

ChemComm

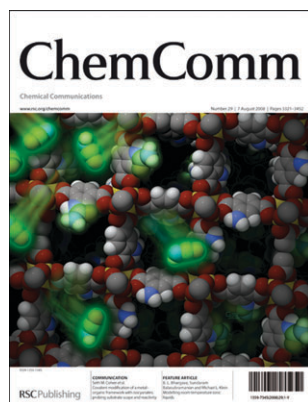
Chemical Communications

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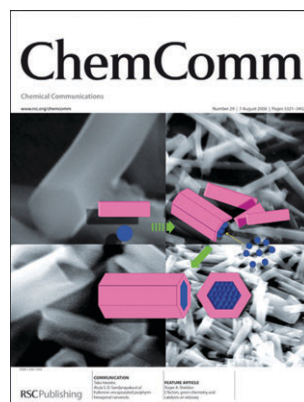
IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (29) 3321-3452 (2008)



Cover

See Seth M. Cohen *et al.*, pp. 3366–3368. Isoreticular metal–organic framework-3 has been chemically modified, in a post-synthetic approach, with isocyanates to generate urea groups within the lattice. Image reproduced by permission of Emily Dugan, Zhenqiang Wang, Marilyn Okamura, Annette Medina and Seth M. Cohen from *Chem. Commun.*, 2008, 3366.



Inside cover

See Taku Hasobe, Atula S. D. Sandanayaka *et al.*, pp. 3372–3374. This image shows a series of organization processes of fullerene-encapsulated porphyrin hexagonal nanorods. Image reproduced by permission of Taku Hasobe, Atula S. D. Sandanayaka, Takehiko Wada and Yasuyuki Araki from *Chem. Commun.*, 2008, 3372.

CHEMICAL BIOLOGY

B57

Drawing together research highlights and news from all RSC publications, *Chemical Biology* provides a ‘snapshot’ of the latest developments in chemical biology, showcasing newsworthy articles and significant scientific advances.

Chemical Biology

August 2008/Volume 3/Issue 8

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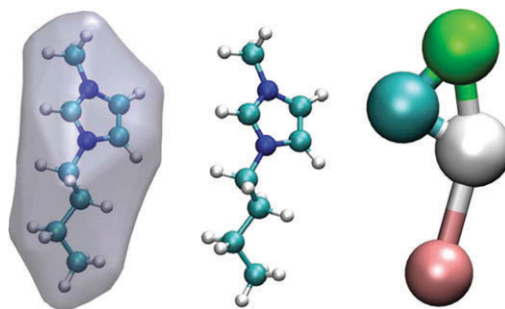
FEATURE ARTICLE

3339

Modelling room temperature ionic liquids

B. L. Bhargava,* Sundaram Balasubramanian* and Michael L. Klein*

An overview of computational studies of room temperature ionic liquids is presented. A hierarchical modelling approach based on *ab initio*, atomistic, and coarse grained molecular dynamics simulations is described.



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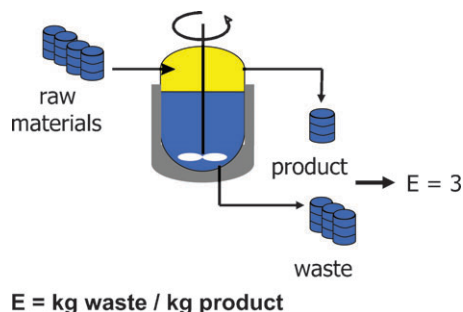
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E factors, green chemistry and catalysis: an odyssey

Roger A. Sheldon

The role of catalysis (homogeneous, heterogeneous, organocatalysis and biocatalysis), alternative reaction media and renewable raw materials in the development of green and sustainable processes and products is reviewed.



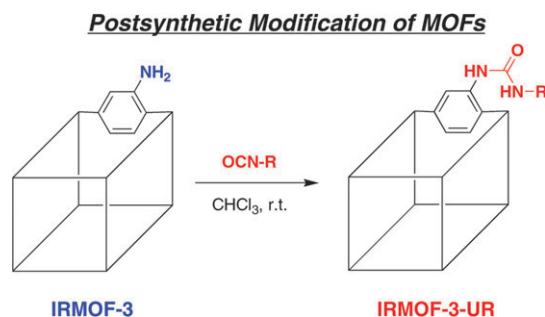
COMMUNICATIONS

3366

Covalent modification of a metal–organic framework with isocyanates: probing substrate scope and reactivity

Emily Dugan, Zhenqiang Wang, Marilyn Okamura, Annette Medina and Seth M. Cohen*

Isoreticular metal–organic framework-3 (IRMOF-3) has been chemically modified, in a systematic postsynthetic approach, with isocyanates to generate microporous frameworks containing urea groups with a variety of substituents.

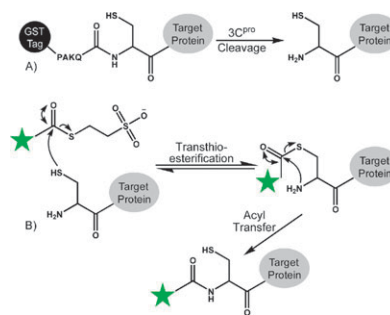


3369

Specific N-terminal protein labelling: use of FMDV 3C^{pro} protease and native chemical ligation

Gillian K. Busch, Edward W. Tate, Piers R. J. Gaffney, Erika Rosivatz, Rudiger Woscholski and Robin J. Leatherbarrow*

We describe an effective method to generate N-terminal cysteinyl proteins by proteolytic cleavage using the enzyme 3C^{pro}, suitable for specific tagging using native chemical ligation (NCL). This 3C^{pro}/NCL system can be exploited for a wide range of protein and applications.

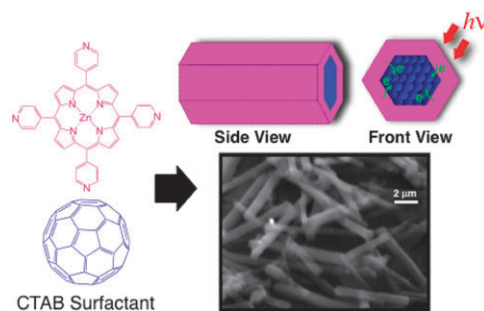


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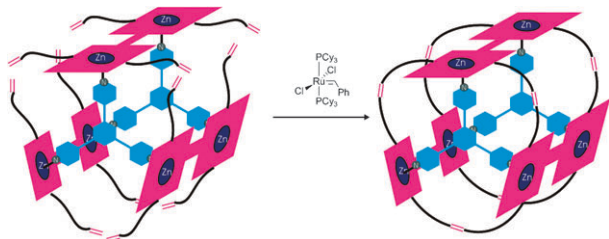
Fullerene-encapsulated porphyrin hexagonal nanorods. An anisotropic donor–acceptor composite for efficient photoinduced electron transfer and light energy conversion

Taku Hasobe,* Atula S. D. Sandanayaka,* Takehiko Wada and Yasuyuki Araki

Fullerene-encapsulated porphyrin hexagonal nanorods prepared in DMF–acetonitrile demonstrate efficient and characteristic photoinduced electron transfer and light energy conversion properties.



