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IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 33(5) 921-1156 (2009)



Cover

See Christophe Den Auwer *et al.*, pp. 976–985. Comparative complexation and coordination sphere characterization between early actinides and iron with an aspartyl-rich pentapeptide ligand: an X-ray absorption spectroscopic investigation. Image reproduced by permission of Christophe Den Auwer from *New J. Chem.*, 2009, **33**, 976.



Inside Cover

See Soo-Hyoung Lee *et al.*, pp. 986–990. Controlled fabrication of conjugated polymer P3HT nanorod arrays using AAO templates. Image reproduced by permission of Soo-Hyoung Lee from *New J. Chem.*, 2009, **33**, 986.

CHEMICAL SCIENCE

C33

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

Chemical Science

May 2009/Volume 6/Issue 5

www.rsc.org/chemicalscience

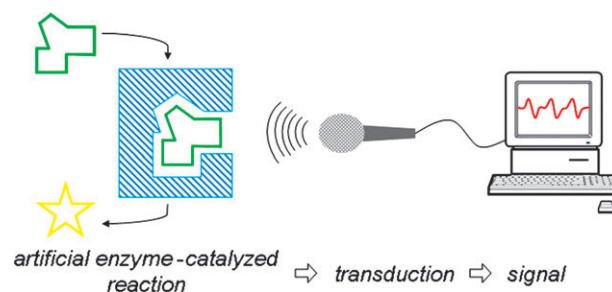
PERSPECTIVE

939

Artificial enzyme-based biosensors

Laurent Vial and Pascal Dumy*

In this Perspective, we provide a concise overview of the research field devoted to the conception of sensors that make use of synthetic rather than native enzymes. Emphasis is given to the advantages of such a substitution.



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Professor Peter Junk

School of Chemistry

Monash University

Box 23

Victoria 3800

Australia

Fax (+61) 3 9905 4597

Tel (+61) 3 9905 4570

E-mail njc@sci.monash.edu.au

Professor Michael J. Scott

Department of Chemistry

University of Florida

PO Box 117200

Gainesville

FL 32611

USA

Fax (+1) 352 392 3255

Tel (+1) 352 846 1165

E-mail njc@chem.ufl.edu

Dr Denise Parent

New Journal of Chemistry

Université Montpellier II

Place Eugène Bataillon C.C. 014

34095 Montpellier cedex 5

France

Fax (+33) (0) 4 67 14 48 79

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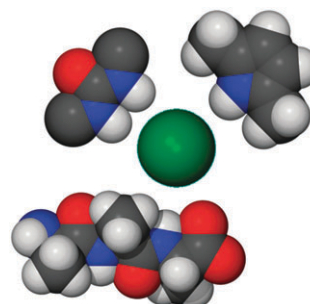
PERSPECTIVE

947

Transport of chloride ion through phospholipid bilayers mediated by synthetic ionophores

George W. Gokel* and Natalie Barkey

This article gives a modern perspective on the transport of chloride ions through membranes that is mediated by a wide range of synthetic transporters.



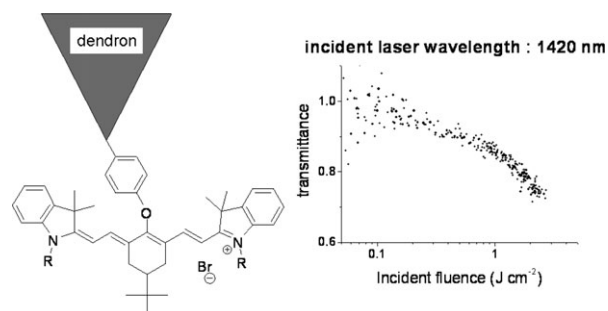
LETTERS

964

Dendron-decorated cyanine dyes for optical limiting applications in the range of telecommunication wavelengths

Pierre-Antoine Bouit, Robert Westlund, Patrick Feneyrou, Olivier Maury, Michael Malkoch, Eva Malmström* and Chantal Andraud*

Cyanine dyes decorated by “click chemistry” with dendrons up to third generation have been synthesized aiming towards functional materials for optical limiting applications in the NIR.

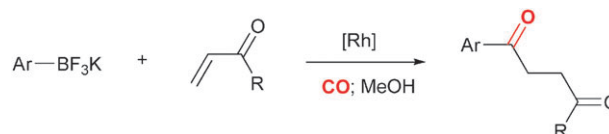


969

Carbonylative 1,4-addition of potassium aryltrifluoroborates to vinyl ketones

Mathieu Sauthier,* Nicolas Lamotte, Julien Dheur, Yves Castanet and André Mortreux

Potassium aryltrifluoroborates have proven to be useful reagents for the carbonylative arylation of vinyl ketones.

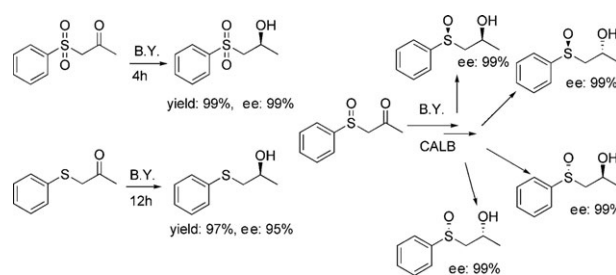


972

A chemo-enzymatic synthesis of chiral secondary alcohols bearing sulfur-containing functionality

Qihui Chen, Ke Wang and Chengye Yuan*

A facile method for the preparation of sulfur-containing chiral secondary alcohols catalyzed by yeast in diisopropyl ether with excellent enantioselectivity and medium-to-high yield is introduced; with combined baker's yeast (B. Y.) and *Candida Antarctica* lipase B (CALB), four stereoisomers of two substituted phenylsulfinylpropan-2-ols were obtained simultaneously with a high efficiency.





Themed Issue: Dedicated to Professor Jean-Pierre Sauvage

In 2009 Jean-Pierre Sauvage will celebrate his 65th birthday, and *New Journal of Chemistry* is dedicating an issue to him. Jean-Pierre has been closely connected to *NJC*, serving on the editorial board from 1998 to 2002, and then on the advisory board for another 4 years. He has been a long time supporter of *NJC*, having published nearly 50 papers in the journal since 1977 on mechanically interlocked molecular architectures.

Papers in the issue include:

Fullerene-rich dendrimers: divergent synthesis and photophysical properties

Uwe Hahn, Jean-François Nierengarten, Fritz Vögtle, Andrea Listorti, Filippo Monti and Nicola Armaroli

Polycationic phosphorus dendrimers: synthesis, characterization, study of cytotoxicity, complexation of DNA, and transfection experiments

Clément Padié, Maria Maszewska, Kinga Majchrzak, Barbara Nawrot, Anne-Marie Caminade and Jean-Pierre Majoral

First enantiomerically pure C₇₀-adducts with a non-inherently chiral addition pattern

Agnieszka Kraszewska, Pablo Rivera-Fuentes, Carlo Thilgen and François Diederich

Photo-induced self-assembly of Pt(II)-linked rings and cages via the photolabilization of a Pt(II)–py bond

Ken-ichi Yamashita, Kei-ichi Sato, Masaki Kawano, Makoto Fujita

Reversible constitutional switching between macrocycles and polymers induced by shape change in a dynamic covalent system

Sébastien Ulrich, Eric Buhler and Jean-Marie Lehn

Redox-driven switching in pseudorotaxanes

Ali Trabolsi, Mohamad Hmadeh, Niveen M. Khashab, Douglas C. Friedman, Matthew E. Belowich, Nicolas Humbert, Mourad Elhabiri, Hussam A. Khatib, Anne-Marie Albrecht-Gary and J. Fraser Stoddart



Professor Jean-Pierre Sauvage

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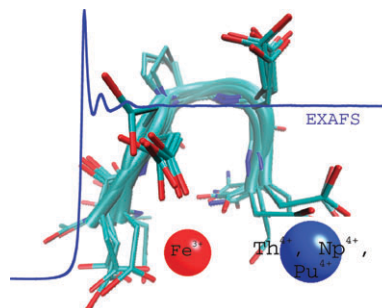
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976

The role of aspartyl-rich pentapeptides in comparative complexation of actinide(IV) and iron(III). Part 1

Aur lie Jeanson, Claude Berthon, St phanie Coantic, Christophe Den Auwer,* Nicolas Floquet, Harald Funke, Denis Guillaneux, Christoph Hennig, Jean Martinez, Philippe Moisy, S bastien Petit, Olivier Proux, Eric Qu meneur, Pier Lorenzo Solari and Gilles Subra

Comparative complexation and coordination sphere characterization of actinide(IV) and iron(III) by an aspartyl-rich pentapeptide.

