate placement could be effected. The broken microcapsule shell needs to be removed from the electronic device to reduce contamination.'

Charlotte Beard

Reference

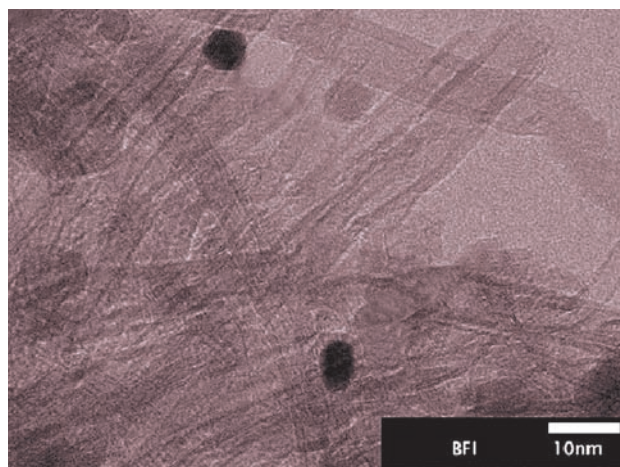
M M Caruso *et al*, *J. Mater. Chem.*, 2009, DOI: 10.1039/b910673a

Metallic impurities in nanotubes can have a large effect on their toxicity

How safe are carbon nanotubes?

Carbon nanotubes are increasingly being used in everyday products such as sporting equipment, biomedical devices and aeroplanes. But questions remain as to how safe these nanotubes really are.

A main factor in nanotube toxicity are the metal contaminants that remain from manufacture, which are typically one to ten per cent by weight, say Martin Pumera and Yuji Miyahara at the National Institute for Materials Science, Ibaraki, Japan. 'Carbon nanotubes are often viewed as homogenous materials, which is of course incorrect – they often contain impurities which are not even listed by the manufacturers,' says Pumera. The pair have used an electrochemical method to assess the effect metals have on nanotube toxicity. They say that their method is quicker and cheaper than laborious and expensive biomedical tests and



could be more useful for initial assessments of carbon nanotube toxicity.

Pumera and Miyahara measured how well five nanotube samples reduced or oxidised two simple biomarkers – hydrogen peroxide and hydrazine. They found that

Small amounts of contaminants in carbon nanotubes could make them toxic

just 100 ppm of iron was needed to dominate the reduction ability, and therefore the toxicity. Pumera says this is very disturbing, as this value is significantly lower than the detection limits of the methods routinely used to assess nanotube purity. 'It is very likely that metallic impurities are responsible for large scatter in results of toxicological studies,' he adds.

Kostas Kostarelos, who works at the Centre for Drug Delivery Research, The School of Pharmacy, London, UK, says 'this work is yet another testament of the imperative need for well-characterised and reproducible standardised carbon nanotube properties. Until this is achieved, comparative studies will continue to be difficult to interpret and predictive assays of complex interactions impacting the toxicological profile of the material will be difficult to establish.'

David Barden

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Unique nanospiral structures could be useful for miniaturising optoelectronics

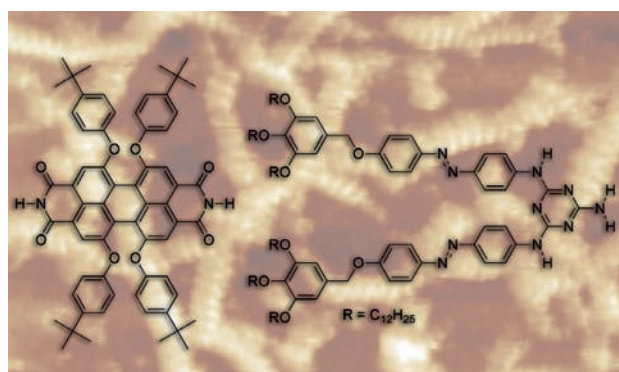
Twist of fate for two-to-one assemblies

A pair of molecules that combine in an unusual 2:1 ratio to give nano-sized spirals have been brought together by an international research team.

Recently, much effort has centred on designing pairs of photo-active molecules that assemble spontaneously to give nanostructures held together by interactions such as hydrogen bonds. Structures containing melamine and imide are particularly interesting as their photoresponsive properties could be used in miniaturising optoelectronics. These two components usually form a 1:1 ratio as they have complementary hydrogen-bonding sites.