3375

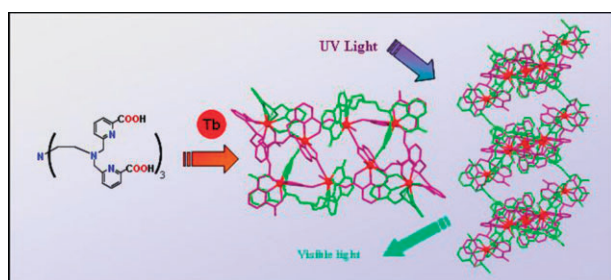


Hollow porphyrin prisms: modular formation of permanent, torsionally rigid nanostructures *via* templated olefin metathesis

Kyoung-Tae Youm, SonBinh T. Nguyen* and Joseph T. Hupp*

Hexa-porphyrin prisms can be template-assembled and covalently locked, *via* cross-olefin metathesis, into permanent torsionally rigid structures that remain stable upon template removal. Synthetic modification of the porphyrin sites can be carried out in a facile manner.

3378

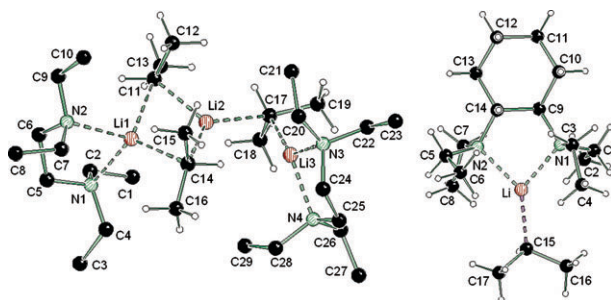


A flexible tripodal ligand linking octametallic terbium rings into luminescent polymeric chains

Xiao-Yan Chen, Claire Marchal, Yaroslav Filinchuk, Daniel Imbert and Marinella Mazzanti*

A new tripodal ligand combining flexibility and high denticity directs the assembly of large octametallic terbium clusters covalently linked into a highly luminescent tube-like chain.

3381

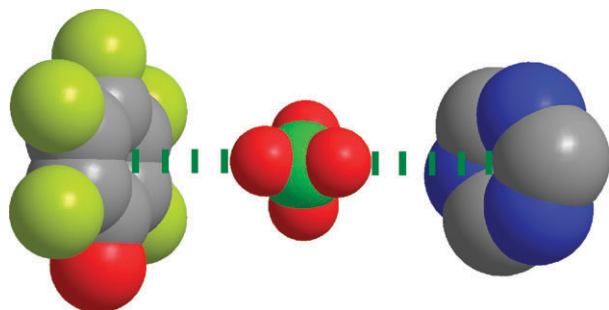


Isopropyl lithium diamine adducts: from a non symmetric aggregate to monomeric *i*-PrLi · (1*R*,2*R*)-*N,N,N',N'*-tetraethylcyclohexane-1,2-diamine

Carsten Strohmann,* Viktoria H. Gessner and A. Damme

By means of isopropyl lithium crystal structures, the transition from dimeric (*i*-PrLi · TMEDA)₂ (**4**) to monomeric *i*-PrLi · (*R,R*)-TECDA (**6**) *via* the non-symmetric aggregate [(*i*-PrLi)₃ · (TEEDA)₂] (**5**) is shown, depending on the steric demand of the ligand.

3384



Concurrent anion... π interactions between a perchlorate ion and two π -acidic aromatic rings, namely pentafluorophenol and 1,3,5-triazine

Rens J. Götz, Arturo Robertazzi, Ilpo Mutikainen, Urho Turpeinen, Patrick Gamez* and Jan Reedijk*

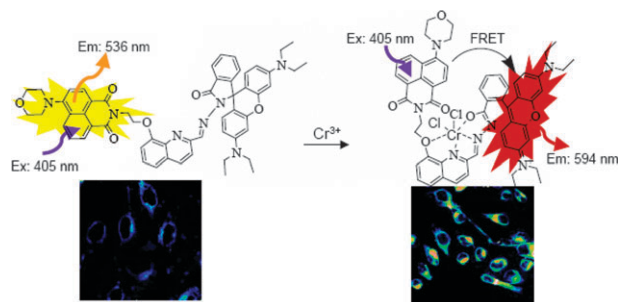
A multifunctional molecule containing both a 1,3,5-triazine and a pentafluorophenoxy group has been designed to investigate the competitive anion- π interactions of these two π -acidic rings. Crystallographic and theoretical data suggest that the two electron-deficient aromatics possess comparable anion binding properties.

3387

FRET-based sensor for imaging chromium(III) in living cells

Zhiguo Zhou, Mengxiao Yu, Hong Yang, Kewei Huang, Fuyou Li,* Tao Yi and Chunhui Huang

On the basis of fluorescent resonance energy transfer from 1,8-naphthalimide to rhodamine, a fluorophore dyad (**FD8**) containing rhodamine and a naphthalimide moiety was synthesized as a Cr^{3+} -selective fluorescent probe for monitoring Cr^{3+} in living cells with ratiometric fluorescent methods.

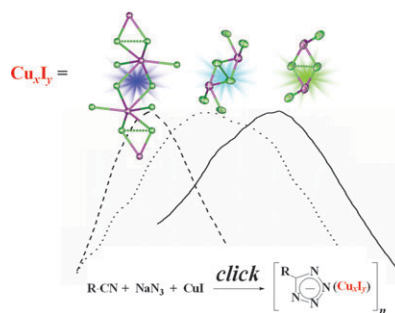


3390

Unprecedented cationic copper(I)-iodide aggregates trapped in “click” formation of anionic-tetrazolate-based coordination polymers

Mian Li, Zhen Li and Dan Li*

A series of unprecedented cationic copper(I)-iodide aggregates, $(\text{Cu}_4\text{I}_2)^{2+}$, $(\text{Cu}_6\text{I}_2)^{4+}$ and $(\text{Cu}_{10}\text{I}_4)^{6+}$, are trapped in the *in situ* formation of anionic-tetrazolate-based coordination polymers, which exhibit structure-related green, cyan and blue luminescence, respectively.

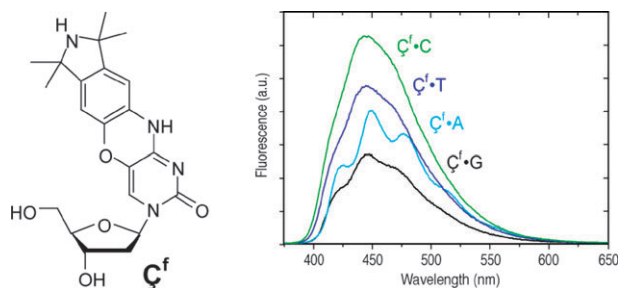


3393

Single base interrogation by a fluorescent nucleotide: each of the four DNA bases identified by fluorescence spectroscopy

Pavol Cekan and Snorri Th. Sigurdsson*

Nucleoside ζ , which contains a rigid nitroxide spin label, is effectively reduced in DNA by sodium sulfide to the corresponding amine, yielding a fluorescent probe (ζ^f). Fluorescence spectra of duplexes where ζ^f is base-paired with A, T, C or G can be readily distinguished. Thus, ζ^f can report the identity of its base-pairing partner in duplex DNA.

