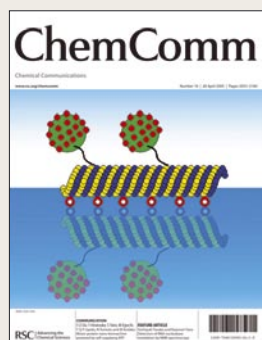


Chemical Science

Crystals changing colour



A rare example of photochromism in the solid state has been discovered by chemists at the University of Victoria, Canada and the University of Washington, US. The team, led by Natia Frank, synthesised a new spirooxazine and found that single crystals undergo a colour change on exposure to UV light that is photochemically reversible and thermally irreversible. The stability of the light-generated form, which is unusual for these compounds, opens up a new class of materials with potential for optical data storage applications.

D G Patel *et al*
Chem. Commun., 2005 (DOI: 10.1039/b417026a)

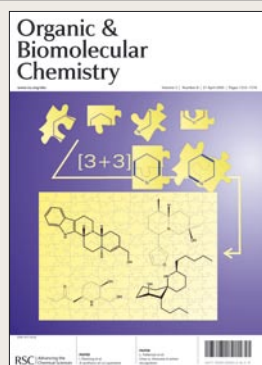
Controlling biominerals



Polymer ligands have been used as models of the amino acids that naturally control the growth of CaCO_3 . Led by Norikazu Ueyama, researchers from Osaka University and the National Institute of AIST Kansai, Japan, have synthesised novel poly(carboxylate) ligands with an amide group neighbouring the carboxylate. They discovered the hydrogen bond between the amide NH and the carboxylate oxyanion plays a key role in controlling morphology during the biomineralization process. The group now hopes to clarify the biomineralization mechanism.

K Takahashi *et al*
J. Mater. Chem., 2005 (DOI:10.1039/b415692g)

Sparteine revisited



One of the challenges facing chemists developing synthetic routes to natural products is stereocontrol. Ian Fleming at the University of Cambridge, UK, and colleagues in Korea have devised an elegant synthesis of racemic sparteine. The key step in their approach is the diastereoselective protonation of a meso dienolate intermediate which sets up the stereochemistry of the target molecule. Few methods exist for preparing enantiomeric sparteine however this strategy shows great promise for achieving this in the future.

T Buttler *et al*
Org. Biomol. Chem., 2005, **3**, 1557

What UV does to ozone



Arthur Suits from Wayne State University in Detroit, US, and colleagues (from the US, Canada and Russia) have studied the break-up of ozone by UV light. Different pathways are possible, leading to the same product. Monitoring these pathways has allowed the electronic states of ozone and its break-up to be better understood. The method could be used to study quantum properties in other molecular systems. Consequently, it contributes to ongoing efforts to control molecular events actively and to build quantum computers.

S K Lee *et al*
Phys. Chem. Chem. Phys., 2005, **7**, 1650

Research highlights

Gas-phase spectroscopy on large molecules confirms their structure

Big proteins analysed

The first infrared (IR) spectroscopic investigation of a 'seriously large' gas phase protein has been completed.

IR spectroscopic studies on proteins have traditionally been carried out on solutions. Scientists have long wanted to carry out similar investigations in the gas phase because this gives fundamental information about the protein without the solvent causing any environmental effects. In the gas phase it is also easy to resolve and isolate different charged states of a molecule – something that can't be done in solution and which therefore offers entirely new and unique information about a protein.

Previously direct IR absorption of gas-phase ions has not been feasible, due to the limited number of ions (typically 10⁶) that can be conveniently prepared, purified, and trapped for optical interrogation.

Gert von Helden from the Max Planck Gesellschaft Berlin, Germany, and colleagues from the US and the Netherlands have now overcome this problem by means of multiphoton dissociation using the

free-electron laser facility FELIX at the Foundation for Fundamental Research on Matter Institute, in Rijnhuizen, the Netherlands.