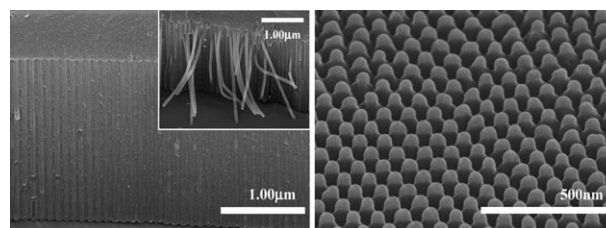


986

A facile method to prepare regioregular poly(3-hexylthiophene) nanorod arrays using anodic aluminium oxide templates and capillary force

Sujin Baek, Jong Bae Park, Wonjoo Lee, Sung-Hwan Han, Jouhahn Lee* and Soo-Hyoung Lee*

Regioregular poly(3-hexylthiophene) (RR-P3HT) nanorod arrays were prepared on the ITO substrate by capillary force in a vacuum oven using a drop-coating of RR-P3HT and anodic aluminium oxide (AAO) templates.

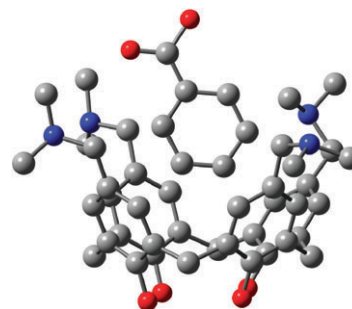


991

Stereochemistry and thermodynamics of the inclusion of aliphatic and aromatic anionic guests in a tetracationic calix[4]arene in acidic and neutral aqueous solutions

Carmelo Sgarlata,* Carmela Bonaccorso, Fabio Giuseppe Gulino, Valeria Zito, Giuseppe Arena* and Domenico Sciotto

Organic anions are included in a tetracationic calix[4]arene in water, and their binding strength changes with pH.

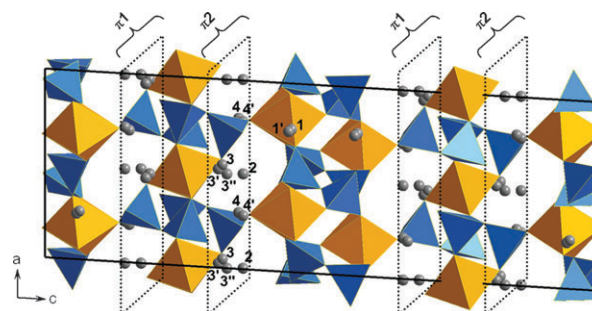


998

Crystal structures of new silver ion conductors Ag₇Fe₃(X₂O₇)₄ (X = P, As)

Eric Quarez,* Olivier Mentr , Yassine Oumellal and Christian Masquelier

Structure of β-Ag₇Fe₃(P₂O₇)₄ (298 K) and location of the π planes. The numbers refer to silver sites.





Chemistry-Biology Interface

Chemistry-Biology Interface theme issue

This theme issue covers topical areas at the chemistry–biology interface from a chemical perspective. The biological consequences of specific molecular interactions have long been a part of scientific (and non-scientific) activities throughout human history. The last century witnessed a myriad of discoveries in the life sciences at molecular detail, and the associated growth of the pharmaceutical and biotech industries. This century has seen a further growth in the field with a resultant increase in publications and journals.

Reviews include:

Nucleic acid encoding to program self-assembly in chemical biology

Zbigniew L. Pianowski and Nicolas Winssinger

Chemical technologies for probing embryonic development

Ilya A. Shestopalov and James K. Chen

Interspecies and interkingdom communication mediated by bacterial quorum sensing

Colin A. Lowery, Tobin J. Dickerson and Kim D. Janda

Small molecule inhibition of microbial natural product biosynthesis—an emerging antibiotic strategy

Justin S. Cisar and Derek S. Tan

Identification of the cellular targets of bioactive small organic molecules using affinity reagents

Benjamin J. Leslie and Paul J. Hergenrother

Expanding dialogues: from natural autoinducers to non-natural analogues that modulate quorum sensing in Gram-negative bacteria

Grant D. Geske, Jennifer C. O'Neill and Helen E. Blackwell

Guest editor:



David Spring

University of Cambridge, UK

"The interface with biology is a fertile scientific pursuit for chemists"

060833

See also:

Molecular BioSystems issue 6, 2008 – Emerging Investigators theme issue

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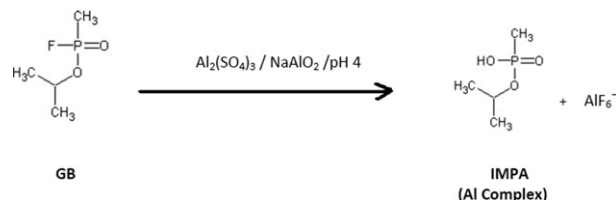
PAPERS

1006

Aluminium sulfate and sodium aluminate buffer solutions for the destruction of phosphorus based chemical warfare agents

Daniel J. Williams,* William R. Creasy, David J. McGarvey, Roderick A. Fry, Vicky L. H. Bevilacqua and H. Dupont Durst

Nerve agents VX and GB (sarin) are sequestered and removed by aluminium sulfate and sodium aluminate mixtures adjusted to pH 4 in solution.

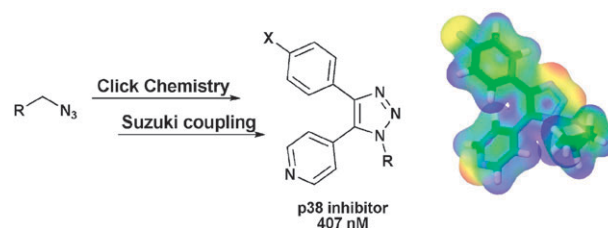


1010

Short cut to 1,2,3-triazole-based p38 MAP kinase inhibitors via [3 + 2]-cycloaddition chemistry

Peter Dinér, Terese Andersson, Jimmy Kjellén, Karin Elbing, Stefan Hohmann and Morten Grøtli*

Azides are easily converted to 4,5-substituted 1,2,3-triazoles in two steps using Click Chemistry and Suzuki coupling yielding p38 inhibitors with nanomolar activity.

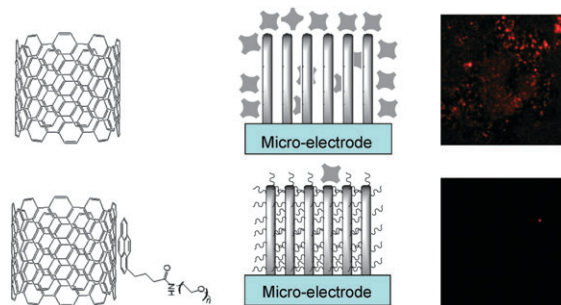


1017

Stable non-covalent functionalisation of multi-walled carbon nanotubes by pyrene-polyethylene glycol through π - π stacking

Jie Liu,* Olivier Bibari, Pascal Mailley, Jean Dijon, Emmanuelle Rouvière, Fabien Sauter-Starace, Patrice Caillat, Françoise Vinet and Gilles Marchand

Stable non-covalent functionalisation of MWNTs arrays by pyrene-PEG for avoiding non-specific adsorption of proteins.