However, when Shiki Yagai at Chiba University, Japan, and Frank Würthner at Würzburg University, Germany, mixed two of these molecules – an azobenzene-functionalised melamine and a perylene bisimide – in a 1:1 ratio, they didn't get the linear structures they expected. Instead, they got small assemblies with ill-defined morphologies, explains Yagai.

To their surprise, adding more of the azobenzene to this mixture



A melamine and a bisimide combine in an unusual 2:1 ratio to give intriguing spiral structures

triggered the formation of what Yagai describes as 'tightly-coiled helical nanostructures,' containing the two components in a 2:1 ratio. He suggests that the additional melamine molecules in the chain reduces the number of hydrogen bonds, making it more flexible and able to curve. When this happens, bisimide molecules can sit in adjacent bends of the helix, and are able to pi-stack, making the structure more stable.

Ronald Castellano, an expert in self-assembly at the University of Florida, Gainesville, US, says 'this

work reminds us of the beautiful complexity that can be achieved from the assembly of relatively simple synthetic building blocks and that there is still much to learn about predicting supramolecular structure on the nanoscale.' He adds, 'this work shows that to access new functional assemblies we must be willing to resist taking the most comfortable or intuitive approach.'

Yagai comments that these helices are similar to those seen in the light-harvesting systems of photosynthetic organisms, and he expects them to attract significant attention from supramolecular chemists. He says that unconventional systems like these could have exciting prospects, because 'switching such a structure into a new morphology might be accomplished by small changes of solvent, coordination of an analyte, a light pulse or an electrochemical stimulus.' The team are now developing smart nanostructures with morphologies and light-harvesting functions that can be controlled by light pulses.

David Barden

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The bioavailability of iron and zinc in barley grain is investigated

Essential elements from cereals

Just how much iron and zinc do you get from your breakfast? Scientists in Denmark have been looking for the answer.

Iron and zinc deficiencies are common nutritional disorders, particularly in the developing world where cereal grains are the most common food type. Measuring total concentrations of these elements in food crops is relatively easy but does not give any information about how much will be taken up by the body. This is a much bigger challenge, which Søren Husted at the University of Copenhagen and his team have set about solving. They say investigating how these elements are bound in the plant can give more information about their bioavailability.

Some elements can be indicators



Analysing iron and zinc in crops could help improve their nutritional value

of the chemical binding form of others, explains Husted, so by analysing iron, zinc, phosphorus and sulfur in the plant simultaneously, they could determine how the iron and zinc are bound. 'Multi-elemental analysis of plant tissue with sufficient robustness and accuracy is absolutely not trivial,' says Husted. But by using a combination of analytical techniques such as mass spectrometry, size exclusion chromatography and enzymatic extraction, his team were able to do just that.

They found iron and zinc have different chemical binding forms in the plant. This is contrary to the general view in the literature, says Husted, and shows that separate research strategies need to be applied in order to increase the

bioavailability of both elements. 'We think that our methods will be an important tool in future molecular plant breeding programmes aimed at improving cereal plants with a higher amount of bioavailable iron and zinc,' he adds.

Husted plans to extend the technique beyond plants. 'We would like to follow the chemical binding forms of iron and zinc from the plant, via the cooked meal, all the way through the human digestion system,' he says. 'This will give important answers to the questions remaining regarding bioavailability of micronutrients.'

Edward Morgan

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S Husted et al, *Metallomics*, 2009, DOI: 10.1039/b905688b

An electrochemical reaction can be followed as it happens inside a spectrometer

Spectra issues dissolve in ionic liquids

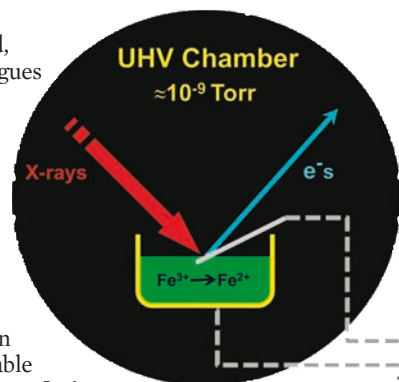
UK scientists have used x-ray photoelectron spectroscopy (XPS) to follow an electrochemical reaction in situ.