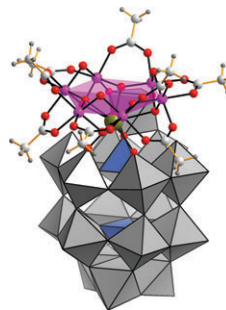


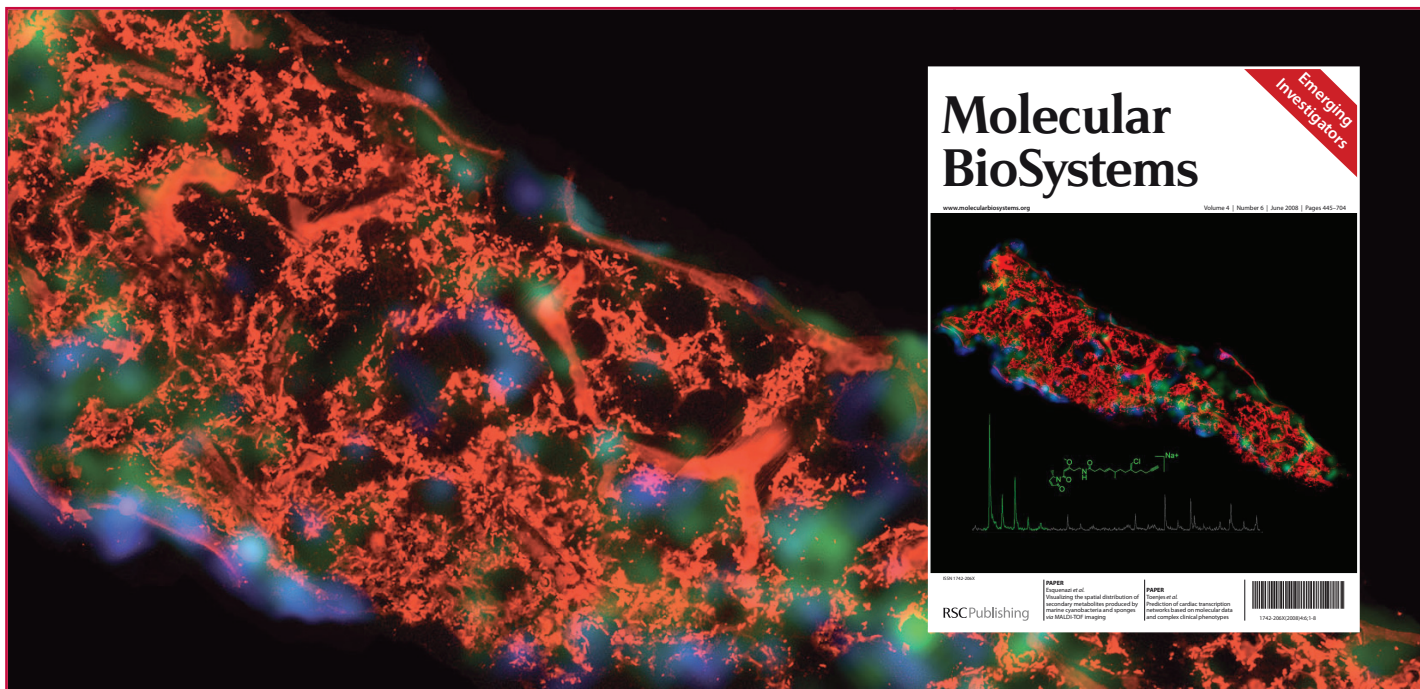
3396

A polyoxometalate-based manganese carboxylate cluster

Xikui Fang and Paul Kögerler*

Partial substitution of organic bridging ligands, while retaining the core structure of a $\{\text{Ce}^{\text{IV}}\text{Mn}^{\text{IV}}_6\}$ coordination cluster, is achieved by metathesis reaction with a di-vacant polyoxotungstate Dawson anion, resulting in a stable adduct.





Emerging Investigators theme issue

Molecular BioSystems issue 6, 2008, devoted to outstanding young scientists at the chemical- and systems-biology interfaces, features novel methods to visualise and manipulate protein function in living cells, the development of chemical techniques to monitor specific protein post-translational modifications, new insights into metabolomics and much, much more!

Papers include:

Visualization of phosphatase activity in living cells with a FRET-based calcineurin activity sensor

Robert H. Newman and Jin Zhang

Conformation and the sodium ion condensation on DNA and RNA structures in the presence of a neutral cosolute as a mimic of the intracellular media

Shu-ichi Nakano, Lei Wu, Hirohito Oka, Hisae Tateishi Karimata, Toshimasa Kirihaata, Yuichi Sato, Satoshi Fujii, Hiroshi Sakai, Masayuki Kuwahara, Hiroaki Sawai and Naoki Sugimoto

A quantitative study of the recruitment potential of all intracellular tyrosine residues on EGFR, FGFR1 and IGF1R

Alexis Kaushansky, Andrew Gordus, Bryan Chang, John Rush and Gavin MacBeath

Direct printing of trichlorosilanes on glass for selective protein adsorption and cell growth

Dawn M. Yanker and Joshua A. Maurer

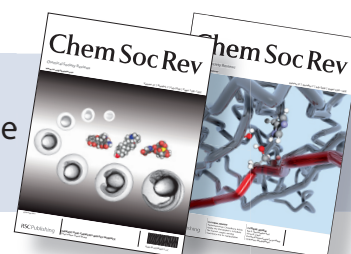
A chemical approach for detecting sulfenic acid-modified proteins in living cells

Khalilah G. Reddie, Young Ho Seo, Wilson B. Muse III, Stephen E. Leonard and Kate S. Carroll

See also:

Chem Soc Rev issue 7, 2008 - Chemistry-Biology Interface theme issue

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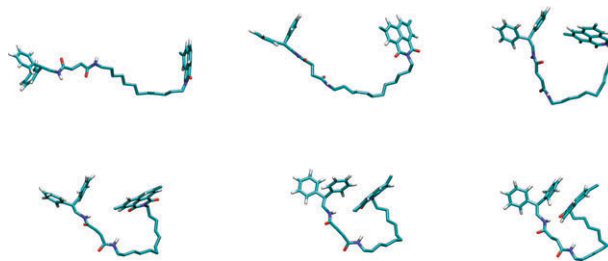
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3399

Can a synthetic thread act as an electrochemically switchable molecular device?

Costantino Zazza, Andrea Amadei, Nico Sanna and Massimiliano Aschi*

Our theoretical/computational study shows for the first time that a recently proposed molecular thread might be an interesting example of a nanoscale molecular device that undergoes a reversible conformational change in response to external stimuli (*i.e.*, oxidation–reduction).

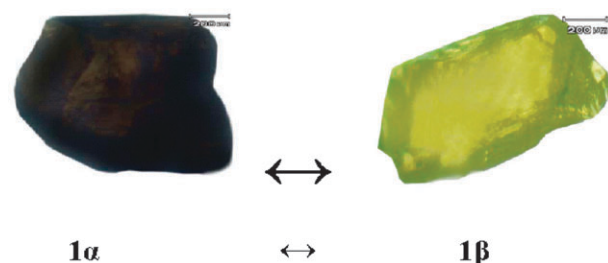


3402

Crystal-to-crystal transformation from a chain polymer to a two-dimensional network by thermal desolvation

Alireza Aslani and Ali Morsali*

Single-crystal to single-crystal transformation of a new lead(II) coordination polymer with ligands 8-hydroxyquinoline (8-Quin) and nitrate, $[\text{Pb}_2(8\text{-Quin})_2(\text{NO}_3)_2(\text{MeOH})]$ (**1 α**) to $[\text{Pb}(8\text{-Quin})(\text{NO}_3)]$ (**1 β**), is reported and the structures of **1 α** and **1 β** determined by X-ray crystallography.



3405

Rhodium-catalyzed (*E*)-selective cross-dimerization of terminal alkynes

Takashi Katagiri, Hayato Tsurugi, Tetsuya Satoh and Masahiro Miura*

Cross-dimerization of various terminal alkynes with different bulky terminal alkynes efficiently proceeds in the presence of a rhodium catalyst system to produce the corresponding (*E*)-enynes with high regio- and stereoselectivity.