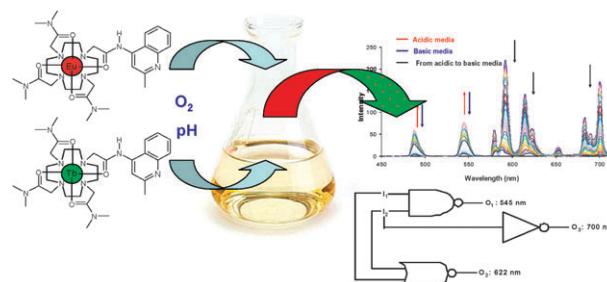


1025

Lanthanide macrocyclic quinolyl conjugates as luminescent molecular switches and logic gate functions using HO^- and O_2 as inputs

Célia S. Bonnet and Thorfinnur Gunnlaugsson*

The synthesis, characterisation and the photophysical evaluation of a new Tb(III) complex **1Tb** (from **1**) is described. The combination of **1Tb** and **1Eu** (also made from **1**) was used for the radiometric luminescent sensing of pH and O_2 , and we show that the Ln-emission outputs could also be expressed in logic gate operation terms.



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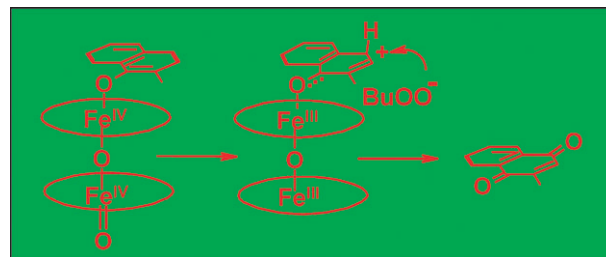
PAPERS

1031

Kinetics and mechanism of the oxidation of alkyl substituted phenols and naphthols with t BuOOH in the presence of supported iron phthalocyanine

Olga V. Zalomaeva, Irina D. Ivanchikova, Oxana A. Kholdeeva* and Alexander B. Sorokin*

Based on $^{18}\text{O}_2$ labeling experiments, EPR spectroscopy with spin traps and kinetic studies, a mechanism including a coordination of substrate and oxidant to a diiron center and two one-electron transfers, has been proposed to explain a high selectivity of oxidation of phenols to quinones.

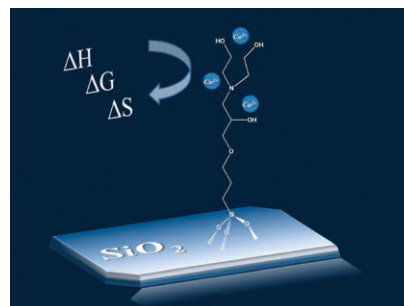


1038

Useful aminoalcohol molecules incorporated in an epoxide silylating agent for silica organofunctionalization and thermodynamics of copper removal

Maurício A. Melo Jr, Fernando J. V. E. Oliveira, José A. A. Sales and Claudio Airoidi*

Ethanolamine and diethanolamine reacted with a precursor epoxysilane compound and were further immobilized on a silica surface. The resulting materials presented ability to take up copper ions from dilute aqueous solution and the energetics of this spontaneous process was determined.

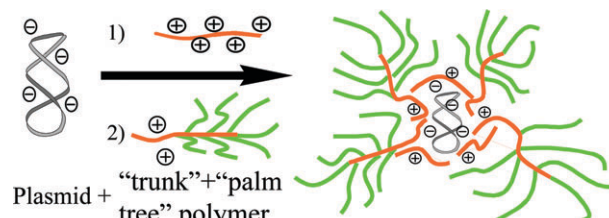


1047

Probing the interaction between DNA and cell transfection polymers with luminescent Ru^{II} complexes

Larisa Kovbasyuk, Cécile Moucheron, Philippe Dubois and Andrée Kirsch-De Mesmaeker*

When DNA is loaded with Ru^{II} [Ru(TAP)₂(TPAC)]Cl₂ complex and titrated with vectorizing polymer(s), the emission of the complex starts to be restored once the polymer distorts the polynucleotide in the DNA–polymer association. This Ru complex acts as a photoprobe of the DNA–polymer interaction.

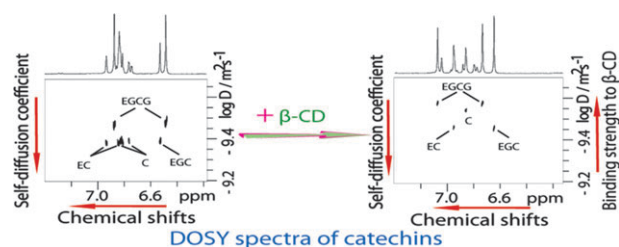


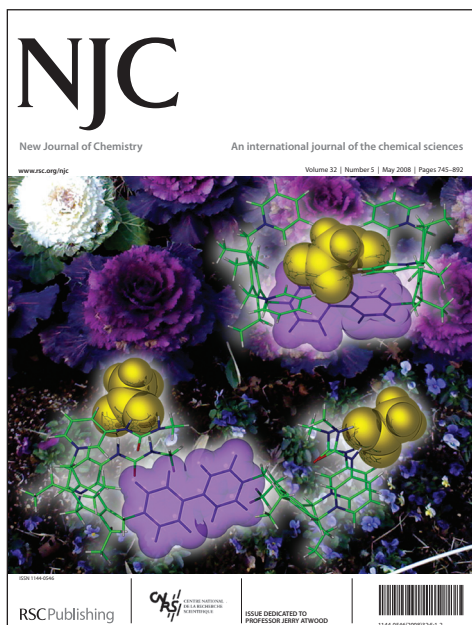
1057

The use of diffusion-ordered spectroscopy and complexation agents to analyze mixtures of catechins

Jun Xu, Tianwei Tan, Lennart Kenne and Corine Sandström*

DOSY has been used to separate mixture of catechins according to their distinct binding affinities to β -cyclodextrin or bovine serum albumin.





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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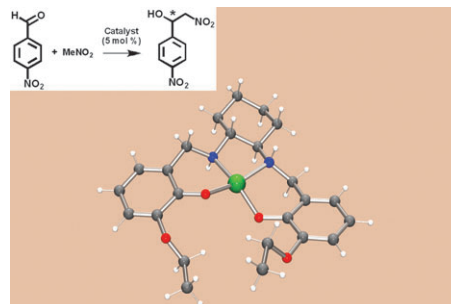
PAPERS

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In search of enantioselective catalysts for the Henry reaction: are two metal centres better than one?

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

Copper(II) complexes of the chiral Schiff bases and a reduced analogue are tested as catalysts for the asymmetric Henry reaction; both yield and enantioselectivity are enhanced when the reduced ligand is incorporated into the catalyst and when a second equivalent of $\text{Cu}(\text{OAc})_2$ is added.

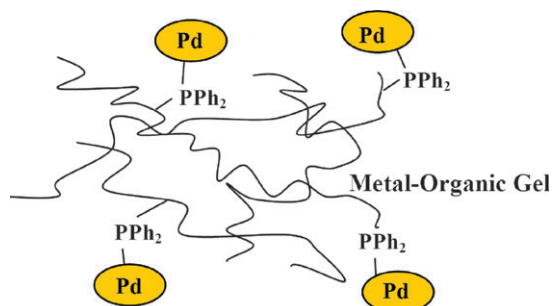


1070

Metal–organic gels as functionalisable supports for catalysis

Jianyong Zhang,* Xiaobing Wang, Lisi He, Liuping Chen,
Cheng-Yong Su and Stuart L. James

Modification of Fe-tricarboxylate based gels yielded phosphine-functionalised metal–organic gels, which can act as a new type of functionalisable porous scaffold. The subsequently functionalised $\text{Pd}(\text{II})$ -immobilised gel and its xerogel showed high activity and could be reused in the catalysis of Suzuki coupling.