Von Helden and his colleagues have obtained the first mid-IR action spectrum of a gas-phase protein (cytochrome c), and have found that it shows the same features of amide I and amide II as the solution spectrum. This provides the most direct evidence to date of the inherent stability of protein structure in the absence of any solvent water molecules.

Excited by the implications of the work, Alan Marshall, part of the team from the National High Magnetic Field Laboratory in

Measurements on gas phase proteins show their inherent stability

Reference
J Oomens *et al.*, *Phys. Chem. Chem. Phys.*, 2005, **7**, 1345

Florida, US, comments: 'It will now be possible to determine not only intrinsic structures of peptides and proteins (zwitterions, salt bridges, effect of charge state on conformation), but also to probe the nature of binding of metal ions and drugs, as well as protein: protein complexes'. John Simons, an expert on gas phase biomolecules from Oxford University, UK, agrees with the significance of the work, commenting 'the authors should be congratulated on a considerable experimental achievement'.

Experimentalists are now waiting for theorists to catch up before the spectra of other big molecular ions can be interpreted.

More calculations about molecular oscillations are needed, and as von Helden says, 'such calculations are currently difficult for molecules with more than about 100 atoms because of the non-linear scaling of the computational costs with system size. Thus, access to experimental IR spectra of large molecules will necessarily drive the improvement of the molecular modelling algorithms'.

Philip Earis

Insulin proteins pass on their structural information and add to amyloid research

Hormone history mirrors prion morphology

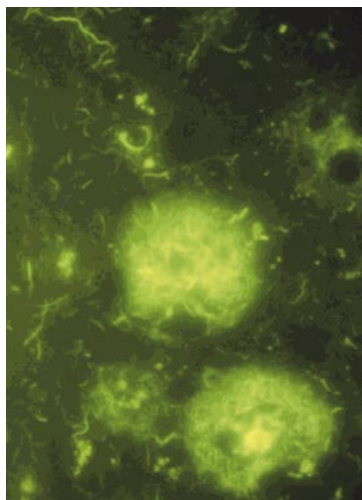
Structural studies of insulin shed light on the prion strain phenomenon and suggest a new approach to biomaterial synthesis.

The insulin protein forms in water as one type of amyloid fibril (type A), but Wojciech Dzwolak at the Polish Academy of Sciences, Sokolowska, and colleagues found that it adopts a more 'curvy' stacked form (type B) when formed in the presence of ethanol.

Dzwolak's team found that insulin types A and B behave rather like prions. When type B is added to an insulin solution in pure water, the type B proteins act as a template for the formation of further type B proteins.

Amyloid plaques in the brain are associated with neurodegenerative disease

Reference
W Dzwolak *et al.*, *Phys. Chem. Chem. Phys.*, 2005, **7**, 1349



'It is only the template that matters,' Dzwolak said, 'not the presence of ethanol, which favours type B, or its absence, which favours type A.' The type of insulin formed is controlled by the history of the template.

The findings have medical and technical implications. Amyloid deposits in the brain characterise a range of poorly understood neuropathologies, from Alzheimer's to prion diseases. On the technological front, fibril morphology could be controlled for the synthesis of biomaterials on the basis of 'solvational history,' suggests Dzwolak.

Bea Perks

A common weed could help decontaminate water in the developing world

Getting to the root of the arsenic problem

A voracious weed could save the lives of people living in areas with arsenic contaminated water, according to UK researchers.

Using dried roots of the water hyacinth, often labelled an 'environmental plague' in the tropical and subtropical world, Parvez Haris and colleagues at DeMontfort University quickly reduced arsenic levels in contaminated water to below the World Health Organization's guideline value of less than 0.01mg/L.

This simple, effective and cheap solution has potential implications in the developing world, where serious contamination of drinking water by natural arsenic in surrounding rocks is threatening the lives of millions. Long term health consequences of arsenic exposure are severe and include skin cancer, nervous system damage and miscarriage.