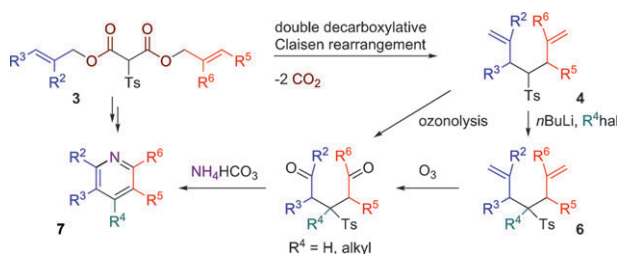


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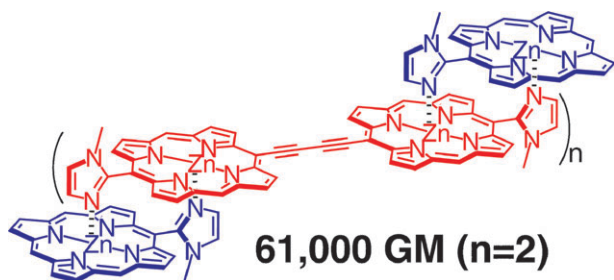
Double decarboxylative Claisen rearrangement reactions: microwave-assisted *de novo* synthesis of pyridines

Donald Craig,* Federica Paina and Stephen C. Smith

Microwave-assisted double decarboxylative Claisen rearrangement of bis(allyl) 2-tosylmalonates provides substituted 1,6-heptadienes, which may be alkylated, and then converted into pyridines by ozonolysis followed by reaction with ammonia generated *in situ* under microwave conditions.



3411

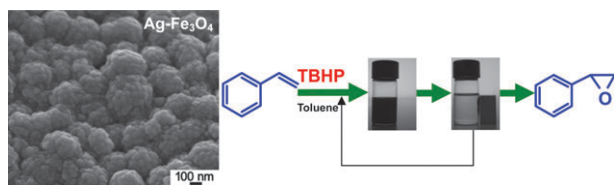


Stepwise elongation effect on the two-photon absorption of self-assembled butadiyne porphyrins

Joanne Dy, Kazuya Ogawa,* Kenji Kamada, Koji Ohta and Yoshiaki Kobuke*

Butadiyne–porphyrin dimer arrays, which were constructed by complementary coordination of the central zinc atom to imidazolyl, were elongated stepwise and their 2PA properties were investigated.

3414

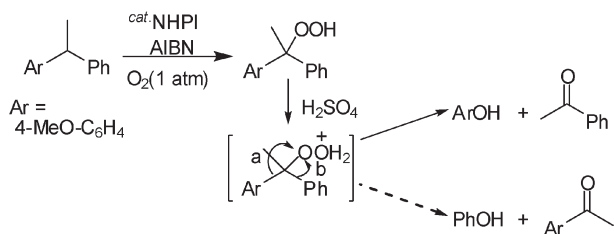


One-pot synthesis of Ag–Fe₃O₄ nanocomposite: a magnetically recyclable and efficient catalyst for epoxidation of styrene

Dong-Hui Zhang, Guo-Dong Li, Ji-Xue Li and Jie-Sheng Chen*

With the assistance of PVP, a novel magnetically recyclable Ag-based catalyst has been synthesized in one pot, and it is found that this catalyst is highly efficient in selectively catalyzing styrene conversion to styrene oxide.

3417

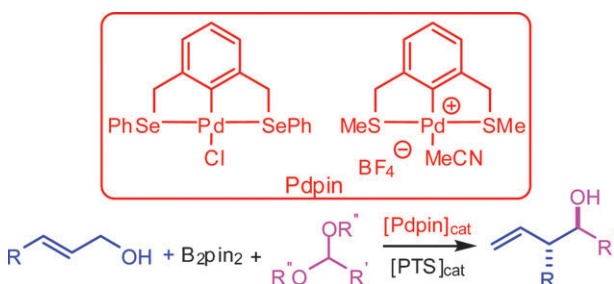


Selective one-pot synthesis of various phenols from diarylethanes

Ryota Nakamura, Yasushi Obora and Yasutaka Ishii*

Various substituted phenols were selectively synthesized by a one-pot reaction through the NHPI-catalyzed aerobic oxidation of 1,1-diarylethanes followed by treatment with dilute sulfuric acid.

3420



Single-pot triple catalytic transformations based on coupling of *in situ* generated allyl boronates with *in situ* hydrolyzed acetals

Nicklas Selander and Kálmán J. Szabó*

Single-pot triple catalytic transformations have been designed for the synthesis of homoallyl alcohols and epoxides from allyl alcohols (and other simple allylic substrates) and acetals. These transformations involve a cooperative sequence of three discrete processes.

3423

Synthesis of 4a-carba- α -D-lyxofuranose from 2,3-*O*-isopropylidene-L-erythruronolactone *via* Tebbe-mediated cascade reaction

Girija Prasad Mishra, G. Venkata Ramana and B. Venkateswara Rao*

A new, efficient and highly diastereoselective approach for the synthesis of 4a-carba- α -D-lyxofuranose from the isopropyl glycoside of 2,3-*O*-isopropylidene-L-erythruronolactone using Tebbe reagent was developed.

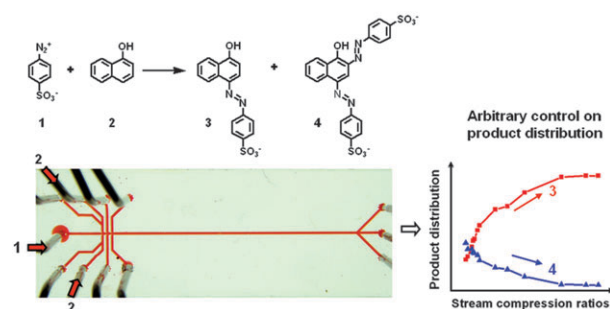


3426

A dynamic micromixer for arbitrary control of disguised chemical selectivity

Karla K. Cotí, Yanju Wang, Wei-Yu Lin, Chia-Chun Chen, Zeta Tak For Yu, Kan Liu, Clifton K.-F. Shen, Matthias Selke,* Anchi Yeh,* Weixing Lu* and Hsian-Rong Tseng*

A new type of dynamic micromixer combining the concepts of parallel multi-lamination and hydrodynamic focusing was developed for arbitrary control of disguised chemical selectivity of the diazo coupling reaction.

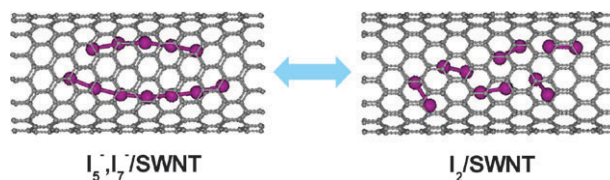


3429

Tuning of hole doping level of iodine-encapsulated single-walled carbon nanotubes by temperature adjustment

Zhiyong Wang, Lu Wang, Zujin Shi,* Jing Lu,* Zhennan Gu and Zhengxiang Gao

The hole doping level of SWNTs can be tuned by utilizing the conversion between polyiodide chains and iodine molecules encapsulated inside SWNTs.