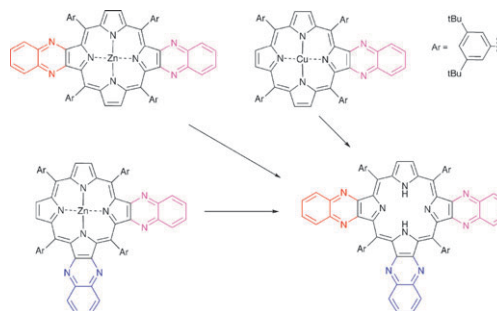


1076

Expansion of the porphyrin π -system: stepwise annelation of porphyrin β, β' -pyrrolic faces leading to trisquinoxalinoporphyrin

Tony Khoury and Maxwell J. Crossley*

Lateral extension of the porphyrin π -electron system by ring annelation of β, β' -pyrrolic faces to give a trisquinoxalinoporphyrin is achieved by three separate pathways. Each of the synthetic routes could have use in elaboration of more complex oligoporphyrin arrays.

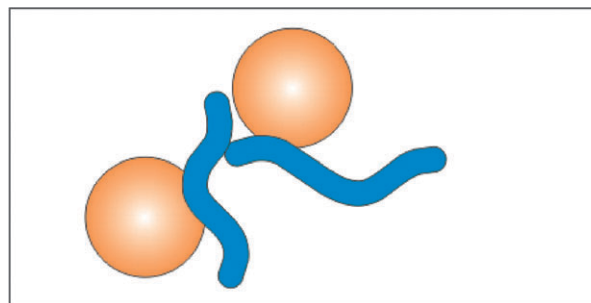


1087

Interactions between dendrimers and heparin and their implications for the anti-prion activity of dendrimers

Barbara Klajnert,* Michela Cangiotti, Sara Calici,
Maksim Ionov, Jean Pierre Majoral,
Anne-Marie Caminade, Josep Cladera,
Maria Bryszewska and Maria Francesca Ottaviani*

Cationic dendrimers interact with heparin and change the kinetics of fibril formation.



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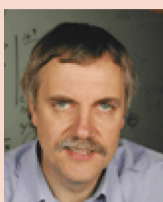
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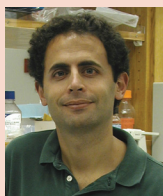
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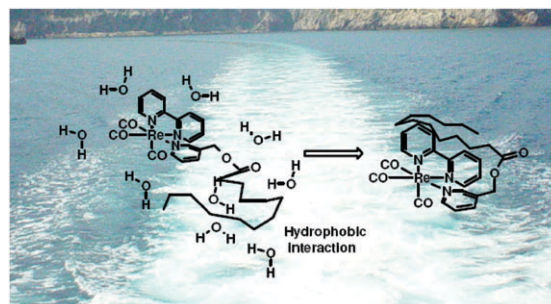
PAPERS

1094

Rhenium *fac*-tricarbonyl bisimine complexes: luminescence modulation by hydrophobically driven intramolecular interactions

Michael P. Coogan,* Vanesa Fernández-Moreira, Jacob B. Hess, Simon J. A. Pope* and Craig Williams

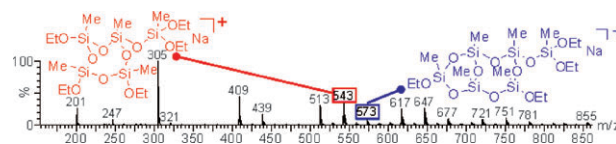
Hydrophobically driven forces modulate the luminescence properties of a myristyl ester functionalised rhenium complex.



1100

New insights on organosilane oligomerization mechanisms using ESI-MS and ^{29}Si NMR

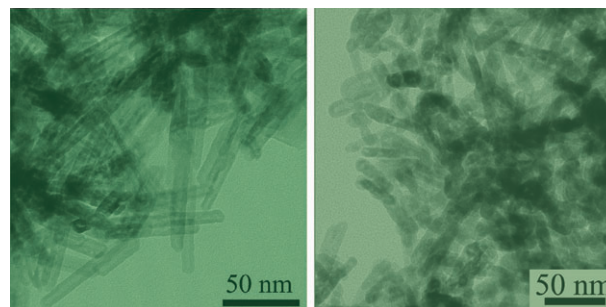
José Planelles-Aragó,* Cristian Vicent,* Beatriz Julián, Eloisa Cordoncillo and Purificación Escribano

The temporal evolution of methyl-diethoxysilane through hydrolysis and condensation reactions is monitored by $^{29}\text{Si}\{^1\text{H}\}$ NMR and ESI-MS techniques at pH 1, 6 and 13, displaying different oligomeric species formed under these conditions.

1109

Corundum-type tubular and rod-like In_2O_3 nanocrystals: synthesis from designed InOOH and application in photocatalysis

Li-Yong Chen, Zhen-Xiang Wang and Zu-De Zhang*

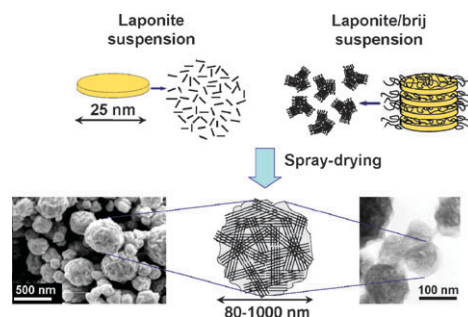
Tubular and rod-like $\text{H-In}_2\text{O}_3$ nanostructures, obtained by thermal decomposition of their precursors, exhibit photocatalysis in the degradation of rhodamine B.

1116

Laponite and hybrid surfactant/laponite particles processed as spheres by spray-drying

Laurent Bippus, Maguy Jaber and Bénédicte Lebeau*

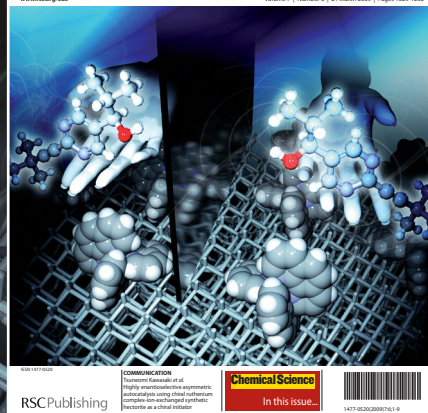
Laponite and brij58/laponite colloidal suspensions constituted of (isolated and stacked) elementary disc crystals and aggregates of stacked discs, respectively, have been spray-dried to form spherical mesoporous laponite particles.



Organic & Biomolecular Chemistry

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Volume 7 | Number 6 | 21 March 2009 | Pages 1029–1232



Organic & Biomolecular Chemistry 150th Issue

Organic & Biomolecular Chemistry (OBC) issue 6, 2009, is the 150th issue of the journal. Since the first issue was published in January 2003, *OBC* has achieved tremendous success. Can any other 'young' journal boast such highly cited papers, published after independent peer review to such exacting standards? Take a look at some of the high impact papers from leading scientists published in this issue of *OBC*.

Perspective:

Design and synthesis of phosphole-based systems for novel organic materials

Yoshihiro Matano and Hiroshi Imahori, *Org. Biomol. Chem.*, 2009, DOI: 10.1039/b819255n

Emerging Area:

Metal-catalysed halogen exchange reactions of aryl halides

Tom D. Sheppard, *Org. Biomol. Chem.*, 2009, DOI: 10.1039/b818155a

Communication:

Highly enantioselective asymmetric autocatalysis using chiral ruthenium complex-ion-exchanged synthetic hectorite as a chiral initiator

Tsuneomi Kawasaki, Toshiki Omine, Kenta Suzuki, Hisako Sato, Akihiko Yamagishi and Kenso Soai, *Org. Biomol. Chem.*, 2009, DOI: 10.1039/b823282b

Paper:

Ruthenium-based metallacrown complexes for the selective detection of lithium ions in water and in serum by fluorescence spectroscopy

Sébastien Rochat, Zacharias Grote and Kay Severin, *Org. Biomol. Chem.*, 2009, DOI: 10.1039/b820592b

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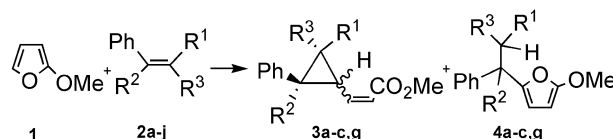
PAPERS

1127

Novel formation of phenylcyclopropanes from the reaction of β -cyanostyrenes and related compounds with 2-methoxyfuran: experimental and theoretical studies

Kuniaki Itoh* and Shigehisa Kishimoto

2-Methoxyfurans react with β -cyanostyrenes to give cyclopropanes. The regio- and stereochemistry have been studied by B3LYP/6-31G* level DFT. The analysis of these reactions is in agreement with the experimental analysis.