During a trip to Bangladesh, one of the most seriously affected areas, Haris witnessed firsthand the suffering of victims of arsenic poisoning. In Bangladesh he saw the

Water hyacinth thrives in contaminated areas and might offer a solution to arsenic problems

water hyacinth thriving on many water surfaces in the area. 'That was my "eureka" moment,' said Haris, explaining what inspired his research.

'Upon returning to the UK, I immediately started working on this plant with my graduate student. To our amazement a powder produced from the root of this plant was able to remove arsenic from water in minutes,' he said, adding, 'it is particularly pleasing to convert a much hated weed to something that can potentially save human lives.'

Turning concept into reality requires field trials. Ultimately Haris hopes to see water hyacinth roots being used in filtration systems to remove arsenic from drinking and irrigation water.

Kathryn Lees

Reference

S W Al Rmalli *et al*, *J. Environ. Monit.*, 2005, 7, 279

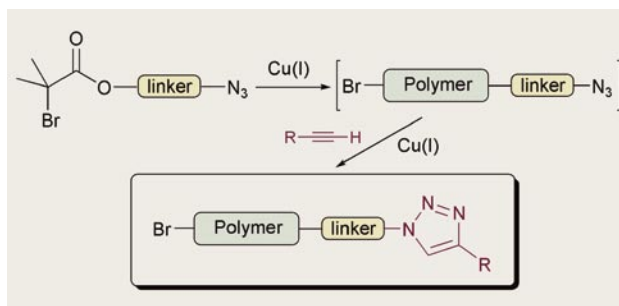
Combining controlled polymerisation and 'click' chemistry

Simple but smart polymers

Convenient and efficient ways to make new macromolecular structures are now possible thanks to an innovative synthesis of a new functional polymer by UK researchers.

Using living radical polymerisation (LRP) to make a linear chain, David Haddleton and colleagues at the University of Warwick, made poly(methyl methacrylate) with an azide group at one end of the polymer chain.

A copper(I) catalyst is used to make the azide end of Haddleton's polymer react with a molecule containing an alkyne group. This forms a five-membered triazole group. The reaction, known as cycloaddition, is an appealing aspect of the synthesis. It is a 'click' reaction: a synthetically easy and efficient transformation with characteristics such as high yields and good selectivity in mild



conditions. Efficient reactions are essential at this stage of the synthesis to ensure the chain ends are successfully modified.

Haddleton's synthesis design has other attractive features. The polymerisation step and the successive reaction to modify the chain ends are catalysed by the same reagent and can be done in the same reactor. This 'one-pot' approach, possible only because

Polymerisation in one pot will make macromolecules easier to synthesise

the chemistry is compatible, means there is no need to isolate chemical intermediates.

LRP is renowned for its ability to control the molecular architecture of a polymer. For example, when LRP is used a functional group can be located exclusively at one end of the polymer chain.

The catalysed reactions combine effectively because they are robust and can tolerate many functional groups, including water. The researchers show the method's versatility by attaching dye molecules to one end of the polymer chain.

In future, this one-pot approach could be used 'to conjugate a range of polymers to proteins, enzymes and surfaces,' said Haddleton.

Alison Stoddart

Reference

G Mantovani *et al*, *Chem. Commun.*, 2005, 2089

Teaching molecular magicians new tricks

arginine can cross these membranes easily. This is one of several phenomena known collectively as 'arginine magic'.

Stefan Matile and co-workers at the University of Geneva have shown that these peptides form complexes with anions to help them cross the membranes. Changing the anions' structure then allowed Matile's group to shed light on the mechanism of arginine's 'magic trick'.

They found the movement of such peptides across bilayer membranes is possible because of repeated complexation/decomplexation of the anions. The resulting changes in solubility of the complexes allow them to adapt to different environments within the membranes.