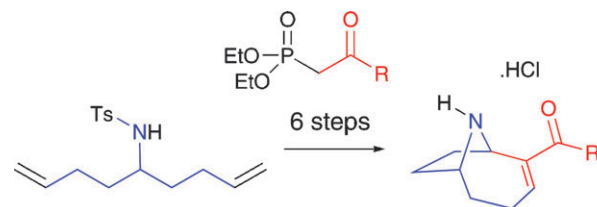


3432

A two-directional approach to the anatoxin alkaloids: second synthesis of homoanatoxin and efficient synthesis of anatoxin-a

Stephen J. Roe and Robert A. Stockman*

A desymmetrising ozonolysis is exploited in a two-directional strategy for the efficient total syntheses of the potent neurotoxins and environmental hazards homoanatoxin and anatoxin-a.



R=Me (anatoxin-a) 10 steps, 27.1% from HCO₂Et
R=Et (homoanatoxin), 10 steps, 14.8% from HCO₂Et

3435



Tracking reactive intermediates in phosphine-promoted reactions with ambiphilic phosphino-boranes

Sylvie Moëbs-Sanchez, Ghenwa Bouhadir, Nathalie Saffon, Laurent Maron* and Didier Bourissou*

Reaction of a phosphino-borane with diethyl azodicarboxylate or PhNCO affords the corresponding 1 : 1 adducts, which were fully characterized by X-ray diffraction and other studies. DFT calculations substantiate the regioselectivity and reversibility of PhNCO fixation.

3438

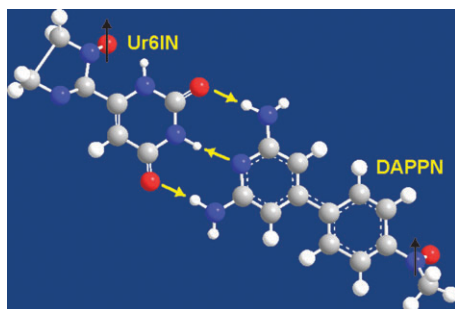


Multidentate thioether ligands coating gold nanoparticles

Torsten Peterle, Annika Leifert, Jan Timper, Alla Sologubenko, Ulrich Simon* and Marcel Mayor*

Multidentate ligands, designed to enwrap metal particles, stabilize Au nanoparticles with a narrow size distribution.

3441

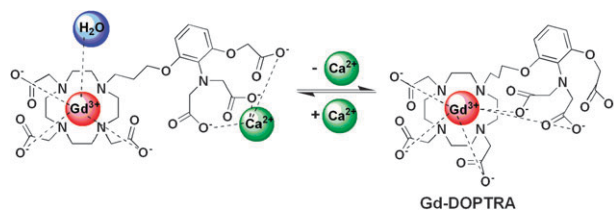


Molecular recognition in a heteromolecular radical pair system with complementary multipoint hydrogen-bonding

Hidenori Murata, Paul M. Lahti* and Safo Aboaku

6-Uradinyl-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazole-1-oxyl (Ur6IN) and 4-(*p*-*tert*-butylaminoxylphenyl)-2,6-di(propylamido)pyridine (DAPPN) form heterospin Ur6IN · DAPPN dyad complexes.

3444



Synthesis and characterization of a smart contrast agent sensitive to calcium

Kirti Dhingra,* Martin E. Maier, Michael Beyerlein, Goran Angelovski and Nikos K. Logothetis*

A novel first-generation Ca^{2+} sensitive contrast agent, Gd-DOPTRA has been synthesized and characterized. The agent shows 100% relaxivity enhancement upon addition of Ca^{2+} . The observed selectivity and sensitivity towards Ca^{2+} in the presence of Mg^{2+} , Zn^{2+} as well as in physiological fluids indicates the prospects of this agent for *in vivo* measurements.

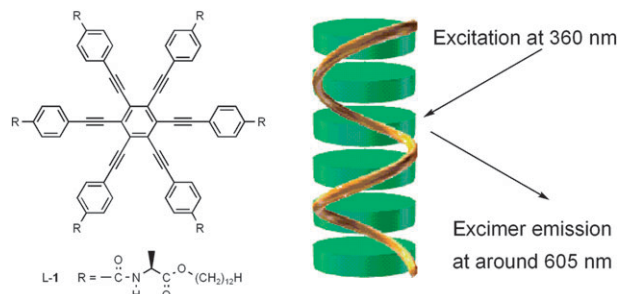


3447

Stable supramolecular helical structure of C_6 -symmetric hydrogen-bonded hexakis(phenylethynyl)benzene derivatives with amino acid pendant groups and their unique fluorescence properties

Koichi Sakajiri,* Takeshi Sugisaki and Keiichi Moriya

A highly stable supramolecular helical structure was formed by the self-assembly of novel C_6 -symmetric hydrogen-bonded discotic molecules, hexakis(phenylethynyl)benzene derivatives with chiral alanine parts, and exhibited orange excimer emission with a large Stokes shift.



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Chemical Biology

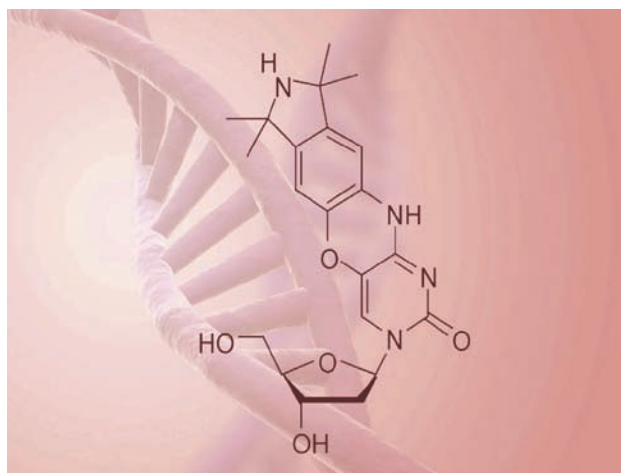
Discriminating probe presents possibility for disease detection

Matching nucleosides

A fluorescent probe can spot the difference between the four DNA bases: adenine, thymine, cytosine and guanine.

Snorri Sigurdsson and Pavol Cekan from the University of Iceland, Reykjavik, have synthesised a highly fluorescent nucleoside (a base bound to a sugar) which can report the identity of its base-pair when placed in a DNA duplex. The fluorescence emitted by the duplex differs depending on which DNA base is paired with the probe.

According to Sigurdsson and Cekan, the probe could find use in detecting single DNA base changes – single nucleotide polymorphisms (SNP) – at sites where variation can indicate disease. Changes within the gene apolipoprotein E, for example, are considered to be an indicator of predisposition to Alzheimer's. The researchers explain that detecting SNPs with their probe could make



it possible to identify genetic diseases or recognise people who might be susceptible to them. Also, the probe would not only detect a SNP but could indicate which DNA base replaced the correct one.

David French from LGC, in Teddington, UK, who has recently

The fluorescent nucleoside can report the identity of its base pair in duplex DNA

studied SNP in the gene encoding sheep prion protein agrees that 'technology that can reliably discriminate between the four naturally occurring bases of DNA to analyse SNPs will be a useful tool for diagnostic tests.'

Sigurdsson plans to investigate the nucleoside's fluorescence under many different conditions. 'Better understanding of the nucleoside's properties will lay the groundwork to develop further compounds that may be better suited for routine-based fluorescence assays,' he says. 'One of the challenges is to find base-discriminating fluorescent nucleosides that emit light at the higher wavelengths detected by instruments currently used in laboratories around the world.'

Rachel Cooper

Reference

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In this issue

Dunking doughnuts into cells

Miniature polymer rings could help reduce cancer treatment side effects

Faster superbug detection

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Beryllium: friend or foe?