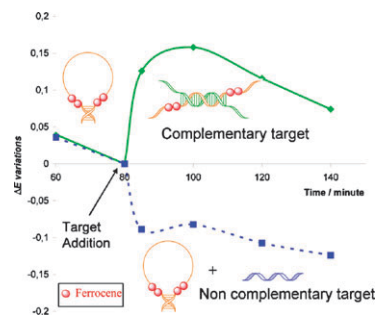


1139

A thermodynamic study of ferrocene modified hairpin oligonucleotides upon duplex formation: applications to the electrochemical detection of DNA

Grégory Chatelain, Hugues Brisset and Carole Chaix*

A new class of ferrocene-modified oligonucleotides is constructed under hairpin form for the electrochemical detection of DNA. The hairpin opening, generated by the hybridization with the complementary target induces significant variations of the electrochemical signal by cyclic voltammetry.

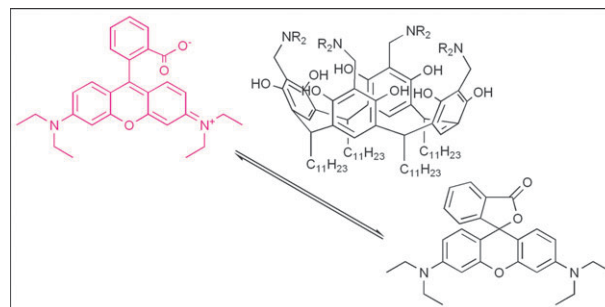


1148

Interaction of aminomethylated resorcinarenes with rhodamine B

Kaisa Helttunen, Piotr Prus, Minna Luostarinen and Maija Nissinen*

Aminomethylated resorcinarenes shift the rhodamine B equilibrium from a red zwitterion to a colorless lactone form. This interaction was investigated using various spectroscopic methods in solution and compared with the effect of non-basic hosts.



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Chemical Science

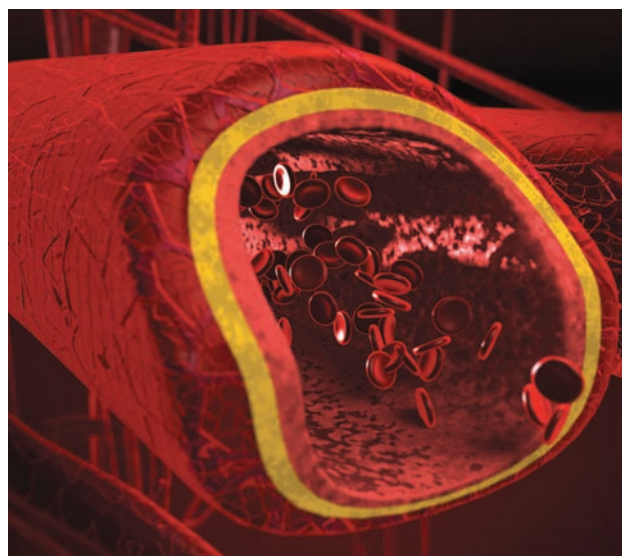
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Korean scientists have found an effective way of making biocompatible implants Polymers keep the blood flowing

Drug-laden polymer coats could make medical implants more biocompatible, according to scientists in Korea.

Dong Lyun Cho and colleagues at Chonnam National University in Gwangju have developed a method of coating stents in polymer and then attaching drug molecules to the surface. Stents are narrow mesh-like metal tubes that can be inserted into the diseased parts of arteries and then expanded to hold them open and keep the blood flowing. However, being foreign objects, stents can cause abnormal cell growth and artery narrowing (restenosis). The stents can be coated with polymers to avoid this. However, for a successful result, the polymer needs to be both biocompatible and strongly fixed to the metal surface, which Cho says is difficult to achieve.

Starting from a diamine monomer, Cho's team created a strongly adhesive polymer film on the stent's surface using a two-stage plasma polymerisation process. This method uses a high-



energy plasma to generate the reactive species needed to get the polymerisation started, and is an excellent way of producing thin pinhole-free films, says Cho. They then used the amino groups on the polymer surface to form amide bonds with α -lipoic acid, a drug

known to inhibit abnormal cell growth.

The new polymer films have high mechanical stability, says Cho, and prevent platelet aggregation in vitro. In addition, when tested on a model cell system, the new stents result in lower restenosis rates. Cho says that the key to these benefits is the α -lipoic acid, since stents coated with a different anticoagulant, heparin, were not as successful at reducing restenosis. Future work, he adds, will involve investigating the long-term clinical effect of their stents.

Ketul Popat from the department of mechanical engineering at Colorado State University, Colorado, US, says that biocompatible surfaces that can prevent inflammation are critical for successful implants. Techniques such as those developed by Cho's team, he suggests, 'will be beneficial in overcoming several of the challenges that current stent technology faces.'

David Barden

The implants hold diseased arteries open and deliver drugs

Reference

S-J Song et al, *J. Mater. Chem.*, 2009, DOI: 10.1039/b813357c

In this issue

Waste not, want not

Bacteria offer an easier way to convert biodiesel waste into useful chemicals

A little more sensitivity

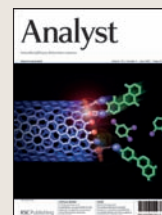
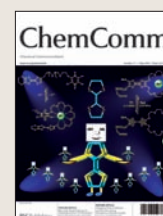
Fluorescent sensors to detect pH changes in a biological cell

Living longer, disease-free

This month's Instant insight discusses our need for better methods to detect age-related diseases

Making logical connections

Henry Rzepa talks about the potential for creativity in both research and teaching activities



A snapshot of the latest developments from across the chemical sciences

Research highlights

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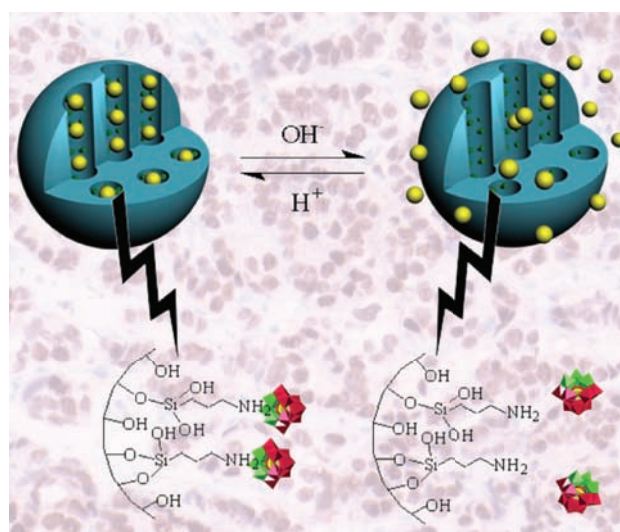
Colon cancer drug could reach its target without being destroyed by stomach acid

Back to basics for drug delivery

Chinese chemists have developed a pH-responsive system that could deliver anticancer drugs to the colon without being broken down by stomach acid.

Enbo Wang from Northeast Normal University, Changchun, China, and colleagues attached a polyoxometalate (POM), through a dative bond, to mesoporous silica spheres. POMs are metal–oxygen cluster compounds that show a wide range of antiviral and anticancer activities. Though they are typically easier and cheaper to synthesise than their small-molecule organic pharmaceutical counterparts, scientists have found it difficult to stabilise and selectively deliver them to their intended therapeutic targets.

Wang tested his silica-bound POM's stability under acidic, basic and neutral conditions, replicating the conditions that they would come across travelling through the human digestive system to get to their target.



He found that the loading and release of the POM from the silica spheres is controlled by the pH value of the surrounding environment. A base triggers the dative bond to break,

Drug release is caused by bonds breaking under basic conditions in the colon

releasing the POM. Acidic conditions, such as those found in the stomach, and neutral conditions don't affect the bond, meaning that the POM will only be released once it has reached the basic conditions in the colon. The team also tested the POM's activity against cancer cells in vitro and found that incorporating the POM into silica spheres actually increased its activity.

