

The chemistry of metal clusters
Nanoparticles in novel catalysts

Investigating biosynthesis pathways
The importance of sustainability

The Chemical Industries Association's new chief executive, Steve Elliott, talks to Sarah Houlton about some of the challenges that are currently facing the chemical industry

The impending European chemicals legislation, Reach (Registration, Evaluation and Authorisation of Chemicals) has been a real cause for concern in the chemicals industry, and is likely to come into force early next year. What concerns remain?

There are currently two opposing positions – that of the Council of Ministers, which is, by and large, a position we support, and the European Parliament's environment committee's position which is rather different. The environment committee's view is extreme, and is a top-down approach that takes us down a route that potentially will see companies withdrawing products from the marketplace without there being an alternative available to use instead.

The environment committee's view also raises significant questions about how Reach will be enforced in that companies are not exactly going to rush to withdraw substances from the market if the alternative is made by a competitor! On the other hand, the Council of Ministers' position should be seen as a more pragmatic bottom-up approach that reflects the way that supply chains in commercial markets work. It says that if you can convince the authorities that you can adequately control a substance for a particular use, then you should be able to manufacture it for that use.

Something will have to give if sufficient MEPs are to be persuaded to vote for a bill that would be workable in practice and deliver the right environmental outcome, while also supporting competitiveness. The issue that's really grabbing the headlines is the 'A' in Reach, authorisation. Part of this calls for the substitution of chemicals that are deemed too 'risky' or environmentally unsound, but there is a danger that will result in important chemicals – and products that require them – vanishing from the market, leaving neither the environment or the economy any better off.

Publicly, there remains much work to do to convince people that companies aren't just sitting back and deliberately selling products that are environmentally unsound. But equally, we should recognise that there is a significant body of influential opinion that is telling us that you can't argue against Reach purely on the basis of how many jobs might get lost or how less competitive we become. We have to make an argument that demonstrates that we think the route the Council of Ministers is taking is the one that not only enhances jobs in companies but also makes a better environmental outcome more likely.

Are you optimistic there will be a workable agreement?

I have to be optimistic that there will be! I think if there isn't it will be extremely difficult, and if the whole thing is thrown out by the Parliament you can imagine the headlines - it won't be the parliament's fault, it will be industry's. We want a workable solution, and then we all need to get on and make sure we can implement it sensibly.

The industry's reputation has taken a few knocks in recent months. How can the industry address this?

There is no easy answer, unfortunately. Even when Reach is finally implemented, it will only address individual substances and it will not give us easy answers to the combinatorial effect of such 'cocktails'. I'm sure the likes of WWF, Friends of the Earth and Greenpeace recognise that, and are continually looking to move the agenda and the challenge on.

The most graphic example of this is biomonitoring. WWF, for example, has sampled the blood of MEPs, and also a group of three 11-year-old children for a television programme. While this sort of thing is a helpful contribution to the debate, I think the way the programme was presented was misleading because it tried to attribute cause and effect with very little evidence. It was, I believe, irresponsible.



Steve Elliott

CV

Born: Macclesfield

Career: He's been with the CIA since 1997, working in a variety of roles in trade, sustainable development and business environment before being appointed chief executive in 2006. Prior to this, he worked at the DTI, a South African trade advisory body, Crown Agents and Price Waterhouse.

Status: His wife Lorraine is a personnel manager, and they have two sons who, Steve says, support the wrong football team. Seven-year-old William supports Chelsea, but he says Archie, 5, doesn't know his own mind, and (as a Manchester City supporter himself) he can't bring himself to say who he supports!

Interests: As well as having a season ticket at Manchester City, Steve referees and coaches under-7s football, and enjoys both music and films.

Did you know: His brother Mike works as an assistant director in the movie industry. He recently worked on one of the worst films ever – the remake of Swept Away made by Guy Ritchie and starring his wife, Madonna. He got to carry Madonna out of the sea after a scene; apparently she was a real trouper, but her hubby wasn't! He's currently in India working with Brad Pitt and Angelina Jolie (on a film, not an adoption case!)

However, it is a good thing from our point of view that there are a number of these biomonitoring initiatives taking place in the US and, increasingly, in Europe. As an industry, through the projects such as the Long-Range Research Initiative, we are trying to join up the advocacy dots and look at providing a proper scientific contribution to the debate. What the examples in programmes like this are never able to demonstrate is when a particular chemical entered the person and, most importantly, what effect – if any – it will ultimately have on their health. While we're not saying that there is no validity in this kind of study, what we are saying is that we must not jump to conclusions such as those that have been seen in the press recently about millions of children being damaged by chemicals. It needs to be taken in perspective.

While industry, government, pressure groups and others working together to try and resolve the issue doesn't exactly make headlines, it is important that we do work together to try and understand the effect that substance A in combination with substance B might have on an individual, depending on their own personal circumstances, lifestyle, place of work and so on. This will all carry on long after we have received a political agreement on Reach.

What else can companies do?

We face a collective problem in terms of boosting the industry's reputation. We have tried in the past to get a number of publicity and promotional campaigns of the ground, but companies collectively have been a little reluctant to step up and fund a significant public campaign, perhaps because they feel that even if they do their bit, a major incident at another company will drag everyone down.

Day after day there are negative views of the industry in the media, and there is rarely any formal response, particularly not from industry leaders. If we are really going to tackle the industry's reputation we can't just dip in and out of the debate – we have to demonstrate that there is some substance behind our position. We have to be much savvier and improve our communications skills so that our message resonates with the public.

We need to continue building relationships with pressure groups as well as government and its agencies. Yes, that will cost money, but in the long run it's money we really can't afford not to spend. There is already some good work going on internationally and, encouragingly, much of this is being done by the companies themselves, not just trade associations. They are recognising that there is business value in it. In 2007 we're increasingly going to find that the 'what are chemicals doing to my children' debate is high on the agenda, so it's important that we don't take our eye off the ball. CIA is determined to play its part in addressing that challenge, including taking people and organisations to task when we believe the 'facts' to be misleading or irresponsible.



Formidable humility

Dear Editor

The article 'Remembering Lord Todd' (*Chem@Cam*, Summer 2006) reminded me of an incident almost 50 years ago, in 1957/58, when Sir Alexander Todd, as he was then, was lecturing to our Part II Chemistry class.

Alexander Todd was a formidable character, but that did not stop one student in the centre of the front row shouting out that Todd had made a mistake. Todd turned, glared and, pointing at the student, said in his Scottish brogue, 'Make sure of your facts, lad-

die!' There was a noticeable gasp from the assembled students, and Todd continued with his lecture.

Two days later at the next lecture, Todd entered the lecture theatre, faced the 80 or so students and said, 'I have an apology to make. You were quite right, laddie!'

Immediately all 80 students applauded and cheered. I remember that lesson in humility although I have long forgotten most of the chemistry.

Yours sincerely, Tony Kallend
Westerham, Kent

Chemistry in a hut

Dear Editor,

I enjoyed reading Dennis Marrian's memories of Lord Todd (*Chem@Cam* Summer 2006) and found my appetite whetted for more in similar vein.

It will be 50 years this autumn since I went up to read Nat Sciences, rather a struggle at first after two years in her Majesty's service, but improving and culminating in an engrossing final year with Part II in organic.

Todd, Emeleus and Norrish were the presiding divinities, and Maurice Sugden my director of studies.

In 1958 we moved over to the then new labs in Lensfield Road – it was very interesting to see the picture on page 5 of Lab 287 which looks identical to our practical organic lab of 48 years ago.

After graduating, I and a friend, Roger Duffett (whose name appears regularly among your puzzle winners) worked very briefly in the Nissen hut in the Cavendish.

Sadly the hut was no longer there the last time I visited Cambridge. I was at the bottom of that small group led by

Perutz and working for a lady who worked in John Kendrew's section.

I recall analysing x-ray pics of myoglobin and feeding the data into the original EDSAC computer, climbing a steel ladder to enter a wire cage which contained the input feeder for the punched tape.

The model of the double helix stood in the 'foyer' of the Nissen hut, looking rather nondescript and yet to achieve the iconic status which it now enjoys.

I soon moved on to work for what was then the smallest of the oil majors, and a year or two later I was pleasantly surprised to find that Lord Todd reappeared at our monthly research meetings, where he was a revered consultant and a good listener.

Perhaps there are among your readers chemists who worked in the Nissen hut and who knew Max Perutz and his co-workers well, and would be willing to share their stories of the events and characters of those legendary early years.

Sincerely, Roger Mowll
r.mowll@btinternet.com

Happy 'grandchildren'

Dear Editor

Thanks for the Summer edition of *Chem@Cam*, entertaining as ever.