Instant insight: Brian Scott and colleagues examine the molecular basis of chronic beryllium disease



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Research highlights

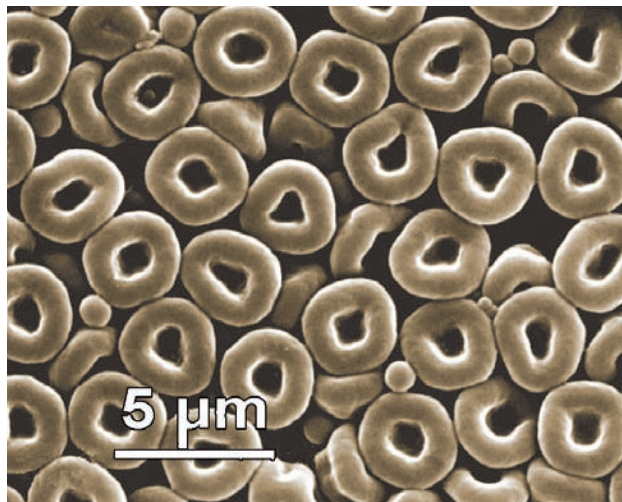
Miniature polymer rings show affinity for specific cell types

Dunking doughnuts into cells

Doughnut-shaped particles could help to reduce side effects from cancer treatments, says a team of scientists from the UK.

Developed by a team fronted by Mark Bradley at the University of Edinburgh, the uniquely-shaped polystyrene particles can penetrate specific cell types in the body, and have a particular affinity for the liver. 'This opens up the possibility of using these particles to deliver therapeutics solely to the liver in cases of disease and could limit side effects associated with the treatment,' says Bradley. Side effects, such as hair loss in cancer treatment, can arise because drugs aimed at cancer cells may also affect similar cell types in other parts of the body.

Bradley explains that the team stumbled on the micro-doughnuts accidentally during their investigations. Whilst using a simple technique called dispersion polymerisation to grow small particles in a polymer mixture, they



Bradley's microscopic polystyrene loops were discovered by accident

found that adding a small amount of dioxane to the usual ethanol solvent gave their surprise result. 'The particles' unique and highly uniform structure was immediately interesting to us and we considered the possible applications they might have,' says Bradley.

Andy Sutherland, an expert in polymer chemistry, at Aston University in Birmingham, UK, says the particles' selective cellular uptake is striking. 'By understanding the basis of this cellular choice it may, in the future, be possible to design polymer constructs that both target specific cell types and allow molecular cargoes to be imported into these cells for therapeutic, diagnostic and imaging applications.'

The team suggests it is the particles' shape that is responsible for their cell specificity. And their unusual shape and uniform, tiny size – thirty times smaller than a human hair – mean they could also be suitable in filtration and purification devices, for example, says Bradley. The next challenge will be to understand how the doughnuts form, he adds.

Katherine Davies

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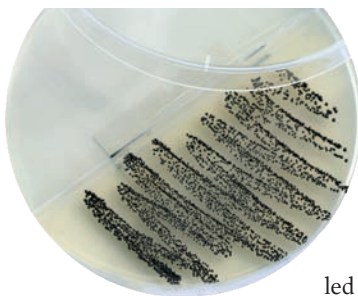
Lab-on-a-chip confines bacteria in droplets for fast antibiotic screening

Faster superbug detection

Chip technology could cut the wait for test results on clinical samples, say US scientists. A team at the University of Chicago has developed a method to detect bacteria in blood plasma samples and simultaneously screen their response to antibiotics.

The group's technique works by mixing a sample with a dye that fluoresces in the presence of bacteria; the mixture is then converted into droplets inside a microfluidic chip. If the sample contains bacteria some of the droplets will contain a single bacterium and fluoresce. Because of the very small droplet size, the occupied droplets will have a high bacterial density, removing the need to incubate samples to increase their concentration before detection.

The team was able to use the method to detect the MRSA (methicillin-resistant *Staphylococcus aureus*) 'superbug', so-called because



Chip technology removes the need for time-consuming sample incubations

of its resistance to several antibiotics. They were also able to find potential treatments for MRSA infections by treating an array of the droplets with different antibiotics and looking at the change in fluorescence.

Rustem Ismagilov, who led the team, explains that his motivation was rooted in improving medical diagnostic tests. Traditional methods of diagnosing bacterial infections rely on time-consuming sample incubations or amplifying the bacterial DNA which, while faster, cannot be used to look at antibiotic response. 'Our technique can potentially provide access to new types of diagnostic tests for bacterial infections and simultaneously identify a treatment regime to provide same-day test results,'

says Ismagilov.

But not only that, 'it could also provide a simple and inexpensive solution to testing for bacteria in other fields where contamination by bacteria is a concern, including the food industry and water management,' Ismagilov adds.

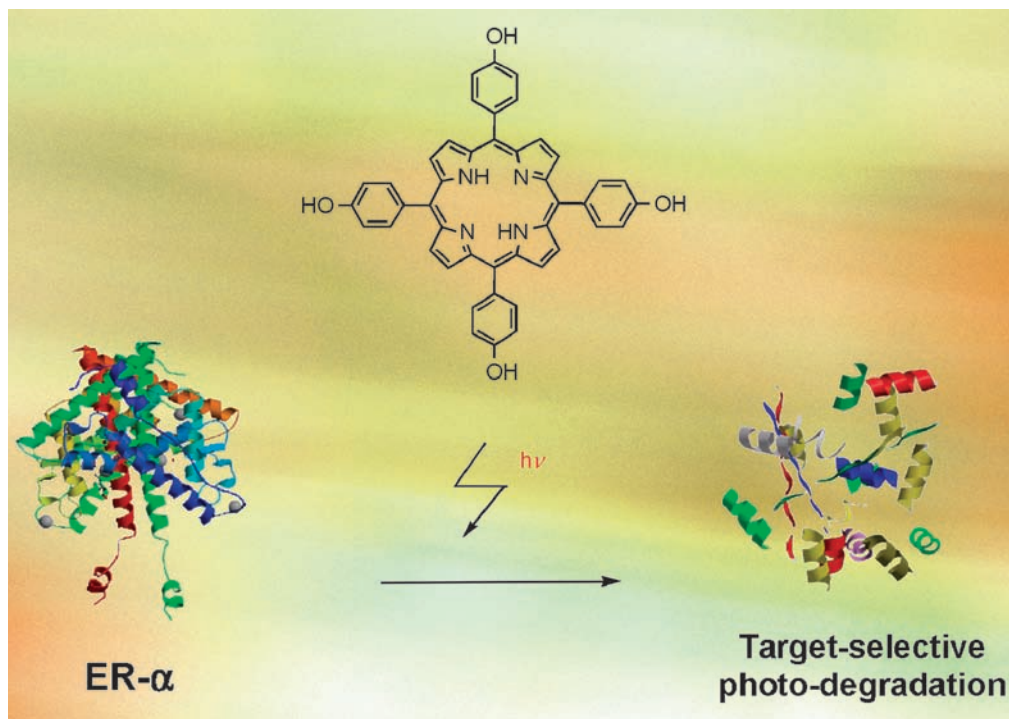
Samuel Sia, an expert in lab-on-a-chip diagnostic devices at Columbia University, New York, US, is enthusiastic about the research. 'The finding that confining a single bacterium to a small volume can decrease detection time is a striking demonstration of the advantages of microfluidics,' he says. Whilst he explains that considerable development and clinical testing will be needed before such an assay could be used for real-world diagnostics, he adds that 'the experimental design is very clever, and the results convincing.' *Kathleen Too*

Reference

J Q Boedicker *et al*, *Lab Chip*, 2008, DOI: 10.1039/b804911d

Selective porphyrin offers therapeutic lead

Protein removal on target



If you're a researcher planning to cure a disease by removing a specific protein, you'll need the therapy to be selective. Hit the wrong target and you'll make things worse – not better. With this in mind, Japanese scientists have identified a light-activated agent that seeks out and destroys a particular protein.