Membrane-penetrating peptides could be used as cellular targets, and some anions could be potential biochemical probes, says Matile. *David Barden*

Reference

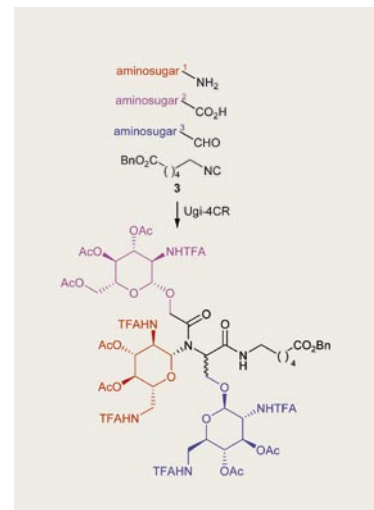
M Nishihara *et al.*, *Org. Biomol. Chem.*, 2005 (DOI: 10.1039/b501472g)

Arginine-rich peptides use anions to cross membranes in biological systems, say Swiss researchers.

Bilayer membranes, which separate aqueous compartments in living organisms, are generally seen as impermeable barriers. But peptides rich in the amino acid

Membrane crossing is easier thanks to a bit of magic from the amino acid arginine

Complex mimetics, simply done



A method to synthesise diverse libraries of carbohydrate clusters quickly and simply has been developed.

Carbohydrate clusters have the potential to lead to new antibiotics and these libraries could be screened for drug leads or developed further to give specific drug targets.

The method combines four compounds in a one-pot process known as the Ugi multicomponent reaction. By using a variety of carbohydrate-containing starting materials, a diverse range of products can be made. The sugar units also have amine groups attached that can interact with bacterial RNA.

The work, by Bernhard Westermann and Simon Dörner from the Leibniz Institute for Plant Biochemistry, Halle, Germany, extends a known reaction to a new application. Any antibiotics developed using carbohydrate clusters would likely develop fewer resistance problems and be less toxic than simple carbohydrates. Using several binding sites on one molecule also gives improved performance, say the researchers. *Vikki Allen*

Reference

B Westermann and S Dörner, *Chem. Commun.*, 2005, 2116

Cancer killing catalysts

Nanophotocatalysts are killing cancer and viruses by producing destructive oxygen species.

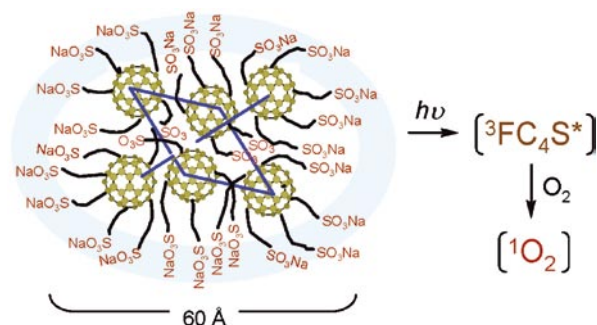
A system where photostable hexa(sulfo-*n*-butyl)[60]fullerene (FC₄S) nanospheres convert light energy into either 'hot' electrons or triplet energy was developed by Long Chiang from the University of Massachusetts, US, and colleagues from the University of Toronto, Canada, and Tohoku University, Japan. These electron or energy forms then pass to molecular oxygen and form a superoxide radical or singlet oxygen, respectively.

Under photodynamic therapy (PDT) treatment, production of these reactive oxygen species can destroy tumour and cancer cells such as fibrosarcoma tumour cells. The fullerene C₆₀ molecule is a good choice for PDT treatment because it generates triplet energy quantitatively. The C₆₀ was tuned for biological applications by

adding micelles to make it less hydrophobic.

FC₄S compares favourably with other PDT drugs and has the added advantage of being photostable. This means a single dose might be possible for multiple treatments.

Following the success of this research, Chiang hopes the principle will be applied elsewhere, for example in cosmesis or other environmental applications such as antibacterial spray and water treatment. *Elinor Richards*



Reference

C. Yu *et al.*, *J. Mater. Chem.*, 2005 (DOI: 10.1039/b500369e)

Reactive oxygen can destroy cancer cells if used in photodynamic therapy

Human genome sequence helps target cancer

The human genome is being used to produce a new generation of drugs that target the genetic changes responsible for individual cancers.