I'm writing about the happy couple on page 18 celebrating their wedding. Both did their PhDs with Steve Loeb at Windsor, Ontario.

Since Steve did his PhD with me, they are my academic grandchildren. Please convey my best wishes.

Keep up the good work.

Cordially, Chris Willis
London, Ontario

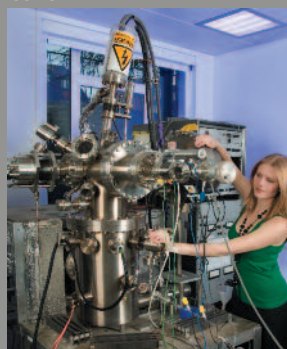
chem@cam

Chemistry at Cambridge Newsletter

Contents

News	4
Research	7
Alumni	13
Chat lines	15
Puzzle corner	19

Cover



Amy Stevens, a PhD student in Richard Lambert's group, using an ultra-high vacuum chamber with mass spec and XPS capabilities

Photograph:
Nathan Pitt and Caroline Hancox

This newsletter is published three times a year by the University of Cambridge Chemistry Department. Opinions are not necessarily those of the editor, the department, or the university.

Editor-in-Chief: Steve Ley
Editor: Sarah Houlton
Photographers:
John Holman, Nathan Pitt,
Caroline Hancox
Editorial Board:
Brian Crysell, Jonathan Goodman,
Rosemary Ley, Jeremy Sanders

Address:
Chem@Cam, Department of Chemistry
, University of Cambridge, Lensfield
Road
Cambridge CB2 1EW
Phone: 01223 763865
e-mail: news@ch.cam.ac.uk
website: www.ch.cam.ac.uk

This publication is supported by
Cambridge University Press

CA Scheme buys ChemDraw

Thanks to the generosity of the Corporate Associates Scheme, the university now has a three-year site-wide licence for ChemDraw Ultra 10 for Macintosh and ChemOffice Ultra 10 for Windows.

Thanks must also go to CambridgeSoft, which produces the package, for giving us a significant discount. They have now also joined the Corporate Associates Scheme.

It is available to anyone within the university who has an @cam.ac.uk email address. Go to <http://tinyurl.com/t4cm5> and follow the instructions.

The next generation

Three recently-appointed university lecturer have been made Next Generation Fellows. The scheme is designed to give young academics a sound financial footing to kick off their independent research careers.

Oren Scherman is the Walters-Kundert NGF, Matthew Gaunt the Philip and Patricia Brown NGF and David Spring the Newman (Frances and Augustus) Foundation NGF. Oren works in the Melville Lab, and Matthew and David are both

in the organic sector.

The department and the new NGFs are all extremely grateful to the generous donors who have given them such a great start to their formal academic careers.

■ Jonathan Burton is leaving us in January to take up a lectureship in Oxford.

His huge contribution to the department will be greatly missed, but this is a great opportunity for both him and Oxford, and we wish him all the best for his future career.

A collection of prizewinners

Various members of the department have received prizes and other honours in the past few months.

Teaching fellow Bill Nolan was one of the recipients of this year's Pilkington Prizes for Teaching. Set up by the late Sir Alastair Pilkington, former chairman of the Cambridge Foundation, the prizes are supported by Cambridge University Press and are awarded annually to recognise excellence in teaching.

Bill received the prize for his substantial contribution towards the development of organic and inorganic chemistry practical classes, and also for being a driving force behind the refurbishment of the teaching labs.

Dave King has been awarded the Jawaharlal Nehru Birth Centenary Medal by the Indian National Science Academy. This is the academy's most prestigious international award, and Dave has been recognised for his contributions to international cooperation and public understanding in science and technology.

Royal Davies has been awarded the Royal Society of Chemistry's 2006 award for optical spectroscopy.

And Alan Fersht has been made PhD honoris causa at the Hebrew University in Jerusalem, and honorary professor of the university of Sichuan.

Rewarding talks

Photos: Nathan Pitt

Dante Gatteschi...



In October, the department hosted a half-day symposium entitled 'From single molecules to extended lattices' in the Pfizer lecture theatre. The meeting was supported jointly by the Royal Society of Chemistry and the Società Chimica Italiana, and a range of distinguished speakers gave talks including the RSC Tilden Lecture by Matt Rosseinsky of the University of Liverpool, and the RSC-SCI Vigani Lecture by Dante Gatteschi of the Università di Firenze.

Cambridge was a particularly apt venue for the Vigani lecture as the Italian John Vigani spent many years studying in Cambridge, and was made the first professor of chemistry in 1702.

The audience of current academics, researchers and undergraduate students from several departments were treated to a feast of science. An enthralling lecture on the use of polynuclear complexes as novel materials for magneto-cooling by Eric McInnes provided an apt counterpoint to the Vigani lecture by Dante Gatteschi on quantum effects within single molecule magnetic devices.

In the second session, Clare Grey from Stony Brook University in the US addressed the current energy crisis, discussing her studies on solid state NMR

methods to explore structures, properties and efficiencies of novel battery materials. The afternoon session finished with the Matt Rosseinsky's Tilden lecture on the new chemistry of multifunctional oxides and nanoporous materials.

The meeting closed with the presentation of awards by the current RSC President Jim Feast to both the Tilden and Vigani Lecturers.

The day was completed with an evening visit to Queens' College where Vigani taught between 1702 and 1705, and where his original cabinet of materia medica including seeds, snakes, scorpions and pigments is still held.

The speakers were entertained with dinner in the Old Senior Combination Room in Cloister Court at Queens' which dates back to about 1450 and which provided an atmospheric reflection of the college as Vigani would have known it. While some architectural aspects of the college may still appear familiar to Vigani, the transformations of chemistry over the last 300 years would undoubtedly have amazed him. *Jeremy Rawson*

...and Matt Rosseinsky



Below: Steve Ley shows off the Nagoya Medal he recently received at a meeting in Japan. While he was enthralling the audience, his daughter was busy giving birth to his first grandchild back home in Cambridge. Read more on page 15



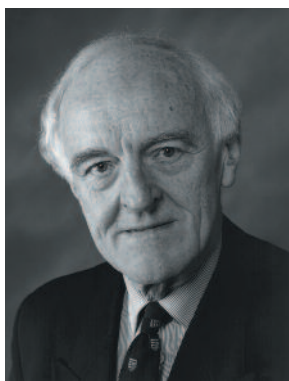
Three new fellows

Congratulations to Ruth Lynden-Bell and Atta Ur-Rahman, who have been made Fellows of the Royal Society. For many years, Ruth was a Fellow at New Hall, and worked in the department. After a time in Belfast as a professor at Queens University, she returned to Cambridge where she has been a very welcome presence in the theoretical sector.

Atta Ur-Rahman is another graduate of this department, having worked with John Harley-Mason. He is now director of the Higher Education Commission Research Institute in Pakistan, and effectively the government's science minister.

One of the new foreign fellows has links to the department, too. Roger Tsien, who was our Todd Professor a couple of years ago, carried out much of his pioneering physiology PhD work here in the 1970s.

ACS prize for David B



David Buckingham: 'surprised and delighted' to receive the Ahmed Zewail award

David Buckingham has been awarded the first Ahmed Zewail prize for molecular sciences. Named after the 1999 chemistry Nobel prize winner and sponsored by publisher Elsevier, it will be awarded by the American Chemical Society every two years for 'significant and creative contributions of a fundamental nature to any of the disciplines of molecular sciences'.

David is to receive the prize of \$20,000 and a gold medal in recognition of his contributions to the understanding of the optical, electric and magnetic properties of molecules. In return, he has to speak at the ACS's meeting in Chicago next March.

'I was already supposed to be speaking at the meeting,

on my recent work on chiral NMR,' David says. 'So I'm now going to have to give two different lectures at the same conference!'

The award came of something of a surprise to him, but he says it's been wonderful hearing from so many old friends who have been in touch to congratulate him.

'I've been officially retired since 1997, and the biggest surprise is that they should think of giving it to someone at the grand old age of 76,' he says. 'The great thing about being "retired" is that I can choose where, when and how I work! I'm still learning new things and the work I've been doing on chirality in NMR has rejuvenated me – as has the new hip I got in August.'

A change at the helm



All change: from Jeremy...

Jeremy Sanders announced earlier this year he wished to step down as head of department in December, almost seven years after he succeeded Dave King in the role.

The next head of department is to be Bill Jones, and he is to take over the reins of responsibility in January.

Jeremy's going to be keeping busy, though – as well as chairing the chemistry panel



...to Bill

for the 2008 Research Assessment Exercise, he is becoming university deputy vice-chancellor and is to be chair of the university's 800th anniversary steering committee, coordinating the university's celebrations of its 800th birthday.

He also says that he hopes to spend more time with both his research group and his family!