'The pH-responsive controlled-release principle is likely to be of benefit for a variety of transition metal-containing drugs,' says Wang. Eric Maatta, an expert in transition metal systems from Kansas State University, Manhattan, US, agrees. He says that 'the strategy will likely be applicable to the delivery of other classes of anti-tumour agents and enhances the prospects for POM-based therapies'. David Parker

Reference

G Sun et al, *Dalton Trans.*, 2009, DOI: 10.1039/b901133a

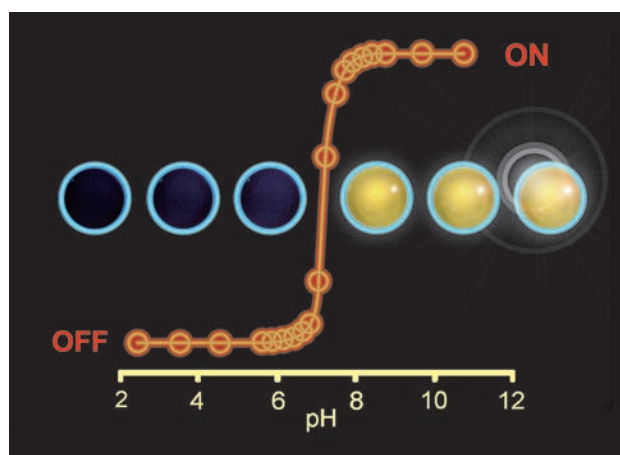
Scientists develop fluorescent sensors to detect pH changes in a biological cell

A little more sensitivity

Fluorescent pH sensors that are so sensitive they can detect changes within almost a pH unit have been developed by Japanese researchers. The digital sensors could be used in molecular computers and to monitor pH changes in biological cells, say the scientists.

Seiichi Uchiyama and Yumi Makino at the University of Tokyo made the sensors by incorporating water-sensitive fluorophores into pH-responsive polymers. The polymers' structures vary with pH, from a hydrated open form at low pH to a dehydrated globular form at high pH. The sharp fluorescence signals given at each stage within a pH unit make them effective digital sensors. Different polymer structures can cover different pH ranges.

Dongwhan Lee, an expert in molecular sensors from Indiana University, Bloomington, US, says that it is the polymers' innovative design that allows them to give such



a sharp fluorescent response to pH change.

'Our sensors can be used to detect a subtle change in intracellular pH,' says Uchiyama. Conventional sensors are sensitive to an 80-fold change in pH whereas Uchiyama's sensors require only a five-fold

The sensors can detect changes within a pH unit

change. As well as changing the operating pH range, modifying the proton-recognising groups on the polymers can also tune the switching direction (on-off and off-on actions).

Uchiyama says that in the future, he hopes to incorporate different ion sensors into the structures to detect biological ions other than protons.

He adds: 'Molecular computing is the most exciting and challenging application for fluorescent digital ion sensors. There are many scientific papers about molecular logic and computing that use conventional fluorescent sensors. Our highly efficient devices could easily be combined with this concept to further develop molecular computing.'

Harriet Brewerton

Reference

S Uchiyama and Y Makino, *Chem. Commun.*, 2009, DOI: 10.1039/b900889f

Bacteria offer an easier way to convert biodiesel waste into useful chemicals

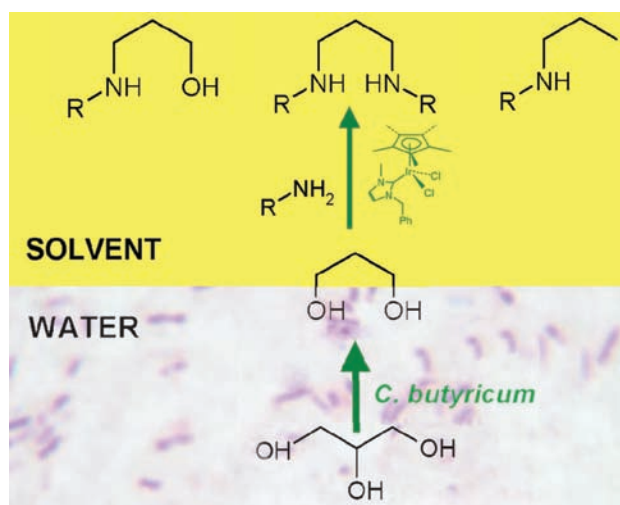
Waste not, want not

UK scientists have converted crude biodiesel waste into useful amines with no need for difficult separation techniques.

Glycerol is produced in significant quantities as a by-product in biodiesel production, making it a cheap renewable feedstock for the chemical industry. For example, using microbial processes to ferment glycerol is an attractive route to 1,3-propanediol, which can be used as a precursor to high value polymers and platform chemicals. However, the fermentation products are produced in dilute solutions along with cell material and other metabolic products, making purification and separation difficult.

Now a team of scientists, led by Andrew Marr at Queen's University Belfast and Gillian Stephens at the University of Manchester, has combined microbial and transition metal catalysed processes to produce secondary amines without having to isolate and purify the diol intermediate.

Marr and Stephens treated glycerol



Glycerol waste was treated with *C. butyricum* to produce secondary amines

Reference
S Liu *et al.*, *Chem. Commun.*, 2009, DOI: 10.1039/b820657k

with the bacterium *Clostridium butyricum*, then centrifuged the mixture of bacteria, 1,3-propanediol and by-products to remove the cells. The team then added a solution of an iridium catalyst, base and aniline in toluene to the solution, creating a biphasic mixture. After 24 hours at 115°C, 20 per cent of the 1,3-

propanediol had been converted to secondary amine.

‘As fossil fuels become less accessible, chemists need to start developing new methods to convert renewable feedstocks into the chemical products and materials that society demands,’ says Marr. ‘Our key advance is to integrate biocatalytic and chemocatalytic processes to avoid the need to separate the fermentation products.’

‘This is an important example of adding value to renewable resources,’ says Mark Harmer, a research fellow at DuPont, Delaware, US. ‘The ability to use all of the components from renewable feedstocks will be key to developing a biorefinery to replace the current oil-based refinery.’

Stephens agrees: ‘The new approach will allow a myriad of chemical products to be derived from a single fermentation mixture. The microbiology can also be changed, allowing conversion of a wide range of feedstocks to diverse fermentation products.’

Vikki Chapman

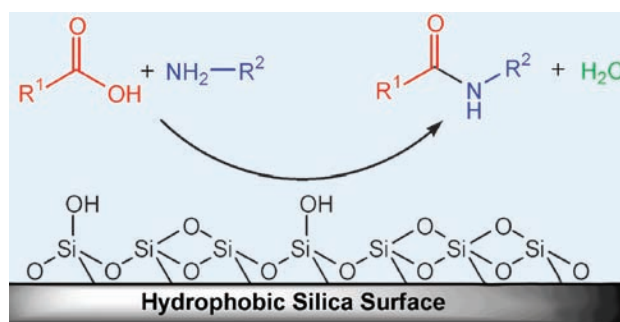
Amide synthesis goes cheap, clean and simple

Greening up pharmaceuticals

UK scientists have come up with a green method for synthesising amides, a fundamental reaction in the pharmaceutical industry, using a cheap and readily available material found lying around in labs.

James Clark and co-workers from the University of York developed a heterogeneous catalyst from silica gel, which is usually used as the stationary phase in column chromatography. They heated the silica gel to 700°C to activate it and then used it in a reaction to combine a carboxylic acid and an amine to make an amide. The only by-product was water, making the method cheaper, cleaner and less toxic than existing procedures. The catalyst remains active for a long time too, even after exposure to the atmosphere, and can be filtered for reuse.

Amides have been synthesised in



Silica gel, used here to make amides, could be the key to a greener pharmaceutical industry

Reference
J W Comerford *et al.*, *Chem. Commun.*, DOI: 10.1039/b901581g

various ways over the years, but the methods are ‘hazardous, complex and expensive’, says Clark. ‘Amide synthesis has been highlighted by the pharmaceutical industry as one of the most important targets for greening.’