Spectroscopic techniques such as infrared and ultraviolet-visible absorption are routinely used to investigate electrochemical reactions, giving important mechanistic and structural information. However, these methods are limited to probing the outer electrons of species and cannot be used to monitor core electronic changes. XPS could fulfil this need but its requirement for ultra-high vacuum (UHV) conditions introduces a critical obstacle: solvent evaporation.

Peter Licence at the University of Nottingham, UK, has overcome this problem using ionic liquids, exploiting both their low volatility and inherent conduction properties. By specifically employing an iron(III)-

containing ionic liquid, Licence and his colleagues were able to monitor iron(III)-iron(II) reduction using XPS. Simple though it sounds, the work has been far from easy. 'We had phenomenal problems,' admits Licence, 'we could do the electrochemistry in UHV and we've been able to [measure the XPS spectra] of the ionic liquids, but to do both at the same time has been a real uphill struggle.' Given the difficulties, Licence is clearly pleased with his team's success. 'This is the first time that anyone has been able to monitor a real chemical reaction in a high vacuum environment,' he says.

Gregory Wildgoose, an expert in electrochemistry at the University of



The reduction of iron(III) to iron(II) is monitored using X-ray photoelectron spectroscopy

Oxford, is similarly enthusiastic. 'This is an important step forward; actually being able to do the electrochemistry inside the spectrometer is a very desirable tool for developing sensors and catalysts.' Wildgoose also praises the team's ingenuity in improving the technique's sensitivity. 'Incorporating the redox probe into the ionic liquid is very clever, enabling a sharp XPS signal, which would be difficult in a normal solute-solvent system,' he adds.

Licence is now eager to apply the technique, and test its limits. 'We're interested in designing more efficient catalysts, new probes, sensors, functionalised electrodes,' he explains, 'we really want to push this technology to see how far we can take it.' Philip Robinson

Reference

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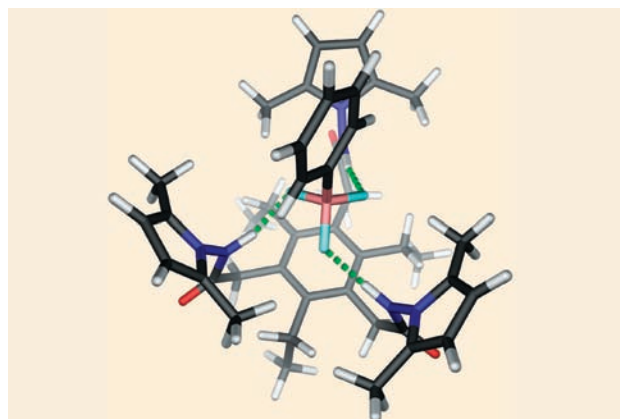
A supramolecular receptor shows that fluorine compounds can form hydrogen bonds

Fluorines make hydrogen bonds

Scientists in the US have shown that fluorine compounds can form hydrogen bonds, a finding that could have implications for the pharmaceutical industry, they say.

Fluorine is often used in drug development as its presence in organic compounds can affect properties such as adsorption, distribution and stability. However, exactly how it interacts with biological molecules remains a puzzle, says Julius Rebek Jr at The Scripps Research Institute, California.

While inorganic fluorides are powerful hydrogen bond-acceptors, there is not much evidence that covalently bound organofluorines form hydrogen bonds. Not much sticks to organic C-F bonds, says Rebek, which is why they have been so useful in products such as Teflon. So the group moved up the periodic table to look at the B-F bonds in fluoroborates. Fluoroborates are covalently bonded but also anionic, which makes their hydrogen



bonding properties interesting for researchers.

Rebek and his team made a supramolecular tripodal receptor with three inwardly directed hydrogen donors. They used the receptor to surround the BF_3^- of a trifluoroborate, presenting it with available hydrogen-bond donors, and found the covalently bound fluorine did form hydrogen bonds. 'This is

A supramolecular receptor helps to understand the hydrogen bonding of fluoroborates

Reference

P Restorp *et al.*, *Chem. Commun.*, 2009, DOI: 10.1039/b914171e

the inaugural case of recognising the BF_3^- group,' says Rebek.

Understanding the nature and strength of hydrogen bonding in this way could be important for drug development, says Rebek. These results could lead to 'the CF_3^- groups that appear in medicines being replaced by the BF_3^- group to improve solubility and, perhaps, bioavailability,' he adds.