The Tardis has landed

Much of the work done in the theoretical sector is extremely hungry in terms of computer power. The latest addition to the department's computing resources is now residing in the basement, and comprises 47 dual dual-core Opteron nodes.

This translates to 47 black boxes in two large, upright cabinets, each of which contains four processor cores. Each node makes up 8Gb of RAM, making a total of 376Gb – compare that to your home PC!

All the boxes are linked together so they can perform MPI, or message pattern interface, jobs. This, essentially, means that all the computers can work on the same problem at the same time. This gives an enormous amount of computing power to apply to the complex molecular dynamics experiments carried out in Stuart Althorpe and Michiel Sprik's groups.

Computer officer Catherine Pitt says the computer was delivered in pieces October, and it took a whole week to build it. 'It even has a remote control power supply, so I can turn it on and off from my office on the third floor!' she says. 'This means I'll only need to go



Catherine peeks through the Tardis

down there if I need to replace a part.'

There is space in the cabinets for further nodes to be added in the future. 'We've called the machine Tardis,' Catherine explains. 'It just looks like a couple of cabinets, but it's absolutely huge inside!'

Winning science writing

Phillip receives his prize at Claridge's. He's pictured with (from the left) Telegraph science editor Roger Highfield, Adam Hart-Davis, New Scientist editor Jeremy Webb, Bayer's Steve Painter and Philip Campbell, the editor of Nature



One of the winners of this year's *Daily Telegraph* Science Writer Awards was Phillip Broadwith, who's doing a PhD with Jonathan Burton.

Phillip wrote about the metathesis reaction which has rapidly become an important industrial process, and won the chemistry Nobel prize for Bob Grubbs, Dick Schrock and Yves Chauvin last year.

'It was an enormous surprise when I got the call from the *Telegraph's* science editor, Roger Highfield, telling me I'd won!' Phillip says. The judges he impressed included David Attenbor-

ough, Bill Bryson, Adam Hart-Davis and Mary Archer.

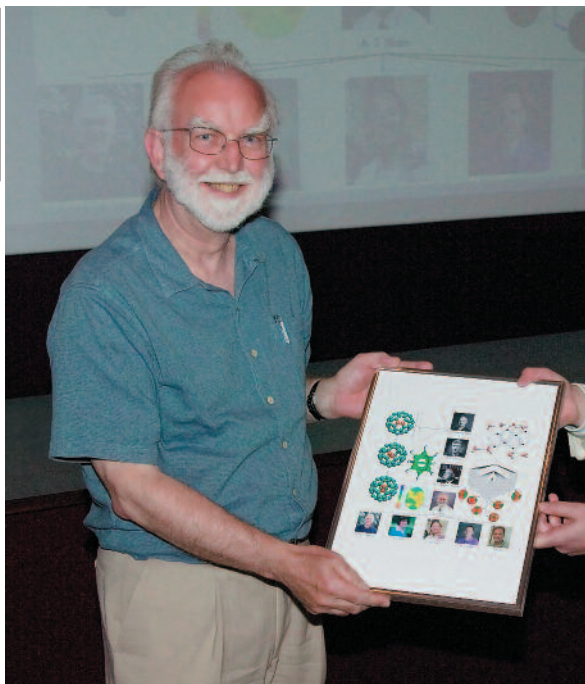
He was presented with a cheque for £1,000 at a ceremony in Claridge's hotel in London. 'I sat next to Adam Hart-Davis at the lunch,' he says. 'He was great fun!'

He also gets the opportunity of a work placement at the *Daily Telegraph*, the Royal Society or the competition's sponsor, chemical company Bayer, and a year's subscription to *New Scientist* and *Nature*.

You can read Phillip's winning article at www.science-writer.co.uk, and there's more from him on page 14 of this issue.

A brace of retirement events

Photo: John Holman



Anthony (left) and Stuart (right) both celebrate their impending retirements in conference style

Photo: Nathan Pitt



This summer, the department hosted conferences in honour of the retirement of two long-serving members of the academic staff.

First up, in July, was one for Anthony Stone of the theoretical sector. Anthony's work over the years has focused on developing the theory of intermolecular forces for polyatomic molecules, so that realistic model potentials are now being applied in a wide range of applications, from the smallest clusters to crystals.

He also published the definitive book in the field, 'Intermolecular forces', and developed software including the Orient programme.

The conference featured talks from a few of his many collaborators, to provide an overview of some of the fields that have been strongly influenced by his research. These were given by Sally

Price of University College London, Richard Saykally of the University of California at Berkeley, Ad van der Avoird, of the University of Nijmegen, Ken Jordan of the University of Pittsburgh, and David Wales from here in Cambridge.

The second conference, in September, was in honour of Stuart Warren – although Stuart has been persuaded to carry on teaching and postpone his retirement until 2007.

Held over two days, it featured many former members of Stuart's group. On the first day, talks were given by Jonathan Clayden, Jason Eames, David Fox, Adam Nelson, Richard Hartley and Peter O'Brien. The next day, Nikolai Kuhnert, Varinder Aggarwal, Iain Coldham, Nick Greeves and Kelly Chibale spoke, before a talk from the man himself.

Aside from his research, Stuart has been a major force in the teaching of chemistry. As Jeremy Sanders said in his opening remarks on the first day, Stuart has been an enormously influential figure in organic chemistry throughout the world for many years. 'He brought a coherence and quality to teaching across what was, at the time, a pair of departments of chemistry,' he said.

'It was when I joined the teaching staff and found myself giving lectures that I really felt Stuart's influence: he set a lecturing standard that one had to aspire to or feel utterly inadequate. Stuart could be critical, but in a constructive way, and I know that my teaching and my lectures are immeasurably better for the experience. I want to thank you for all you have done for us, and for the teaching that you will still be doing for us next year.'

Photo: John Holman

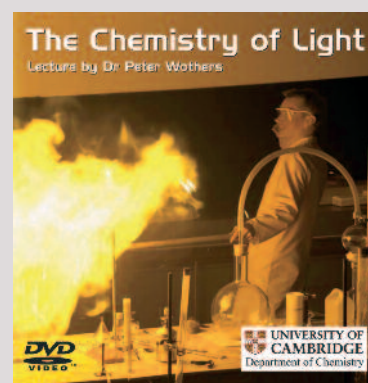


When you're moving house, it's usually a fairly straightforward (if stressful) affair. Not so when you're moving labs. When Stuart Mackenzie arrived in Cambridge this summer, it took a crane to get the table he's leaning on in the photo on page 8 into the building!

At this year's Open Day, Peter Wothers' lecture 'The chemistry of light' was filmed, and a DVD has been produced. It provides a fantastic opportunity to relive the lectures with close-ups and replays, as well as links to additional material.

Copies of the DVD cost £5. Send a cheque, payable to the University of Cambridge, to DVD sales, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW.

All proceeds will go towards future Science Week activities.



The hole story

Photo: Nathan Pitt



Rachel O'Reilly is creating functional hollow nanoparticles, and hopes to use them to make selective homogeneous catalysts

Micelles are common structures in nature and everyday life. This is how soap works – one end of the soap molecules likes to be in water and the other end likes to be in oil, and when they are suspended in water the water-hating parts all clump together. It leaves the parts that are happy in water on the outside, forming micelle or nanoparticle structures that range from about 10 to 100nm in size.

MODIFIED MICELLES

Conventionally, polymeric micelles are made using covalent chemistry to join the two parts of the molecule together. Rachel, however, has been using a mixture of both specific covalent and non-covalent chemistry because of the fascinating possibilities this provides for modifying the micelles.

'Once we've formed the micelles, we can stabilise them by forming covalent bonds selectively between the outer parts of the micelle to form a rigid shell on the outside,' she explains. 'By tailoring the micelles so that the bond that holds the inside parts to the outside parts is non-covalent and easy to break, we can cleave it and remove the interior, hydrophobic, part to leave a robust hydrophilic cage structure behind.'

Where the bonds have been broken, functional groups are left behind on the inside of the cage. 'Previously, polymeric cages have been formed using harsh ozone degradation chemistry which

gave ill-defined functionality,' she explains. 'This novel strategy gives extremely well defined, functional and robust hollow polymeric scaffolds.'

It is relatively simple to 'tune' the size and function of the nanoparticles, and small hydrophobic molecules can permeate through their shell into the hollow core, giving fascinating possibilities for using the nanoparticles for encapsulation.

How the polymers are made in the first place is important. At the end of each of the two parts of the polymer chains there is a group that will form a non-covalent bond with the other part of the polymer. Rachel uses a range of controlled radical polymerisation techniques which means she can control the functional groups at the ends of the chains.