Peter Dunn at Pfizer, Kent, UK, who is part of the industry group that identified amide synthesis as a prime target for greening, says:

‘What I find most interesting about this research is that the authors have used standard silica, which can be found in any synthetic chemistry laboratory. They took a material that was just lying around in the lab and discovered that it can be easily converted to an effective catalyst for this important transformation.’

‘Green chemistry should always challenge the more traditional chemistry community to reconsider established practices and to apply its skills and intelligence to design greener and more sustainable processes and products,’ says Clark. ‘We want to extend this particular type of chemistry to as wide a range of substrates and products as possible and then see where else we can apply the “simple is beautiful” and “complex isn’t clever” philosophies.’
Mary Badcock

Prostate cancer is easier to detect by combining biology with Raman scattering

Working together to spot cancer

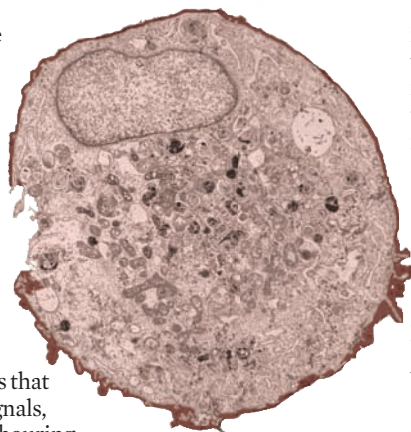
UK scientists have designed a method to detect prostate cancer using surface-enhanced resonance Raman scattering. Duncan Graham, from the University of Strathclyde in Glasgow, and his colleagues, combined the technique with a biological method called an enzyme-linked immunosorbent assay, or ELISA, to detect prostate specific antigen, whose elevated levels in serum indicate the cancer's presence.

ELISA is used to detect antigen levels in patients after prostate removal to ensure that all malignant tissue has been removed. Blood serum samples are fixed to a surface then a specific antibody is washed over the surface to bind to any antigen in the samples. Linked to the antibody is an enzyme dyed with a reagent that fluoresces when the antibodies bind to their antigens. This is normally

detected by fluorescence spectroscopy, but only one target at a time can be detected due to the large spectral overlap of dyes used for different targets.

Raman spectroscopy is used to investigate molecular bonding and can provide a unique vibrational 'fingerprint' for target molecules. For molecules that produce weak Raman signals, a highly scattering neighbouring surface such as gold can increase their response – this is surface-enhanced resonance Raman scattering (SERRS).

The team analysed antigen levels in human serum samples using ELISA, but in the final step used gold nanoparticles with SERRS to



Elevated prostate specific antigen levels indicate the cancer's presence

measure antigen concentration. They were able to detect picograms per millilitre antigen levels, lower than the current limit of nanograms per millilitre in cancer screening. Richard Van Duyn, an expert on SERRS from Northwestern University, Evanston, US, cautions that there are several other competing high-sensitivity approaches to measuring prostate specific antigen, such as surface plasmon resonance, but he agrees that SERRS has a 'bright future in solving biomedical problems'.

Graham says he hopes that in the future, he will be able to use SERRS to detect multiple proteins that indicate the presence of disease.

Hilary Burch

Reference

R Stevenson *et al*, *Analyst*, 2009, DOI: 10.1039/b902174d

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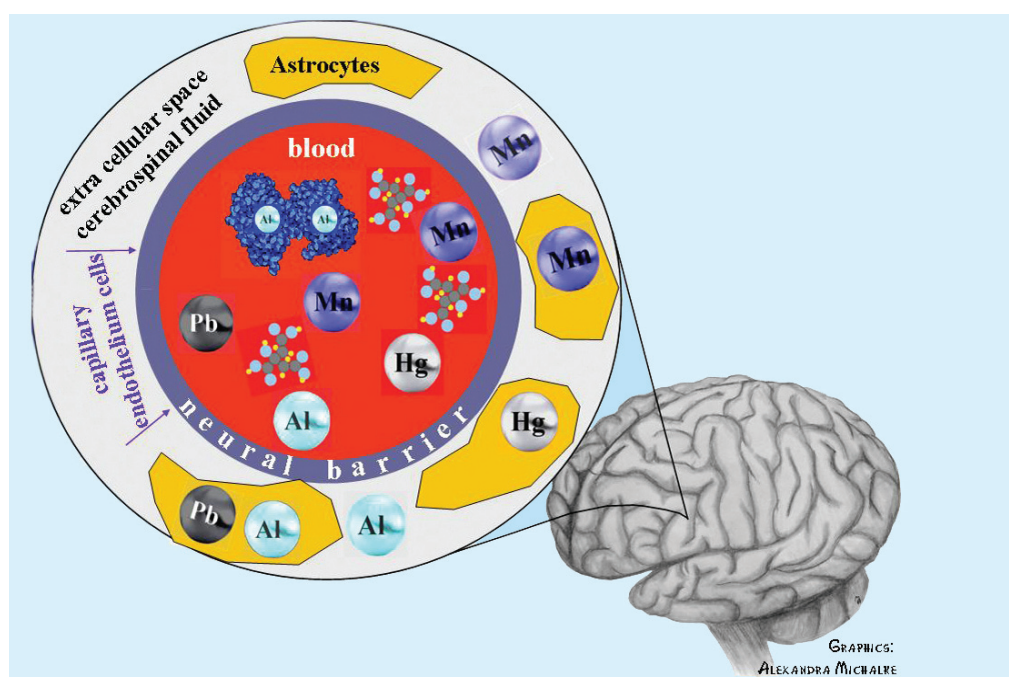
Living longer, disease-free

Bernhard Michalke and colleagues at the Institute of Ecological Chemistry in Germany discuss our need for better methods to detect age-related diseases

Humans are living longer, particularly in industrialised countries. But with this extended lifespan comes an increased chance of suffering from age-related dementia and nervous system disorders such as Alzheimer's and Parkinson's diseases. These diseases severely reduce an individual's quality of life and are a heavy financial burden on national health systems. Any possible therapeutic cures have so far been limited.

The changes in the body's nervous system that can cause these diseases are the focus of neurotoxicology studies. Research has shown a link between exposure to metals such as aluminium, lead, manganese and mercury and nervous system degeneration. Elevated metal levels were found in the blood and brain samples of neurological disorder sufferers that had industrial manufacturing backgrounds. Exposure can happen in several ways, for example, aluminium is used as an additive in processed food and is present in cookware, contaminated water, medication and antiperspirants. Lead can be found in paints and water pipes in old houses, and glassware, some jewellery and tobacco. Occupational exposure occurs in lead smelters, lead refining and battery manufacturing. Exposure to elevated manganese levels occurs by mining and processing the element. Welding manganese alloys produces toxic fumes and dry-cell batteries and fireworks could contain manganese too. High mercury level sources include fish and dental amalgams. Occupational sources are combustion of fossil fuels or waste, the chloralkali industry, battery production, mercury alloys and polymer synthesis.

There have been many investigations into the metals' neurological and toxicological



GRAPHICS:
ALEXANDRA MICHALKE

effects, but the characterisation of their chemical forms (or trace element speciation) has not always been considered. Knowledge of trace element speciation can lead to a better understanding of how metals cross neural barriers and their potential role in causing disease in the human brain.

During the past few years, speciation analysis has become a valuable tool in highlighting neurotoxic chemical species and their pathways. Powerful techniques have been applied to human samples, mostly blood serum. More research is needed on other components that either transport species to the brain or are present in neuronal tissue or fluids. Some studies on cerebrospinal fluid and brain tissue have shown promise, but obtaining samples can be difficult. Results can also be hampered when the elements being studied are in low

Trace element speciation analysis shows how metals cross the neural barrier to cause disease in the brain

concentrations or their chemical forms are not stable. For example, in studies on the role of species such as aluminium-citrate, manganese-transferrin and manganese-citrate, forms in which the metals are able to cross the blood-brain barrier, in neurodegenerative diseases, even sample preparation, separation and storage time can change their identity or alter their concentration, making analytical quality control a challenge. These challenges and limitations illustrate that element speciation analysis in human body fluids is not an easy task. Until these problems are resolved, there will continue to be a lack of speciation data – data that could be the key to helping us live longer.