Professor Luigi Fabbrizzi, an expert in anion binding in synthetic receptors from the University of Pavia, Italy, says the receptor could be 'a useful tool for [finding] many drug compounds of pharmaceutical interest possessing fluorinated fragments. More sophisticated receptors could be developed, capable of interacting with fluorinated compounds in more competitive solvents including water, which would allow the monitoring of many drugs in physiological fluids.'

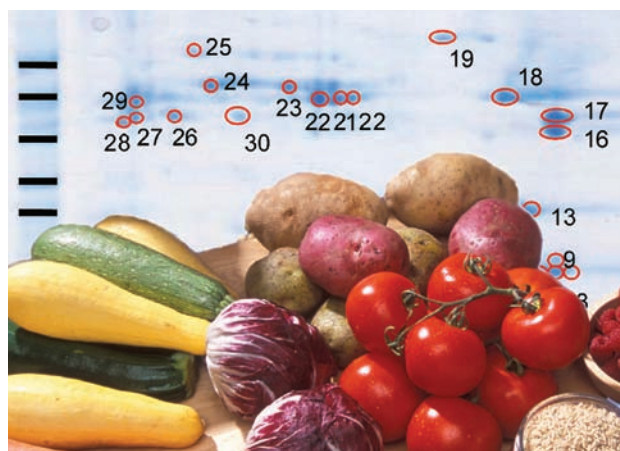
Rebek's group are currently looking at commercial applications of the receptor. Nicola Wise

Understanding our food

Monika Pischetsrieder and Rainer Baeuerlein from the University of Erlangen-Nuremberg, Germany, look at how the safety of GM food can be assured before it reaches supermarket shelves

Fifty-five genetically modified (GM) food or feed items are currently awaiting authorisation by the European Union. Evaluating the safety of GM organisms, which is carried out by the European Food Safety Authority, usually takes more than three years and includes a rigorous risk assessment. In order to simplify the process, the concept of substantial equivalence has been introduced. This means that a GM tomato, for example, is regarded as safe if it has the same composition as a traditionally produced tomato. But what does 'the same composition' mean? Usually, analysing substantial equivalence focuses on the main components, such as sugar and protein concentrations as well as critical nutrients and anti-nutritional factors, such as vitamins or solanine (a toxic tomato component). However, it has been argued that genome modification may lead to unexpected random effects with unknown consequences for the consumer. And these random effects may be overlooked if it is only the main components that are analysed. To combat this, untargeted analytical methods, which promise to give a systematic view of food composition, were introduced into the safety assessment of GM food. The most promising approaches for this purpose are omics-methods.

Proteomics, or proteome analysis, was originally developed for biomedical research to search for diagnostic markers (indicators of disease) or new drug targets, for example. The proteome is the entire complement of proteins in a biological sample such as a cell. Since proteins are the primary products of gene expression (where information from a gene is used to make a protein), a random effect caused by genetic modification of a plant should be reflected in the



proteome. So proteome analysis could indicate if a new GM food is indeed substantially equivalent to a traditional food and can be regarded as safe without further evaluation. The goal of proteome analysis is to depict the composition and concentrations of all cell proteins or other biological samples as completely as possible. Since a cell contains several tens of thousands of different proteins, sophisticated methods for protein separation must be applied. This is achieved either by two-dimensional gel electrophoresis (gel-based methods) or by two-dimensional liquid chromatography (shotgun methods). After separation, proteins are usually identified by two-dimensional mass spectrometry. However, taking into account that one shotgun experiment can generate up to 100,000 mass spectra, it is obvious that with this method, data interpretation, evaluation and management cause a bottleneck.

In other areas of food science, researchers have also used proteome analysis to give an overview of protein composition in biological samples. To study a particular food's effect on the body – physiological or nutritional activity – the food item is

traditionally administered to cultured cells or animals and the response of selected diagnostic markers is recorded. Alternatively, any changes to the whole proteome that can be seen as a reaction to the treatment reduce the chance to overlook any unexpected beneficial reactions or toxic side-reactions. As a result, the process of identifying bioactive food items or components, which affect metabolism and health, should be largely accelerated.