'For example, if we have a complexing ligand on the end of the outer hydrophilic part of the polymer, we can bind a metal atom to it,' she says. 'The interior, hydrophobic, part of the polymer contains another ligand that binds to the metal. When we've made the cage, we can add a competitive ligand to strip out the interior, either leaving the metal behind, or removing it so a different one can then be introduced.'

Rachel also uses existing polymer self-assembly strategies but has been investigating modifying them to incorporate functional monomers which contain tethered catalysts to enable their placement within a specific domain of the nanoparticle. For exam-

ple, many metal catalysts contain phosphine ligands, so if the hydrophobic monomers used to make the nanoparticle contained phosphine groups, these can be introduced into the inner core and allow the transition metal to be directly attached.

Because the structures are hydrophilic on the outside, they are water-soluble, so maybe catalysis could be performed selectively within their 'protected' core domain in aqueous solution. Such metal catalysts are usually heterogeneous – they're suspended in the reaction mixture rather than being in solution – and Rachel thinks this could have big advantages. 'They would be easy to recycle and reuse, but would have none of the disadvantages of being heterogeneous such as a lack of reactivity, difficulty of recovery and possible processing problems.'

This simple structure can then be modified to make it more complicated, perhaps by using responsive polymers. 'An exciting possibility is that if we use polymers containing groups that respond to external stimuli, it could give us "smart" functional nanoparticles,' Rachel says. If such a particle was tailored to change its solubility by altering the temperature, for example, this could make them much easier to recover and re-use – important for expensive transition metal catalysts.

Chiral nanoparticles also offer fascinating possibilities. 'We have been making chiral monomers and using them to make chiral micelles and nanoparticles, and have been investigating what effect the chirality has on reactions within the core domain' she says. 'If the core consisted of chiral monomers units and we then encapsulated a metal catalyst, would that improve its selectivity?'

CV Rachel O'Reilly

Born: Hollywood, Northern Ireland

Education: After school in Northern Ireland, she came to Cambridge for her first degree, and moved to Imperial for a PhD with Vernon Gibson.

Career: Rachel spent two years in the US with both Craig Hawker at the IBM Almaden research centre in San José and Karen Wooley at Washington University in Saint Louis. She was awarded a Royal Commission 1851 Research Fellowship in 2004 and a Royal Society fellowship, with which she returned to Cambridge in September 2005.

Status: Boyfriend Andrew Dove – a fellow chemist – is an academic at Warwick. They did their PhDs together at Imperial, but Rachel claims they are now trying to diverge into different research areas!

Interests: She's fascinated by geology, which she studied as part of her degree, and loves travelling to look at rocks. She also claims that she's been trying to learn to play golf for ages (very badly).

Did you know? Rachel represented Northern Ireland as a high-board diver when she was at school. 'I'm rather shortsighted, so it made it much easier to be brave as I couldn't see how far up I was!' she claims. She was pretty good at it, too – finishing third in the All-Ireland championships when she was 14.

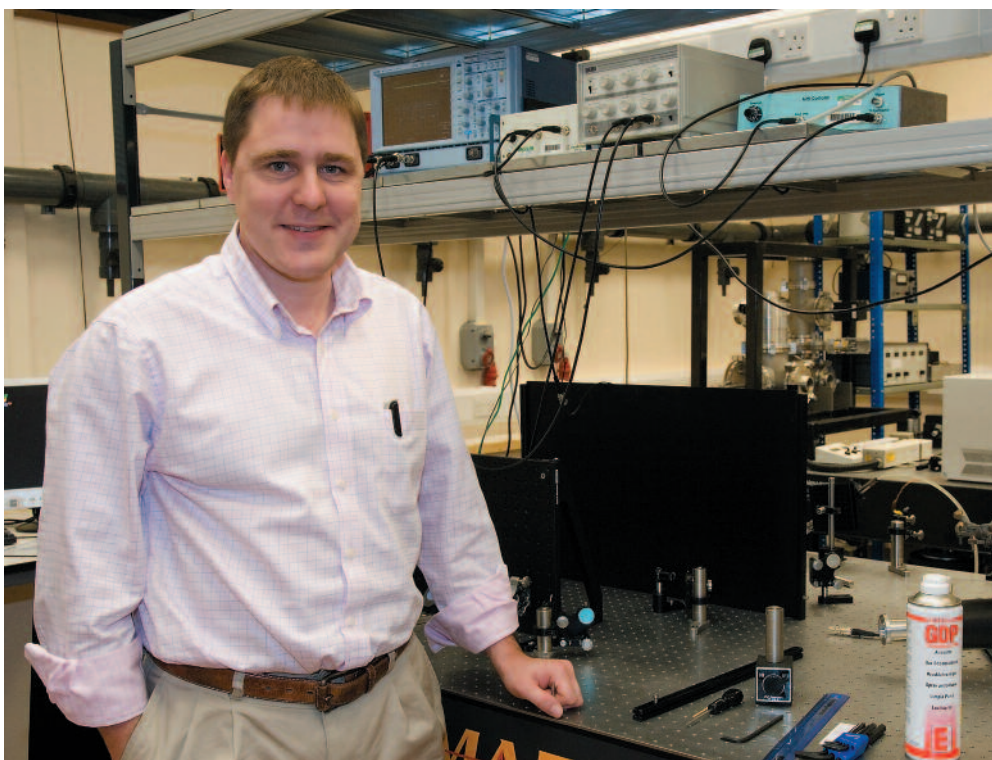


Photo: Nathan Pitt

The curious world of cluster chemistry

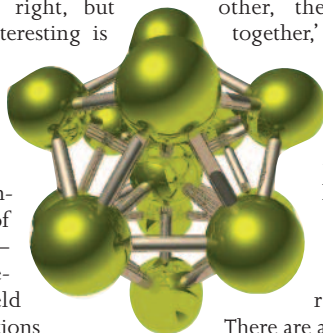
Clusters containing small numbers of molecules or atoms have some rather unusual properties. Stuart Mackenzie is looking at how they are held together, and the unusual chemistry you can do with them

Clusters are a major focus of Stuart Mackenzie's science. 'We're looking at how they are held together, which is interesting in its own right, but for me what's most interesting is to see if you can use them to do things that wouldn't ordinarily be possible', he says. 'They're fascinating!'

A cluster is an agglomeration of a handful of individual moieties – whether atoms or molecules – that are held together by weak attractions such as van der Waals forces or hydrogen bonds.

The molecules are not fundamentally altered, but these forces mean they are kept in a fixed orientation compared to each other. 'If you imagine a cluster of

water molecules, it's quite a floppy structure, but instead of the molecules rotating independently about each other, they are weakly locked together,' Stuart explains.



Metal clusters are particularly fascinating. 'In the size of cluster we look at, there is very little metallic about them!' he says. 'They consist of maybe 2 to 50 metal atoms, and have some quite remarkable properties.'

There are astonishing differences in reactivity between one cluster of, say, 19 rhodium atoms, and another that is made up of 20 atoms. There could be as much as three orders of magnitude of difference in their behaviour. In other words, by adding just one more atom to

a small cluster it becomes hugely more – or less – reactive. The reasons behind this are not very well understood at all.'

Equally fundamentally, and probably related to the reactivity, the actual structures of the clusters are not well understood. 'While it's possible to do theoretical calculations that suggest what they might look like, it's much more difficult to prove that it looks like you think it does,' he explains.

'For example, if you take six tennis balls, you might arrange them as an octahedron, with four balls in a square plus one above it and the other below. But you could also arrange them spread out flat, or even in a line. While chemical intuition might suggest that some arrangements are more likely than others, it's hard to demonstrate it. And, importantly, how does the arrangement change how reactive the cluster is?'

The electronic structure of the clusters is clearly important in reactivity, and Stuart claims that spectroscopy is now reaching the point that it will be possible to say something about how the geometrical structure itself affects the reactivity, too. 'We're interested in trying to find ways to generate these clusters in individual isomeric forms, and then study their reactivity and see which factors are important,' he says.

This reactivity has several practical implications, such as in the decomposi-

Stuart Mackenzie

Born: Durham

Education: His degree was in chemistry and physics at Leeds. 'I didn't want to do chemical physics or physical chemistry – I was quite clear that I wanted to do some of both!' he says. This was followed by a PhD at Oxford with Tim Softley on the high resolution photoionisation of small molecules.

Career: A postdoc with David Nesbitt in Colorado piqued his interest in clusters. He returned to the UK in 1997, first as a research fellow back in Oxford, before moving to Warwick as a lecturer in 2000. He moved to Cambridge this summer.

CV

Status: He met his wife, Christiane Timmel, at Oxford. She's another chemist, and is still there as a Royal Society University Research Fellow, working on oscillating magnetic field effects and heading up a new EPR facility. Their first child is due in January. 'If you see me looking even more bleary eyed early on next year, you'll know why!' he says.