Reference
B Michalke, S Halbach and V Nischwitz, *J. Environ. Monit.*, 2009, DOI: 10.1039/b817817h

Read more in *JEM Spotlight: Metal speciation related to neurotoxicity in humans* in issue 5, 2009 of the Journal of Environmental Monitoring.

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Making logical connections

Henry Rzepa tells Carl Saxton about the potential for creativity in both research and teaching activities



Henry Rzepa

Henry Rzepa is a professor of computational chemistry at Imperial College London, UK. His research focuses on modelling the shapes, properties and reactions of molecules and in presenting this information in internet-friendly ways.

Why did you decide to become a chemist?

We lived on a farm in Scotland. Once, my mother came down with flu and my father was away. I decided to make my mother a cup of tea. I had only a tenuous grasp of proportions and the resulting brew was close to one part water to 10 parts tea leaves. She drank it nonetheless. Thus encouraged, I started mixing anything I could find on the farm to see what would happen. By age 14, I had my own laboratory at home. After completing a synthesis of benzidine (nowadays firmly banned as being far too toxic) and reading a textbook on valence theory, the future course of my professional life was firmly set.

What first got you interested in theoretical chemistry?

The textbook on valence theory I allude to above, but more firmly, after completing a PhD in physical organic chemistry and reaction mechanisms. I realised that all those linear free energy relationships I was measuring were not really telling me anything really fundamental about why the molecules I was studying behaved the way they did. I decided that only quantum mechanics was going to do this. At just the right time, Michael Dewar visited the department, and after his inspiring talk, I expressed an interest in working for him. A week later, a package weighing certainly more than a kilogram containing about 50 reprints for me to read arrived. I was hooked!

What projects are you working on at the moment?

One area of research is about unravelling the origins of stereo- and chemoselectivity in metal-catalysed reactions. A good example is rationalisation of the heterotacticity in magnesium-catalysed lactide polymerisation, in terms of how isopropyl groups interact with phenyl faces and other groups.

The second area is the discovery and understanding of new forms of 'chiral aromaticity'. We, and others, have over the last decade shown how some aromaticities can originate from helical (twisted) arrangements of conjugated systems. The first glimmers started some 45 years ago, with the espousal of Möbius molecules by Heilbronner, but it's probably only in the last five years that lots of nice examples of this type of molecule have started to come to light.

The third theme is related to our aim of activating the internet for chemical application.

What do you think the journal article will look like in twenty years' time?

Perhaps the biggest change I foresee is that the readership of the scientific article will not consist of just 'humans', but of what we refer to as 'machines'. The journal article will become semantically enabled, and software agents will be able to assimilate the article logically and infer logical connections to other knowledge. They will distil all this information down to a set of suggestions for the human to make those previously uncharted connections which we call discovery or indeed inspiration. As such, the boundaries and dimensions of what is now a well-defined article will soften and blur.

What are your thoughts regarding RSC Prospect?

If I say it is ahead of its time, you must understand that I view it as very much central to our vision of the future. It is part of that semantically enabled vision I spoke about earlier. Currently, Prospect is still aimed squarely at human readers. But it's just a small step away from the full machine-human symbiosis that I mentioned before. If only all publishers were so innovative.

You have been active in teaching for 31 years – how has the face of teaching changed?

Well, in many ways, students are still students! The very best were capable of astounding me 31 years ago with their enthusiasm and ability, and that still happens to this day. Observing how many students manage the transition from school to being able to cope with the real world in the four years they spend at university is one of the rewards of my job.

Has there been a lot of interest in your lectures as podcasts?

The students certainly appreciate being able to replay lectures (in audio), and the enhanced visuals that podcasts can deliver. In one year, my podcasts made it into the iTunes top ten charts! However, preparing podcasts is very time-consuming, and only one other colleague has thus far tried it. So to some extent, we have really not achieved the critical mass of podcast materials in chemistry that would make the genre mainstream rather than just an oddity.

If you weren't a scientist, what would you be?

Were it not for my total lack of any skills, I would have enjoyed being a composer.

Essential elements

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Lab on a Chip goes YouTube™

Are you interested in watching the latest advances in microfluidics on video? The new *Lab on a Chip* YouTube™ video channel makes it possible by visualising all the latest scientific research in the field of miniaturisation. 'Many of the articles we receive for *Lab on a Chip* include video footage. These videos are currently captured on our journal website together with the scientific article, but we felt it was essential to share all this interesting information, not only with the scientists who regularly read *Lab on a Chip* but with the wider scientific community,' states Harp Minhas, editor of the journal.

One of the videos included

illustrates how researchers at the University of St Andrews, UK, use the unusual curving properties of laser beams to hurl microparticles and cells over walls. The scientists were looking into optically redistributing microparticles and cells between microwells.



'I think it is a great idea to establish such a video channel, in particular within the field of microfluidics where the vast majority of results are recorded

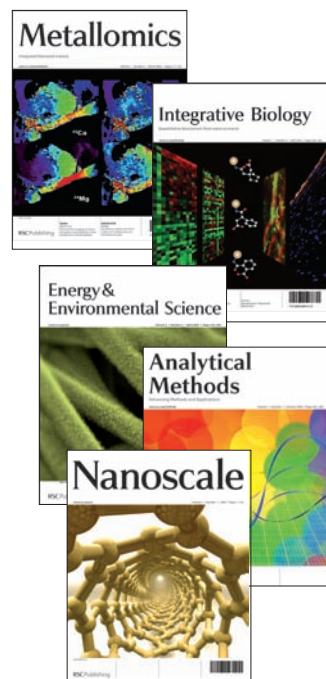
and presented as video files,' comments Jörg Baumgartl, who led the research. The associated article is published in *Lab on a Chip* as an advance article at www.rsc.org/loc.

'All scientists are keen to increase the visibility and impact of their work and this ties in with the RSC goal to communicate the chemical sciences as widely as possible and engage a wide audience,' adds Harp Minhas. 'Videos are a universal language and aid the understanding of scientific work on an international level. YouTube™ represents the perfect medium to help us achieve this goal.'

To find out more go to www.youtube.com/labonachipvideos

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Out and about

The Third *ChemComm* International Symposium on Organic Chemistry was held in February in China. The RSC partnered with three universities – Peking University, Sichuan University and the Shanghai Institute of Organic Chemistry – to host the three one-day meetings. With over 700 delegates attending and key speakers from across the world, the symposium was a huge success.

Sarah Thomas, editor of *ChemComm* comments: 'The lectures presented during the symposium were of outstanding quality and covered the whole breadth of organic chemistry from transition metal asymmetric catalysis, organocatalysis,

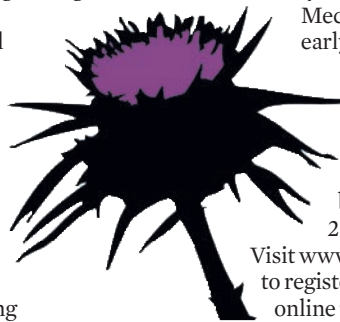
mechanistic studies to the synthesis of both natural and non-natural products.' Abstracts of the research presented at the symposium, and biographies of the presenters can be found at www.rsc.org/chemcommsymposia

The RSC is also organising the 42nd IUPAC Congress which will be held in Glasgow, UK, in August. The programme features around 50 symposia, which will demonstrate the impact of the chemical sciences, highlighting

exciting innovations with an overall focus on 'Chemistry Solutions'. Key themes for this event are: Analysis & Detection, Chemistry for Health, Communication & Education, Energy & Environment, Industry & Innovation, Materials and

Synthesis & Mechanism. An early bird discount of £50 is available for those who register for the meeting before 5 June 2009.

Visit www.iupac2009.org to register your place online today!



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Deputy editor: Sarah Dixon

Associate editors: Celia Gitterman, Joanne Thomson

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