Information from the sequencing of the human genome has already provided elegant new drugs, says Paul Workman, director of the Cancer Research UK Centre for Cancer Therapeutics.

Imatinib, a drug used in cases of chronic myeloid leukaemia and gastrointestinal stromal tumours, is one example. Drugs like this target specific mutations in cancer cells and significantly reduce the toxicity

Drugs have been created using the human genome

associated with more traditional, less selective treatments.

Treatments linked directly to cancer genomics also hold the promise of personalised drugs to match the molecular make-up of individual patient's tumours. There are challenges associated with this genetic approach, not least the development of drug resistance. Workman believes that these challenges will be overcome within the next 10 years. *Chris Incles*

Reference

P Workman, *Mol. BioSyst.*, 2005 (DOI: 10.1039/b501751n)

Metals cause fast breakdown of pesticides

Processes for decomposing pesticides and chemical warfare agents are being unravelled by Canadian scientists.

Phosphate triesters and phosphorothioate esters are close relatives of pesticides and chemical warfare agents. Stan Brown and his team at Queen's University have looked at how two metal-ion containing systems catalyse their methanolysis reactions.

During methanolysis a methoxide group coordinated to either La^{3+} or Zn^{2+} displaces part of the phosphorus-containing molecules making them break down. These reactions are fast and in alcohol

Reference

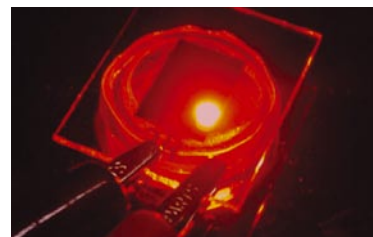
T Liu *et al.*, *Org. Biomol. Chem.*, 2005, **3**, 1525

solvents the metals promote phosphate triester decomposition by up to a billion-fold.

This research sheds light on an unusual class of metalloenzymes, the phosphotriesterases, and how they catalyse the breakdown of pesticides like paraoxon, an organophosphate cholinesterase inhibitor.

Providing 'practical and simple ways of applying catalytic alcoholysis reactions to decontaminate pesticide laden sites and objects contaminated by chemical warfare agents,' is the ultimate goal of this work, said Brown. *Kathryn Sear*

Bright future for OLEDs



An iridium complex has been developed as a red-light emitting material for use in organic light emitting diodes (OLED).

Shinjiro Okada and co-workers from the Canon Company in Atsugi, Japan, fine-tuned substituents of the ligand 1-phenylisoquinoline to optimise their design for a red phosphorescent iridium complex.

Research over the last 15 years has focused on OLED displays as replacements for liquid crystal displays (LCDs) in the flat panel industry, covering everything from watches to flat-screen TVs. They are especially suited for mobile devices like phones and digital cameras.

Advantages of OLEDs include low power usage, a wide viewing angle and small size. OLEDs emit their own light and give brighter, sharper images than LCDs.

Okada thinks future work will be aimed at blue phosphorescent materials. *Helen Lunn*

Reference

S Okada *et al.*, *Dalton Trans.*, 2005 (DOI: 10.1039/b417058j)

Solvent guess work taken out of gel design

A simple chemical alteration can make a molecule that normally forms gels in organic solvents switch to making gels in water.

Jan van Esch and colleagues in Groningen, the Netherlands, have demonstrated that simple chemical modification of cyclohexane *bis*-urea compounds transforms them from being organogelators (low molecular weight compounds (LMWs) that cause gelation in organic solvents) into hydrogelators (molecules that bring about gelation of water and water-based solutions).