Interests: Lots of sport, such as league cricket and badminton, and he used to play university squash. He also loves classical music, and says he enjoys travelling – his wife is German so they spend a fair amount of time there. And, with a home in Oxford and most of his research group still being in Warwick, he's rather well acquainted with the motorway.

Did you know? Science was only Stuart's second choice of career. Apparently, at the age of about 8, he had a burning desire to be a ballet dancer. 'Considering the effect that my 20s had on my waistline, I think perhaps I chose wisely!' he claims.

tion of nitrogen oxides on rhodium – the reaction that takes place in a car's catalytic converter. 'We do experiments in a very high vacuum on maybe 1,000 of these clusters at a time,' Stuart explains. 'Although this is not a particularly good representation of what goes on in a catalytic converter in the real world, this is the only way that we will get any idea about how the structures affect the reactivity.'

By using high-powered mass spectrometry techniques, his group has already found that whenever two nitrogen monoxide molecules are adsorbed on a rhodium cluster they decompose, forming a nitrogen molecule.

'This is almost certainly what goes on

in a catalytic converter,' says Stuart. 'We can now look at the kinetics of the reaction and, in principle, the reaction dynamics as a function of the shapes and sizes of the clusters.'

In parallel with this work, he's trying to find a way of generating these clusters in a known structural form by using lasers. 'It's really hard!' he says. 'We can't produce very many of them – maybe a million in a laser pulse. That might sound like a lot, but it's actually chemistry on an attomole [10^{-18}] scale.'

'We then have to carry out some form of spectroscopy on them to transform them into the shape we're interested in. We're finally getting there with this – we ionise them extremely carefully, and then try to identify the differ-

ent structures on the basis of their ionisation energies and vibronic structure.

Clusters of small molecules also offer fascinating possibilities. 'If we take two molecules, while we may know that they will react with each other, it's currently impossible to make them approach each other in a preferred orientation,' he says.

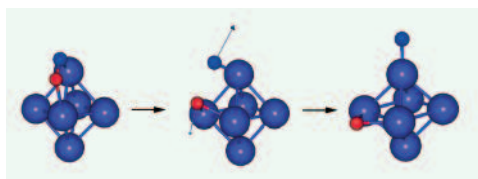
'If, for example, you have a hydrogen molecule and a hydrogen chloride molecule, whether they actually react at any point during a reaction depends on which way round they are when they encounter each other. So, clearly, it makes a big difference.'

At the moment, there is no experimental way of forcing the molecules to

meet in the best orientation for reaction. Stuart is trying to use the weak forces that hold clusters of molecules together to make them do just that before triggering a chemical reaction by breaking a bond with a laser pulse.

Small clusters of just two or three water molecules, for example, are quite floppy in themselves, but hydrogen bonds hold them together. So instead of being isolated molecules that are moving independently of one another, they are loosely tied together by these weak forces. The individual molecules are still clearly identifiable as they have not been changed at all, but they now have preferred orientations with respect to each other.

Stuart thought it might be possible to



A little light reflection

A third focus of Stuart's chemistry – away from clusters – is in collaboration with a group of electrochemists and interfacial scientists at Warwick, using cavity ring down spectroscopy (CRDS). In this technique, the first step is make a cavity using highly reflective mirrors, and then inject a pulse of light in. The light rattles back and forth, with a little bit leaking out each time it encounters a mirror. By measuring the rate at which light is lost it is possible to determine how much was absorbed in each round trip.

'It's an extremely sensitive technique for measuring absorption,' Stuart says. 'And it's now making the leap from gas phase measurements into condensed phases where it's probably going to have more impact as there are far more practical applications.'

He's now looking at what happens when the light is completely reflected internally at a surface in order to look at what's going on at the interface a few nanometres above it. 'We're using evanescent wave CRDS, which is sensitive to this type of interface,' he says. 'Coupled with the dynamic ultramicroelectrochemistry applied in solution above the interface, it should be possible to measure what is going on at the surface.'

The technique is in the instrument development stage at present, but plans are afoot to apply it to problems such as lateral proton diffusion in lipid bilayers or charge propagation in conducting polymer films.

Above left:
An NO molecule
dissociating on a
rhodium 6 cluster

use this phenomenon to carry out chemical reactions under restricted geometries. 'If you zap a bond in a water molecule within one of these clusters with a high-powered laser, then a hydrogen atom will be fired out in a specific direction towards one of the other molecules within that cluster – which does not need to be another water molecule – and react with it.'

They have found that it is indeed possible to carry out reactions with known geometry in the gas phase – something that had only previously been possible when the molecules were adsorbed onto a surface.

'Nature only typically gives you one orientation, however – the lowest energy structure,' Stuart says. 'If you have a water molecule and a hydrogen chloride molecule in a cluster, and you're happy with firing the H atom towards the Cl end of the HCl, then that's fine. But if you want to fire it at the other end, or fire the OH instead, you have "rearrange" the structure by some high resolution spectroscopy. That makes it far more complicated!'

'We've not got very far with this yet, but we have worked out what many of the problems are. Some of them may be fundamental and very difficult to overcome. If the cluster falls apart when more energy is put in to it, you've got to be pretty quick doing your chemistry.'



Stuart and group – not quite their normal lab attire! From the left: Kath Ford, Mark Ford, Stuart's wife Christiane Timmel, Jay Bomphey, Stuart, Raffaello Da Campo, Dan Harding, Mikhail Mazurenka and Marie Anderson

Much of Finian Leeper's chemistry is focused on enzyme biochemistry, but he's also got a sideline in making radiolabelled compounds

Thiamine diphosphate, or TPP, is a coenzyme derivative of vitamin B1 that is essential in the action of a number of important enzymes in the body. These include pyruvate dehydrogenase, the enzyme that links glycolysis to the citric acid cycle. It is also involved in a number of other enzymes that humans don't have, which could be targets for herbicides or medicines. Finian Leeper is making inactive derivatives of TPP that will enable crystal structures of the enzymes to be determined when they are bound to the substrate or in its various intermediate states to get a better picture of how they work.

'The enzyme reaction goes through several intermediates where the substrate is covalently bound to TPP,' he explains. 'We are trying to mimic these intermediates in the hope that this will tell us more about the enzyme's mechanism of action. This would then help us design a really good inhibitor of it.'

The best compound they've found thus far, deazaTPP where a nitrogen in

Biosynthesis models



Photo: Nathan Pitt

Finian Leeper: looking at the action of enzymes

the thiazolium ring has been replaced by a carbon atom, binds 25,000 times more tightly to the enzyme than TPP itself. 'We are hoping to work towards being able to inhibit TPP dependent enzymes in a live cell,' he says. 'DeazaTPP inhibits any TPP enzyme we can find. We're now looking for a more specific inhibitor.'

He adds that there's a fairly obvious way to go about this. 'The reaction with the enzyme takes place at the carbon between the sulfur and the nitrogen in the thiazolium ring,' he says. 'We think the trick will be to introduce substituents on the equivalent carbon in deazaTPP to make it more specific. The next challenge will then be how to get it inside a cell, as it doesn't diffuse through cell membranes.'

Another project in his group is on the biosynthesis of prodigiosin. This bright red coloured compound is made by *Serratia marcescens* bacteria, has immunosuppressant activity and is being investigated as a potential cancer treatment. Prodigiosin itself is in preclinical trials, and clinical studies are being carried out on an analogue by Canadian company Gemin X Biotechnologies.

In collaboration with George Salmond in biochemistry, they have discovered that there are 15 genes involved in the biosynthesis. 'We have now established what these genes all do,' he says. 'This was done by blocking each gene in turn, and then analysing what the modified bacteria produced to find out whereabouts in the biosynthetic pathway the synthesis was stopped.' The next step is to study the isolated enzymes involved in the biosynthesis and explore whether they can be used

to make analogues of prodigiosin in a predictable way.

A third focus of his chemistry is a little different – he's looking at ways of making radiolabelled compounds for use as diagnostic agents in positron emission tomography studies. In PET scans, a metabolically active molecule that includes a short-lived radioisotope that emits positrons is injected into the body. As the isotope decays the positrons it emits interact with electrons and are annihilated with emission of gamma-rays. Detection of these gamma-rays gives a 3D image of functional processes in the body, particularly in the brain.

SPEEDY SYNTHESIS

However, because the half-lives of the isotopes are so short, this poses synthetic challenges. Typical isotopes include ^{18}F , which has a half-life of 110 minutes, and ^{11}C , whose half life is just 20 minutes. 'The synthesis has to be very quick – no longer than half an hour!' Finian says. 'The biggest problem is purification, which takes time. We are trying to develop new methods using polymer-supported reagents that remove the need for purification, which will make the synthesis faster.'