Another hot topic in food science is authentication. With the growing global market, food adulteration is an emergent problem. In some cases, detecting the replacement of valuable ingredients or whole foods by cheaper substitutes can be difficult for food control. Particularly if a new food adulteration problem is arising, there is the need to react quickly and to create a reliable analytical solution. By comparing the proteome of the original ingredient with the substitute, the proteins that are only expressed in the substitute can be quickly and efficiently identified and further used as markers for food adulteration. Finally, proteome analysis is applied in food science to systematically reveal the effect of food processing on food proteins, to identify food allergens and to develop a means to improve food quality.

To understand complex interactions between food production, composition and their effects on the human body, it seems that proteomics researchers have the method and technique bases covered. Now, the challenge for scientists is to find a way to handle and interpret the complex data generated.

Read more in Monika Pischetsrieder and Rainer Baeuerlein's tutorial review 'Proteome research in food science' in issue 9, 2009 of Chemical Society Reviews.

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M Pischetsrieder and R Baeuerlein, *Chem. Soc. Rev.*, 2009, DOI: 10.1039/b817898b

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Riding high

Philip Mountford on jockeying, bribing techniques and the challenges ahead for chemistry. Interview by Amaya Camara-Campos



Philip Mountford

Philip Mountford is a professor of chemistry at the University of Oxford, UK. His research interests centre on the synthesis, bonding and reactivity of organometallic compounds of the transition metals and lanthanides.

I have heard you used to ride horses, how did you end up as a chemistry professor?

I rode a lot as a child and teenager, so after my A-levels I took up a position in a horse racing yard as an assistant. After a year or so I didn't quite make the grade for the big stage so I decided to go to university. I am sure my racing background helped in the interview. I already had my A-level grades and so the interviewer asked, half-jokingly, if I had any tips, not really expecting a serious answer. But as it happened I had been with somebody the day before who had a hot tip, I passed that on and the horse won. Sure enough, a few days later I got an offer to read chemistry!

Why did you specialise in inorganic chemistry and catalysis?

I was initially most interested in organic chemistry but it was Dr Peter Pye who really inspired my interest in transition metal organometallic chemistry. I don't think we really covered much catalysis back in 1985, but all these fascinating metal-mediated transformations really grabbed me. In my group, I like to think we make interesting compounds with some sort of *raison d'être*: could be an unusual molecular or electronic structure or some sort of stoichiometric or catalytic transformation.

What are the challenges ahead for catalysis?

I think that improving selectivity (in the way nature can), efficiency, using non-toxic solvents and cheaper (and/or more abundant) metals are some of the main targets. This is really with regard to known reactions. I think there are transformations waiting to be discovered which we haven't really dreamed of. In that regard, there is a role for blue-skies exploratory studies. This is harder and harder to get funding for nowadays – which is ironic since our past successes are built more or less on this paradigm.

Are the current global economic problems affecting funding in the UK?

I think we are already seeing the effect of the recession from an industrial funding point of view. The present (perceived or real) difficulties in gaining government funding stem from other reasons. I think we all recognise that, whatever the colour of the next UK government, there will be significant public sector cut-backs which must surely impact on the funds available to research councils. I also suspect – from a chemistry point of view – we will see more research funding focussed towards immediate or medium-term industrial or

technological goals. This is not unreasonable of course, but we must continue to 'horizon-scan' as well as being a technological arm of the government.

Which is your favourite metal to work with?

That's quite difficult. I worked a lot with tungsten as a graduate student and research fellow (my first serious encounter with a metal). My group has worked with many metal-organic compounds, and I think they would expect me to say titanium as we have used it very successfully. But I have a sneaking admiration for samarium which, as a fairly large early lanthanide, is a bit of a wild thing but can be pinned down with the right ligands.

What makes a good researcher?

I think there are several sorts of 'good' researcher. You need the dedicated, systematic types who are able to really drill down into a problem for months and years with focus and dedication. Then you need the 10-ideas-a-day types who set the agenda and make a sort of creative tension which us mere mortals can feed off for years as they disappear over the horizon. If I look at the successful academics in my area, I see people who are focussed, hard-working, receptive to ideas and able to inspire students and co-workers to try their best and share in a common vision.

What are your views about the current world food crisis and how can chemistry help the situation?