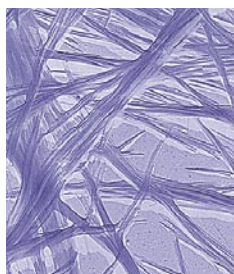
Hydrogen-bonding between the urea parts of the compound means these LMWs can self-aggregate

well in all solutions. But to form gels, the LMWs must also have a strong enough interaction with the surrounding solvent. For water-based solutions van Esch's team found the right solvent compatibility level for the LMWs by adding peripheral groups with the right hydrophilic/hydrophobic balance for gelation to occur.

This logical and elegant approach to hydrogelator design is in direct contrast to the serendipitous way in which most other hydrogels have been discovered, and has added to the understanding of their structure-property relationships. *Sue Askey*

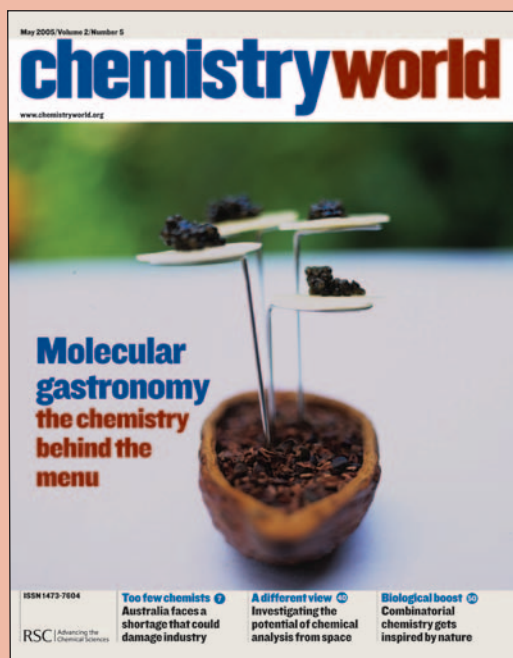
Reference

M de Loos *et al.*, *Org. Biomol. Chem.*, 2005 (DOI: 10.1039/b500837a)



Chemical changes aid gel formation

chemistryworld



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A “must-read” guide to current chemical science!

Chemistry World provides an international perspective on the chemical and related sciences by publishing scientific articles of general interest. It keeps readers up-to-date on economic, political and social factors and their effect on the scientific community.

Featuring:

- Chef Heston Blumenthal devises some unusual dishes based on sound chemical principles
- Global cooperation develops opportunities in chemical analysis from space
- Nanoemulsions deliver molecules through biological membranes to tackle major infectious diseases
- Nature provides the inspiration for recent modifications to classical combinatorial chemistry
- Whatman restructures its business and is now on the acquisition trail

This month in Chemistry World

Agricultural angst

It's all happening down on the farm this month. A UN report evaluating major global ecosystems blames much eco-disarray on increasingly intense agriculture. Separate studies in the US suggest that human health near farmland is at risk from pesticide drift, particularly in California where a third of the nation's pesticides are sprayed. And GM isn't about to solve the problem. The

GM debate, well reported and recently added to in the UK, has entered the US with the admission that biotech giant Syngenta had been distributing an unapproved GM crop for four years. Chemists could help, but are there enough of them? Australia is seeing a marked decrease in numbers of students opting to take up chemistry. Join the club, as some UK chemists might say.

A nose for novel antibiotics

Bad news for noses: researchers are developing a nose replacement using carbon nanotubes, and another team has combined lab analysis and stats to replace a connoisseur's nose when aging sherry. But there's still plenty for real-life noses to do, and plenty we might rather they didn't. A sneeze is the most effective way to transmit

flu, an infection that continues to vex researchers. Antibiotics won't help but they might not even help a bacterial infection if antibacterial resistance isn't overcome. Headline hitting superbugs even became an electoral issue in the UK. Perhaps a novel antibacterial polymer developed in the US holds some of the answers.