Because only tiny amounts of the radioisotope are used, it means less than 0.1% of product has to be separated from the more than 99.9% of unreacted starting material. 'Attaching it to a resin is a way of overcoming that,' he explains. 'We are working alongside the Wolfson Brain Imaging Centre in Cambridge on this, and have already managed to demonstrate that it is possible to make radiolabelled compounds in this way.'

Born: Esher

Education: After prep school near Esher he went to Downside School in Somerset before coming to Cambridge, studying natural sciences at St John's. He stayed on to do a PhD with Jim Staunton on the biomimetic synthesis of polyketides.

Career: He went to McMaster University in Canada as a postdoc with Ian Spenser for 18 months, and returned to Cambridge as a research fellow at John's. He was appointed as demonstrator in 1982, and is now a senior lecturer.

Status: His wife Marion is a primary school teacher. They have two children; Emily has just finished a PhD in cosmology at Portsmouth and now works for a defence company, and son Jerry is at Staffordshire University studying film, radio and TV studies. 'He would only consider A-levels that no-one in the family had done before!' Finian claims.

Interests: He loves sport and still plays cricket for the department team. He used to play rugby – in the second row – and in his four years in the John's first XV they won three league titles and three cups. He retired gracefully to spend more time on his PhD! He adds that in the summer far too much of his time is taken up by mowing the lawn.

Did you know: In his spare time, Finian also enjoys computer programming. He wrote a computer game Cambridge version of Monopoly. 'There are quads instead of houses, colleges for hotels, and you don't go to jail – you go to the university library!'

CV
Finian Leeper

A Nobel week

The Lindau meetings are a great opportunity for young scientists to meet Nobel laureates. This year, the UK group included Aurora Cruz Cabeza from Cambridge. She reports on an inspirational week

Many years have passed since Paul Dirac proposed a mathematical argument for the existence of God to students on a blackboard in Lindau. Although today he would probably have used a PowerPoint presentation, after all these years the essence, aims and atmosphere of the Lindau meetings remain untouched.

Since 1951, selected young scientists have been able to interact with Nobel Laureates in an informal and relaxed environment in Lindau, by Lake Constance in Germany. The major aim of the meeting is to promote the interaction between the scientists of tomorrow and the great scientists of today.

The 56th Lindau meeting – the 18th exclusively dedicated to chemistry – was held in the summer, with 500 students and 23 Nobel laureates in attendance, most of them chemists. The progressive internationalisation of the meeting has enabled students from all over the world to participate and has also made the selection procedure more competitive, with an astonishing 11,000 applicants this year.

A GREAT PRIVILEGE

Since 1997, a small group of students from the UK have been attending the Lindau meetings, and there were six of us from the UK this year, nominated by the Royal Society of Chemistry.

It is an absolute privilege for any young scientist at the dawn of their scientific career to have the opportunity to attend a meeting of this nature. As one laureate mentioned at the beginning of the week, 'It is specialisation that brings up the problem but only multidisciplinary knowledge that brings up the brilliant solution.'

The laureates' lectures covered a wide spectrum of scientific topics: from important catalytic systems for organic synthesis to enzymatic catalysis of key importance to life; from the understanding of fundamental techniques in physics to its applications in fields such as medicine; from the discovery of new materials to their applications in different fields; and from the identification of the environmental problems to the proposal of green and sustainable solutions.

After the morning lectures, the afternoons were filled with discussions, discussions and more discussions. We were

eager to learn and find answers. The laureates were equally eager to help and guide. The discussions were not merely scientific, but included valuable career and personal advice to future scientists.

'No one can do it alone,' said Peter Agre (reflected in the 230 acknowledgements given by Kurt Wüthrich in his presentation). 'Do not forget to hear the music and smell the flowers,' said John Hall. Then there was William Lipscomb's answer to an unmotivated student: 'If you do not have frustration, your problems are not going to be solved.'

Apart from the specific topics, general concerns were voiced about alternative energy sources and global warming, the main points addressed in the round table discussions. 'Energy is one of the major challenges of the future' said Walter Kohn who, although awarded the Nobel prize for his work on density functional theory, is now focused on the issue of solar energy.

Experts in the field like Paul Crutzen and Sherwood Rowland, who were awarded the prize for their work in atmospheric chemistry, agreed on the importance of finding solutions to global warming.

However, to date, there has been insufficient effort invested into seeking solutions and the responsibilities now lie with the present and future generations of scientists. As Ryoji Noyori pointed out in the opening of his lecture, 'Green chemistry is a responsible and a creative science,' and it is for us to become, not only creative and innovative, but also responsible scientists.

Social activities included an opening



Aurora prepares to waltz with Peter Agre...

formal dinner with dancing, a mid-week classical concert and a boat trip to the Isle of Mainau to end the week. I was very privileged to share some strawberries with Walter Kohn while discussing women and science, to dance a waltz with Peter Agre while he advised me on my career, to enjoy a nice lunch with Sir John Walker (the only British Laureate at the meeting) while discussing ways to improve scientific education in schools and to have a coffee with Sherwood Rowland during the boat trip to Mainau.

MOTIVATIONAL SPEAKING

These unique experiences influenced me greatly and provided me with great motivation for my future career. Additionally, the interaction with the brightest young scientists from all over the world – present and future colleagues – was of extreme value to me and I am sure will have a positive influence on my future scientific endeavours.

Many of the 'real' problems of the world were brought into context. For example, Aaron Ciechanover introduced his lecture by reminding us that 'half of the population is living on \$2 a day', and that 'winning the Nobel Prize is not at all important; the important thing is to help people in one or another way'.

Many believed that education is the only solution for the world's problems. Walter Kohn emphasised that 'We need to invest in education for women at all levels'. As a woman, I was very pleased to hear so much encouragement from the laureates towards the female students. William Lipscomb, who is 86, pointed out that the situation is changing and that he was pleased to see more and more women now in science, saying that 'We are getting half of our talents back.'

As Ryoji Noyori mentioned, we are responsible for creating a civilised society in the world. We are all responsible for lighting up the world and people's minds by investing effort in responsible research and education.

...and shares strawberries with Walter Kohn



The shape of things to come

Polymorphs – different crystalline forms of the same molecule – can cause real problems for the pharma industry. Although they're chemically the same, they have different physical properties, such as solubilities, dissolution rates and even the rate at which they are absorbed by the human body.

The altered properties mean the drug is different, and therefore cause real problems with regulators if a new form suddenly appears in a production process. This has happened on numerous occasions, for example in Abbott's anti-HIV drug ritonavir. The company lost a lot of money when the process suddenly threw up a new polymorph that was thermodynamically more stable and much less soluble.

It cost the company an enormous amount of money while it tried – and failed – to get the process to make the original form again. They ultimately completely reformulated the product as a liquid gel capsule using the new polymorph in pre-dissolved form – but this requires refrigeration, unlike the first version.

Part of the drug development process is to try and find all the possible polymorphs of a drug molecule, but even

then it is all too easy to miss one that can then cause problems. Postdoc Antonio Llinàs, who works with Jonathan Goodman and Bobby Glen in the Unilever Centre for Molecular Informatics and also with the Pfizer Institute for Pharmaceutical Materials Science, has discovered a way of generating the most thermodynamically stable polymorph of a drug.

Toni has been working on a project to generate a theoretical model to predict solubilities for some time, and realised early on that accurate and reliable solubility data were needed to build a good model. 'The data in the literature are really poor, and so we have had to generate our own database of accurate solubility information,' he says.

'I soon realised that to do this I had to fully characterise the compounds – not just the starting materials, but the precipitate itself. And I was really excited to find that most of the precipitates I was generating were new, and not only that, they were new polymorphs.'

Unfortunately, because they are looking at patenting the work, Toni can't say too much about precisely how he makes the polymorphs. However, he believes it could be extremely important for the



Photo: Nathan Pitt

pharmaceutical industry. Not only do polymorphs cause production problems, if a rival company can discover a different polymorph it can be used to invalidate a drug patent.

'Because the new method is so good at finding stable polymorphs, it will be really useful for pharma companies,' he says. 'Applying it to all their drugs as they are being developed would make it much more difficult for someone else to come up with a more stable polymorph they have not found themselves.'

Antonio: looking for polymorphs

The Corporate Associates Scheme

Accelrys

Akubio

Amura

Astex Therapeutics

Astra Zeneca

Biotica

Boehringer Ingelheim

BP Institute

Bristol-Myers Squibb

Cambridge BioTechnology

Cambridge Display Technology

CambridgeSoft

Dow

ETRI

GlaxoSmithKline

Thanks to the generosity of the department's Corporate Associates, we have been able to benefit the education and environment for students and staff. For example, the Associates pay for university-wide access to SciFinder Scholar and ChemOffice. They also make significant contributions to the library for journal subscriptions. Moreover, plans are afoot to provide new undergraduate chemistry exam prizes, departmental summer studentships, and new faculty teaching awards.