The food crisis seems to me as much a societal and political problem as an agricultural one. You see waste and abuse of food (often shipped all around the world as we ignore the rich seasonal variations in our own countries) in many 'developed' countries, but yet ruinous governments in others where much more could be done to solve local problems. Chemistry can help in so many ways: pest-control for crops; improved fertilizers; GM; medicines against cattle infection. These seem to me the more obvious impacts but, also, since the food crisis is amplified by man-made climate change, efforts channelled by chemists towards the better use of energy and reduced CO₂ emissions could also indirectly help.

Do you still ride horses today?

Actually I don't ride any more. Between my children, my wife, keeping up with friends and then the day job, I don't have much time for serious hobbies. I do cycle to work every day as regular exercise.

Your favourite food?

Chocolate!

Essential elements

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New journal *Chemical Science*

The recent ACS Fall 2009 National Meeting in Washington was the occasion for the release of some exciting news for researchers from across the chemical sciences: invitations were distributed, an audience gathered, a few words were spoken and then the ribbon was cut, revealing the news that in 2010 a new journal – *Chemical Science* – would join the RSC portfolio.

Editorial director, James Milne, describes this new venture as a milestone in the development of the RSC publishing portfolio. 'During recent years, RSC journals have attracted significant growth in submissions, while impact factors have increased to lead the field. The launch of *Chemical Science* will truly complement RSC Publishing's world renowned communications and



David MacMillan cuts the ribbon to reveal RSC's new journal, *Chemical Science*

review flagship titles.'

At the forefront of the most exciting developments, and helping to define the important areas by publishing the most significant cutting-edge research,

Chemical Science will be a dedicated home for findings of exceptional significance from across ALL the chemical sciences.

Editor-in-chief David MacMillan of Princeton, US, will lead a dynamic international team of associate editors who will drive the scientific development and make decisions on the content. 'I am extremely honoured and excited to be working with the RSC on the launch and development of *Chemical Science*,' he says. 'This is an opportunity to bring forward a very new type of journal and a new way of disseminating edge publications from the world of chemistry. I look forward to being part of this new approach to publishing the world's most pioneering studies in the chemical sciences.'

Free access to Chemical Science will be available – find out more at www.rsc.org/chemicalscience

Further news...

October sees the publication of the 100th issue of the *Journal of Environmental Monitoring (JEM)*. Editor Harp Minhas, announced it a milestone event, as the journal undergoes a significant change in its subject approach. Minhas explains: 'The impact of environmental research is of special concern to our readers. From now on all submitted articles will provide a statement explaining how the research impacts the environment directly and how the work provides insight into environmental processes.' www.rsc.org/jem

In a separate journal development, new titles *Nanoscale* and *Analytical Methods* have published their first articles online, just months after the initial launch announcement in March.

Nanoscale, a collaborative venture with the National Center for Nanoscience and Technology, Beijing, China, publishes experimental and theoretical work across the breadth of nanoscience and nanotechnology, while *Analytical Methods* will appeal to scientists with an interest in the latest research methods demonstrating the link between fundamental and applied analytical science.

Read the articles for free at www.rsc.org/methods and www.rsc.org/nanoscale. Register for free online access to all Nanoscale and Analytical Methods content throughout 2009 and 2010 at www.rsc.org/free_access_registration

MedChemComm coming soon

MedChemComm, a new, peer-reviewed journal from RSC Publishing was announced recently at the 3rd International Symposium on Advances in Synthetic and Medicinal Chemistry in Kiev, Ukraine, and the ACS Fall 2009 National Meeting and Exposition in Washington DC, US. Launching in mid 2010, the journal will focus on medicinal chemistry research, including new studies related to biologically-active chemical or biochemical entities that can act as pharmacological agents with therapeutic potential or

relevance.

The new journal will be owned by RSC Publishing and will be the official journal of the European Federation for Medicinal Chemistry (EFMC). It will complement the existing RSC Publishing portfolio of bioscience journals, providing authors in the field with a dedicated subject-specific publication. Monthly issues will contain a mix of vibrant and concise research and review articles.

The co-editors-in-chief will be Gregory Verdine, Harvard University, US, and Anthony

Wood, Pfizer, UK. Wood comments: '*MedChemComm* is very important, especially when one considers the mission of the journal is to emphasise the role of chemistry as a powerful vehicle to conceptualise new understanding of biological systems and processes. It is a means to design new tools to modulate these selectively by exploring multiple modalities of intervention.'

Free access to MedChemComm will be available for 2010 and 2011. Find out more at www.rsc.org/medchemcomm

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