Chemists in space

Environmental monitoring from space shows conclusively which countries are polluting most, and with what. Envisat, the European Space Agency's satellite, is providing some startling data about nitrogen dioxide emissions, amongst other things, globally. This is expensive science, but a cost worth bearing to stop us destroying our planet? Another cost some might say is worth bearing is for the food at Heston

Blumenthal's restaurant, the Fat Duck. His gastronomic creations don't come cheap, but any scientist who knows his onions should take a visit to see how vacuum desiccators can come in useful in the kitchen. Nanotechnology destined for cosmetics in the form of nanoemulsions have found a vanity-free application – their antimicrobial properties can be used to kill potential biological weapons, like anthrax.

Getting funny looks

Any readers who have ever attempted to see the hidden 3-D images in Magic Eye stereograms will no doubt remember the frustration of trying to cross and uncross their eyes and the elation when a lesser-spotted rhinoceros leaps out of the page all of a sudden. It's now time to warm up the eye muscles again and take part in Haidinger's brush experiment.

There are two methods to see this phenomenon, those traditionalists will be easily identified from the black-bottomed bucket they will be carrying, while those who prefer to move with the times might start getting some strange glances from work colleagues wondering why a flat screen monitor demands such close scrutiny.

Essential elements

We have lift off!

The countdown is over and the first print issue of *Molecular BioSystems*, a chemical biology journal with a particular focus at the interface between chemistry and the -omic sciences and systems biology, launches this month. Everyone involved, from editorial and production staff, through marketing and sales teams, to authors, referees and readers, are waiting for feedback from the scientific community.

The content of the new journal speaks for itself: a Highlight from Paul Workman at the UK's Institute of Cancer Research looks at the role of genomics in cancer drug development, while the first Review covers novel gene discovery systems. The first



Opinion looks at why systems biology is called systems biology, and the first Method reports on the use of electrophoretic and

mass spectrometric strategies for profiling lipopolysaccharides. Communications and full papers complete the range of high quality material from international authors in this impressive first issue.

In a recent Editorial¹ Thomas Kodadek and Caroline Evans (*Molecular BioSystems*' Editorial Board chair and editor respectively) described the new journal as 'a forum for the publication of novel work at the interface between chemistry and biology'.

● Read the first issue and judge for yourself at www.molecularbiosystems.org

¹ *Chem. Commun.*, 2005, 2067

And finally.....



Physical Chemistry Chemical Physics (PCCP) has been selected by the National Library of Medicine to be indexed and included in *Index Medicus*/MEDLINE - the world's most comprehensive source of life sciences and biomedical bibliographic information. Coverage will begin from 2005 and represents a significant milestone for the journal, recognising the quality of biophysical research published within it.

A number of RSC Journals are now indexed in MEDLINE and all chemical biology content is showcased free of charge in the *Chemistry Biology Virtual Journal*.

● To find out more, visit: www.rsc.org/pccp or www.rsc.org/chembiol



As clear as crystal

'Dealing with nearly 1300 manuscripts and 3000 cif files a year means my day is never dull!' says Kirsty Anderson, crystallographic data editor at the Royal Society of Chemistry.

Kirsty joined the RSC in 2001 after obtaining her PhD in Chemical Crystallography from Bristol University. She is responsible for the assessment of crystallography in all papers submitted to the RSC's primary research journals - a unique role in the publishing industry.

'It is important to recognise that we publish chemistry journals rather than purely crystallographic journals' says Kirsty. 'I read every paper I assess thoroughly and although



I am obviously keen to maintain high crystallographic standards, I am initially interested in whether the science in the paper is backed up by the diffraction

data as well as the technicalities of the structure itself.'

Kirsty is also closely involved with the RSC's electronic-only journal *CrystEngComm* and has been instrumental in the creation of *CrystEngCommunity*, a web resource for all scientists interested in crystal engineering and supramolecular chemistry. Future challenges include the further development of *CrystEngCommunity* as well as designing a new crystallographic web resource to aid authors with their submissions.

● If you have any comments or queries about crystallography or *CrystEngCommunity*, contact Kirsty at crystals@rsc.org

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