Corporate Associate membership not only provides essential support for the department, but also provides numerous benefits to help members work with us and achieve their business objectives. Members enjoy many benefits through their enhanced partnership with the Department, such as:

- Visibility within the department;
- Invitations to recognition days and networking events at the department;
- Access to the chemistry department library and photocopying/printing facilities;
- Regular communications about

upcoming events, colloquia, and updates about the department;

- Complimentary subscriptions to Department publications, including Chem@Cam;

- Access to emerging Cambridge research via conferences, special briefings and various publications;

- Priority notification of and free access to research lectures within the department;

- Ability to hold 'Welcome Stalls' in the department entrance hall;

- Preferential conference rates for Corporate Associate members;

- Free access to the teaching lectures held within the department;

- The full services of the Corporate Relations team to facilitate interaction with students, staff, and other parts of the University of Cambridge to help achieve your corporate objectives.

If your organisation would be interested in joining the Corporate Associates Scheme, then please email Jane Snaith at cas-admin@ch.cam.ac.uk, or call 01223 336537.

We look forward to hearing from you!

Jeol

Johnson Matthey

Medivir

Merck Sharp & Dohme

Research Laboratories

Novartis Institutes for

Biomedical Research

Pfizer

Proctor & Gamble

Roche

The Society of

Chemical Industry

Shell Global Solutions

Solexa

Syngenta

Unilever



Spot the difference

Ah, the 1970s. Great fashion, great hair-styles... and they come back to haunt you. When Brian Crysell passed on the above photo, shamefully (and to Brian's surprise!) Chem@Cam only recognised two of the faces. Once Brian supplied the full set of names, it was one of those 'ooh, of course!' moments.

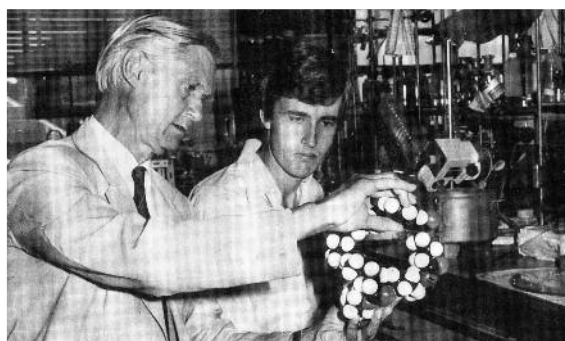
If you're struggling to identify these models of 1970s style, then from the left it's Dudley Williams, Ian Fleming, Jeremy Sanders, Jim Staunton, Tony Kirby, Stuart Warren and Andy Holmes.

Back in the lab

Chem@Cam's regular old photos correspondent, NMR technician Brian Crysell, recently found a copy of the Science and Engineering Research Council's Bulletin from Spring 1984 lurking in the back of a cupboard.

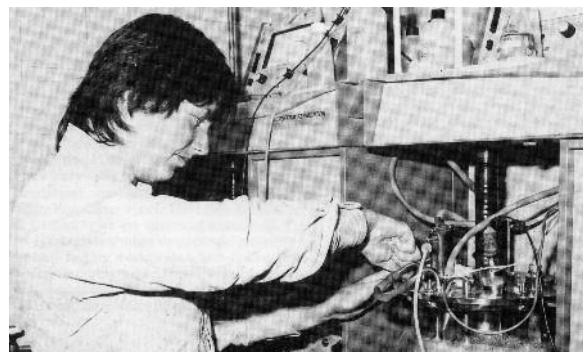
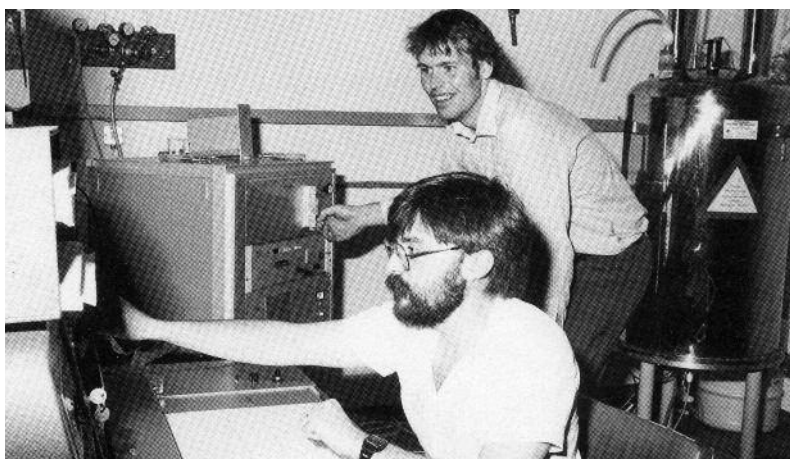
Flipping through it, in between articles on condensed matter physics and ion beam fusion, he spotted a few familiar faces in a piece on the biosynthesis of the pigments of life.

Alan Battersby doesn't appear to have changed at all in the intervening 22 years – unlike the other current member of staff!



Above: Alan Battersby and Simon Bartholomew discuss a molecule that mimics the natural haem system;
Below: Adrian Carpenter and Finian Leeper operating the 400MHz NMR

Below: Hans-Ullrich Hoppe working with oxygen-sensitive intermediates on the biosynthetic pathway to vitamin B12;
Bottom: Jeanette Brown adjusts the fermenter



Cricketing faces: nearly there!



Dear Editor
I have done a little more cricket spotting and am able to supply the names of five more of the group from the 1950s.

Standing, from the left: second P.K. Grant, third F.A. Hart, fifth J. Golden, sixth H.W.W. Brett and 13th F.H. Newth.

One more to identify, and then we have a full team!

Yours sincerely
Geoffrey Liptrot,
Cambridge

This one continues to produce more names!

Does anyone have any further suggestions to add to the identities we already have? The photo was taken in 1955, and is of the teams for the Cambridge v Oxford chemistry labs cricket match.

Geoff Liptrot is standing 10th from the right. The other names we know are Les Johnson (seated, extreme left); Andy Holmes-Siedle (seated, third left); Peter Sykes (standing, eighth from right); and Jeff Watkins, who sent the photo in, is sitting in the centre. Let us know if you recognise anyone else in the picture!

Sustainable development?

In the current atmosphere of government and public concern over climate change, CO₂ emissions and energy consumption, there is an increased emphasis on making chemistry 'sustainable'. But what does sustainability mean in the context of chemistry and what can we do to make it a reality?

Sustainable development is defined as 'development which meets the needs of the present generation without compromising the ability of future generations to meet their own needs'. Much progress has been made since that definition was proposed 20 years ago, but we are still a long way from achieving true sustainability in chemistry.

To satisfy our desire for medicines, fuels, plastics and so on, the chemistry involved must balance economic viability with environmental and social responsibility. As pressure increases to minimise the environmental impact of industry, for example by reducing energy demand and emissions, innovative solutions must be found and implemented appropriately.

MANAGING WASTE

A key challenge to sustainability comes in waste management. Almost every process that chemists use produces waste, and that waste is often toxic and difficult or costly to dispose of safely. Traditional 'end-of-pipe' technologies to clean up effluents are often capital- and energy-intensive. Thus a large amount of effort in recent years has been directed towards developing cleaner, more efficient processes that

Environmentalists love to talk about sustainability. But what does it mean for the chemical industry? Phillip Broadwith reports

produce less waste and use less energy.

The economical use of energy is a central concern in any process; the most effective way to improve sustainability is to reduce energy demand by improving efficiency. Yet some processes, such as the generation of chlorine via electrolysis for use in water treatment, have intrinsically high energy requirements. Therefore some way must be found to offset this by producing the energy in a sustainable fashion.

INTEGRATED APPROACH

An integrated approach to waste and energy management, such as the 'Verbund' system employed by the German chemical company BASF, can significantly improve sustainability. By siting complementary plants close to one another, raw material, energy and transport costs can all be reduced, since heat or material by-products generated in one process can be piped directly into other processes on site. Other companies are now beginning to employ this strategy that fell out of favour in recent years as a cost-effective way to increase efficiency and sustainability.

This is all very well for industrial-scale chemistry, where a plant or process is designed for the long term and can be fully optimised. But, in the research laboratory – whether indus-

trial or academic – the nature of the chemistry changes on a daily basis, so it is not always possible to use the most sustainable technology.

Certain processes are inherently wasteful, such as the use of silica chromatography for purification of synthesised compounds. This produces a large quantity of organic solvent waste, which must be disposed of by incineration. However, there is often no realistic alternative in a research environment.