Kazunobu Toshima and co-workers at Keio University, Tokyo, have discovered a porphyrin derivative that selectively fragments a hormone receptor protein upon irradiation with visible light.

Whilst porphyrin derivatives have been used in photodynamic therapy (PDT) to target cancer cell DNA, Toshima's research is the first time the approach has been applied to proteins. 'We've proved that certain porphyrins degrade not only DNA but also proteins with high selectivity. This could lead to new drugs for PDT,' says Toshima.

Toshima's porphyrin works under mild conditions. What's more, only catalytic amounts of the porphyrin are needed to effectively degrade the target protein, since the protein is actually damaged by reactive

The light-activated porphyrin selectively degrades a hormone receptor protein

oxygen species produced by the porphyrin when it is irradiated with light.

The porphyrin is structurally similar to the hormone oestradiol – one of the oestrogens. Toshima suggests this structural similarity could be the basis of the high selectivity for the target protein, human oestrogen receptor- α . The porphyrin should have a higher affinity, and therefore spatial proximity, to oestrogen receptor proteins, he says. 'The life-time of reactive oxygen species is very short so the selectivity is generated by the location of the porphyrin agent.'

'This is the first example of target-selective protein degradation by visible wavelength photo-irradiation using a porphyrin derivative,' comments Aiping Zhu, an expert in biomolecule photochemistry at the University of Michigan, Ann Arbor, US. 'This exciting result opens up a route for organic photochemical agents as protein photocleavers to control specific functions of certain proteins.'

Russell Johnson

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S Tanimoto, S Matsumura and K Toshima, *Chem. Commun.*, 2008, DOI: 10.1039/b806961a

News in brief

Detecting mercurial proteins

European scientists have used a mercury derivative to detect low abundance proteins, a common challenge for scientists trying to identify trace proteins linked to disease.

Making light work of heavy metals

High energy x-rays are shedding light on plants with possible implications for heavy metal decontamination. A team in Japan has used the rays to image the metal distribution in a cadmium-accumulating plant.

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This month in Chemical Science

Fluorescent green logic

Japanese scientists are applying logic to the protein that causes jellyfish to fluoresce green.

Strontium strengthens imitation bones

Strontium offers a new approach to bone replacements, thanks to recent work by French scientists.

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This month in Chemical Technology

Tubular cells

Japanese researchers have developed a new method for growing cylinders of living cells.

Navy's sensing mission

In this month's interview, Frances Ligler talks about portable, automated biosensors for fast, on-site detection of pathogens, toxins, pollutants, drugs and explosives.

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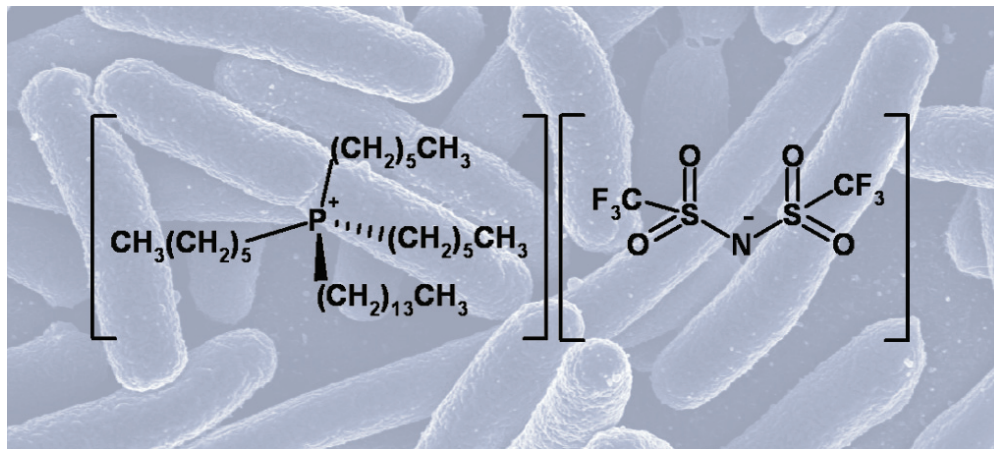
Infrared study suggests link between ionic liquid accumulation rate and toxicity

Why ionic liquids might make you ill

Ionic liquids are often praised for their green credentials, yet they can be highly toxic. Now, researchers from the University of Manchester, UK, have shown that the liquids' interactions with living cells can be studied using Fourier transform infrared (FT-IR) spectroscopy. Their aim is to help scientists understand ionic liquid toxicity mechanisms in order to design safer variants in the future.

Gill Stephens and colleagues used FT-IR spectroscopy to show that the more toxic of the ionic liquids that they studied accumulated in bacterial cells faster than the less toxic ones, suggesting that there may be a link. They also found that the compounds accumulated in the cell membranes, not the cytoplasm inside. Previous research has suggested that ionic liquid toxicity is due to the fact that they disrupt membranes, says Stephens, and these results provide direct support for that idea.

'I would be reluctant to say that this will be the only toxicity mechanism for ionic liquids though,' says Stephens. For



example, ionic liquids can bond to enzymes and disrupt their structures, she explains. Research into this effect is ongoing in her laboratory.

Konrad Kulacki, at the University of Notre Dame, US, who studies the effects of ionic liquids on aquatic ecosystems, says that Stephens' work may help in assessing ionic liquids' environmental impact. 'It is important to study the mechanisms of ionic liquid toxicity, so we can

Ionic liquids accumulate in the membranes of bacteria such as *Escherichia coli*

use this information to design safer compounds,' he adds.

Reinforcing this point, Stephens says that 'there are so many possible ionic liquid structures that finding ones with impeccable environmental credentials is like looking for a needle in a haystack.' Understanding exactly how the compounds affect living cells will therefore help to narrow the search, she says.

Danièle Gibney

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Model membranes

Patricia Bassereau tells Michael Brown about the importance of the membrane in cellular functions and her thoughts about the future of women in science



Patricia Bassereau

Patricia Bassereau is a researcher at the Curie Institute in Paris, France. Her work involves identifying the role of the membrane in cellular functions. She aims to set up biomimetic systems to identify the physical parameters of cells and her long-term goal is to develop a realistic physical model of cell membranes.

Who or what inspired you to become a scientist?

I did not have a role model that inspired me to become a scientist in my family. When I was at school I liked the physical sciences, and I was drawn to the intellectual challenges that they had to offer. I love discovering new things and finding out how things work.

Do you think that there are enough women in science?

There are still some challenges to be overcome. In France, the social structure has enabled many women to work in science; however, this may change in the future. I fear that the number of women in science may decrease, as the younger generation may not be enthusiastic about the stress of a highly competitive life coupled with a low salary.

Your research is on the role of the membrane in cellular functions. What motivated you to work in this area of physical chemistry?

Initially I was working on soft matter, surfactant systems and self-assembly systems. This sometimes involved membranes. I was later working on polymer films. I was interested in cell biology more than 10 years ago. My interest in membranes and cellular functions was increased by two interesting developments in the area. Firstly, theoreticians were developing models that changed the way of thinking about membranes. At the same time, cell biologists realised that proteins were actually incorporated into cell membranes as well as inside cells, and that understanding the properties of membranes was key to other cellular functions. These two strands of thinking helped me return to this area with a new perspective.

Why is it necessary to develop model membranes?

Model membranes are interesting from a physicist's point of view as you can have a simple system of parameters and principles, which can easily be compared to theories.

What are the main areas of research that you are working on at the moment?

There are different aspects that are interesting in our present work. One question is how proteins can deform membranes. Many proteins involved in cell trafficking deform membranes. To study proteins, you must also study the membrane; the two are very much linked. By studying the deformation of the membrane by different proteins

we are able to control the physical parameters that help us understand the mechanism behind the deformation, and the cell processes. At present, we understand that there are two types of proteins, ones that deform the membrane and others that are sensitive to curvature. We hope that by using these model systems and measuring the mechanical properties of the protein assembly, we will be able to further understand this type of mechanism.

We use a lot of membrane nanotubes. By pulling on the cell membrane you can form a nanotube. The diameter of the nanotube can be controlled, and you can then measure many parameters in a controlled environment. By creating these nanotubes you can probe the membrane tension in the cell. So, in a constituted system you can collect mechanical information on the biomembrane.

What achievement are you most proud of in your research?

The achievement I am most proud of is when we used a simple biomimetic system using molecular motors to pull on the cell membrane. This resulted from a close collaboration with cell biologists and theoretician physicists.

Collaborations form a large part of modern scientific research. Which scientist, past or present, would you like to work with and why?

I enjoy working with the theoreticians at the Curie Institute, Jacques Prost and Jean-François Joanny. The close collaboration with these colleagues has been really inspiring.

What is challenging in biophysics at the moment?

There are people like me who have been working on membranes, but there are also people that have been working on cytoskeletons and it is very difficult to combine the two strands. It is clear that in a cell everything is related. Having control of a complete biomimetic system where the membrane and the proteins link the cytoskeleton to the membrane would help us to understand the shape of cells and cell adhesion. Another area that is challenging is neuron research. I think this will be developing in the future.

If you weren't a scientist what would you do?

When I was at school, apart from science, I liked humanities subjects and literature. If I wasn't a scientist, I would like to write science fiction novels.

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Beryllium: friend or foe?

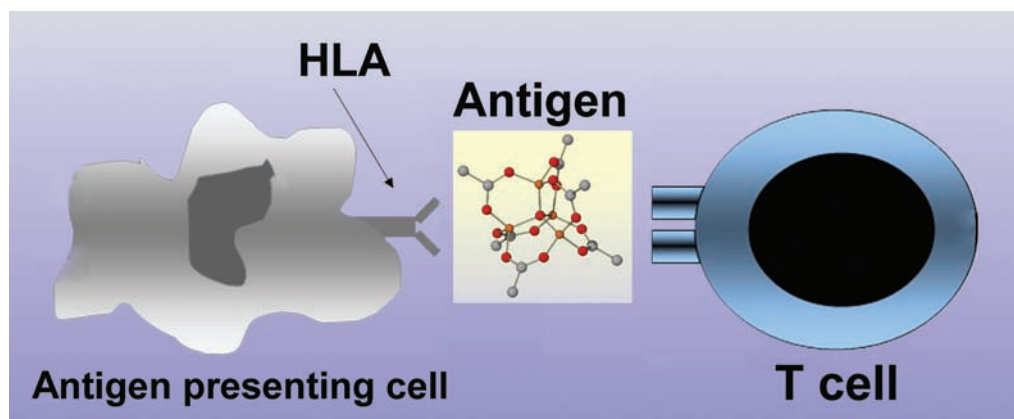
Brian Scott and colleagues at Los Alamos National Laboratory, US, examine the molecular basis of chronic beryllium disease

Beryllium pervades today's technologies, from cars and computers through to dental prosthetics. Its popularity is related to its unique properties: it is lightweight, six times stiffer than steel, has a high melting point (1285 °C) and heat absorption capacity, and is non-magnetic and corrosion resistant. Beryllium also reflects neutrons and is used for nuclear power and weapons applications. In the year 2000 the US used 390 tons of beryllium, with an estimated value of \$140 million.

But, the metal has negative health effects: in susceptible individuals, beryllium exposure causes a lung disorder called chronic beryllium disease (CBD) – a debilitating, incurable and often fatal condition. Given beryllium's widespread use, this toxicity makes it imperative to better understand beryllium's chemistry under biological conditions and how this leads to disease and potential cures and therapeutics.

It is thought that the immune response to beryllium is triggered when the unwittingly-inhaled element is detected by antigen presenting cells (APC, see figure). An unknown beryllium species serves as the antigen which binds to a human leukocyte antigen (HLA) molecule on an APC's surface. The beryllium antigen is then presented to a T cell – a white blood cell with a key role in immune response. Research over the past six years at Los Alamos has resulted in a more complete picture of beryllium's speciation under biological conditions, including its interactions with proteins and the subsequent immunological consequences.

Through the study of several biologically relevant small molecule complexes of beryllium, it was discovered that beryllium has a high propensity to displace hydrogen atoms in strong hydrogen bonds. These bonds, often formed between amino acids containing carboxylate



A beryllium antigen (centre) binds to an HLA molecule on an antigen presenting cell and is presented to a T cell to trigger an immune response

and alcohol groups, help provide the framework supporting protein structure and function. Extending this model to real biological systems, it was shown that beryllium displaced all 12 strong hydrogen bond atoms in transferrin, an iron transport protein found in blood plasma. This presents a potential pathway for beryllium to enter cells with transferrin receptors. These binding studies represent a new paradigm for beryllium binding in biological systems.

Related to its propensity to displace hydrogen bond atoms, beryllium is known to form polymetallic clusters with carboxylate groups. So it has been predicted that beryllium will also form clusters in proteins with many adjacent carboxylate residues. A striking discovery was that the HLA molecules of CBD patients contain a larger number of carboxylate residues than the HLA molecules of people without CBD. And ^9Be NMR binding studies point to a carboxylate bridged cluster of beryllium atoms as an integral structural feature of the antigen (see figure).

Microarray studies have led to other insights into the mechanisms governing beryllium immune response. Cell adhesion genes

and chemokines (small proteins that mediate cell migration) are upregulated in cells treated with beryllium. This suggests a mechanism involving chemokine gradients to attract immune cells to sites of inflammation. Additionally, immune cells treated with beryllium show altered intracellular signalling and cytokine release in response to lipopolysaccharide – a toxin found in bacterial outer cell membranes. This suggests that prior exposure to beryllium may alter the host immune response to subsequent bacterial infections. The implication that cell adhesion molecules and chemokines are linked to CBD potentially opens the door to using molecules that downregulate these immune molecules to inhibit progression of disease symptoms.

A multidisciplinary, molecular based approach to studying CBD has identified relevant beryllium species, their interactions with proteins and the potential roles they play in disease. This may not only lead to potential cures and therapeutics for CBD, but also lend insight into mechanisms of other metal and autoimmune diseases.

Read more in the feature article 'The bioinorganic chemistry and associated immunology of chronic beryllium disease' in ChemComm.

Reference
B L Scott *et al.* *Chem. Commun.*, 2008, 2837 (DOI: 10.1039/b718746g)

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Footnote:
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With the conference season in full swing, RSC Publishing staff are spread around the globe at a number of major conferences over the coming weeks.

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In September, the focus is Turin, Italy, for the 2nd Annual EuCheMS meeting. The wide-ranging themes provide scope for showcasing RSC products – including the recently announced *Metallics* and *Integrative Biology*, both launching January 2009.

If you're travelling to these or other conferences, look out for RSC Publishing staff – they will be happy to meet you.

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