Fortunately, there are many other ways to improve the sustainability of research-based chemistry – much effort has recently been directed towards making chemical transformations more efficient. Advances in chemical and enzymatic catalysis allow reactions to proceed more economically, often at significantly lower temperatures. Improvements in the understanding of reaction mechanisms mean that competing processes can be avoided or eliminated. Better atom economy in reactions means that more of the atoms from the starting materials end up in the final product molecule, reducing the amount of waste by-products.

Advances in spectroscopic and analytical techniques, especially NMR for structural characterisation and assay screening for evaluation of biological properties, mean that much smaller quantities of trial compounds are required. This is especially significant in the total synthesis of complex molecules, where it may be necessary to start a synthesis of around 20 steps with reactions on kilogramme scale to get enough product for testing.

Perhaps the most crucial aspect in the campaign for sustainability comes in the debate over future energy supplies. Chemistry plays an important role in the development of the new technologies required; including generation of biodiesel fuels or stronger, lighter materials for offshore wind turbines.

Chemistry is also inextricably linked to the reduction of industrial and household energy demands; from improving insulation materials to reduce the need for heating, to developing appropriate fuel technology for use in the third world. Clearly, sustainable chemistry is a key factor in achieving overall global sustainability to allow future generations to make the most of the opportunities and resources available to them.

BASF's Verbund site in Ludwigshafen, Germany, makes the most of having several stages of production in one location



Life begins at 40



Most people think that a 40th birthday is a great excuse for a party. Not so Shankar Balasubramanian – he celebrated the end of his 30s by climbing Mount Kilimanjaro.

'I turned 40 in September, at about the same time as two of my friends from undergraduate days,' he says. 'One of them thought we should celebrate on a beach on a remote Pacific island, but I thought we should do something more challenging. My wife suggested Kilimanjaro, and it sounded like a good idea.'

Challenging was the right word. It was the first time Shankar had climbed a mountain, and his first time at altitude. 'It's actually not that difficult a climb,' he explains. 'The only technical issue we really had to wrestle with was the altitude – there are no glaciers or serious rock climbing involved. As it's a volcano it's steep so you gain altitude pretty quickly.'

The climb to the top took the three of them four-and-a-half days, which allowed time to adjust to the altitude along the way. 'It's a spectacular climb,' he says. 'You start in the tropical rainforest, then the landscape turns more alpine. It then becomes a desolate desert, with volcanic rocks and no life,

and as you get close to the summit you start to see some ice.'

The last stretch towards the summit is by far the toughest part of the climb. The night before, they camped at 4,500m, and woke at midnight to head for the top, which is at 5,850m. 'It was very cold – about -20°C – and very dark. It's also pretty steep, with a lot of volcanic ash and scree which makes it difficult to get a secure footing.'

The push for the summit took eight hours, and as they neared the top the sun came up and the temperature rose above freezing. 'It was really uplifting to see the sun rise over the summit,' he says. 'It was really enjoyable, and I'd recommend it to anyone who likes a bit of a challenge and wants to see some of the beauties of the planet.'

It may have been his first mountain, but Shankar's caught the bug and is really keen to go up even higher. 'Perhaps the next one should be Aconcagua in Argentina,' he speculates. 'But as it's higher up – almost 7,000m – it's more dangerous and you have to take much longer to acclimatise. I'll definitely need to get permission from my wife for that!'

Anita with Jacob (right), and Eloise with Rose and Steve (below)



Glamorous grannies

There must be something in the water – there's been something of a spate of secretaries becoming grannies for the first time in the past few months – two of them on the same day and in the same hospital in November.

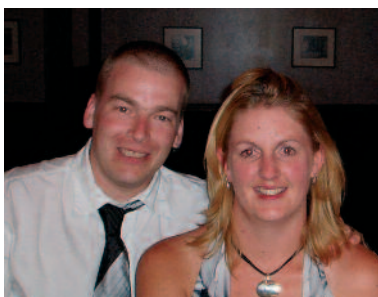
Sue Harding started it off when her daughter Kathryn gave birth to Lucy in March, swiftly followed by Poppy being born to daughter Helen in June. Then Rose Ley's daughter Becky gave birth to Eloise Rosa, and all of four hours later Anita Hudson's daughter Joanna produced Jacob William.

While Becky was in labour, grandad Steve was in Japan giving his Nagoya Medal lectures – and couldn't resist mentioning the natural product synthesis that was going on at home.



Just the one wedding to report this issue – former Chem@Cam cover star Steve Andrews married Zoe Davis at Queens' College on a beautifully sunny day in August. Zoe's a science teacher in Cottenham, and Steve's a PhD student in Steve Ley's group. Just to keep it in the family, fellow Ley group member James Bull was best man

Love is in the air



The happy couple... Tim in a tie with no drink in his hand? What's going on?!

When technician Tim Layt went for a weekend in Amsterdam with his girlfriend Kirsten Scholefield recently, he came over all romantic. He sneaked out of their room early one morning while Kirsten – who used to work on reception – was still asleep, leaving a note that he'd gone for quick smoke.

Not a bit of it. He'd spotted a diamond factory just across the road from the hotel and went shopping instead. Somehow, he managed to contain his excitement until dinner that evening and popped the question after the main course.

'I didn't go down on one knee,' he admits. 'But she said yes straight away anyway! She thought something was up because I kept checking the ring was still in my pocket. She didn't know what,

though – and was really surprised when I asked her.' The happy couple then proceeded to find a bar and drank rather a lot of champagne to celebrate.

Don't expect wedding photos in the near future, though. Kirsten's a Kiwi, and they're going to get married back in New Zealand – in at least three years' time. 'We've got to give all our friends time to save up enough money so they can afford to come out for the wedding..'

Regular readers of Chem@Cam may remember we printed photos of Tim from the night the happy couple first got together. 'It was at the Christmas party four years ago,' he says. 'I was dressed as a red dragon. That's my dating advice – wear a dragon costume if you want to get the girl!'

A great sporting day out

The annual departmental sports day took place at the Leys School sports ground. Teams of staff and students took part in a variety of sporting events, from five-a-side football and cricket to croque and rounders. John Holman and Caroline Hancox were on hand with their cameras to take photos



Right: Mike Todd-Jones does his best Ian Botham impersonation; below: Robin Freebairn and John Coston add one to the score



Above: Mark Hopkin, Tim Layt and Chris Smith; Below: Matt Bushen and Michael Pedley admire Christian Fink's heading skills; below right: Matt Bushen and Ewan Galloway; left: Matt juggles the ball



Left: Joe Piper and Beth Sawyer dancing on the footy pitch; Right: Andrew Mason, Catherine Bacon, Faye Dodds, Richard Horan and Chris Smith



Two secretaries move on...

Photos: Nathan Pitt



Anna Parsyan and Celia Jones both left us recently, and are both pictured here clutching flowers. Celia, who was the Melville secretary, is on the right, and Anna, who worked for Dave King and Carol Robinson, is in the middle on the left. Surrounding her are Julie Lee, Joanne Castle, Anne Railton, John Holman, Vicky Spring, Anthea Bramford and Anita Hudson at the back, and Liz Alan and Jane Snaith at the front



Comings & goings

New Staff

Anthony McPherson
Custodian
John Sproule
Night security
Irma Kvarinskaite
Cleaner
Kirstin Walker
Senior Accounts Clerk

Retired

Michael Ladds
Robin Sarin

Leavers

Celia Jones
Nathan Haridien
Patricia Ferraro-Cordoba
Anna Parsyan

...and Mike retires

Mike Ladds retired from the workshop at the end of October, after an astonishing 35 years' service in the department. At a reception in his honour, Jeremy Sanders presented him with a parting gift (below) and many members of the department both past and present came along to wish him well for the future

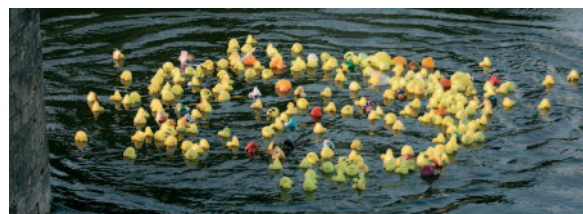
Photos: Nathan Pitt



A quacking good time on the river



The river Cam has never seen so many rubber ducks!



For over 364 days a year the river Cam is covered with punts, rowers and swans but on one day in July, it was swarming with ducks... rubber ducks!

The duck race was organised by Rob Clay Rivers, who's doing a PhD in Chris Dobson's group, looking at Parkinson's disease at the molecular level. Once he finishes said PhD next year, he plans to head to Peru to do mission work, and the race was part of a fund-raising effort for the UK Christian Charity Latin Link.

Never mind nice weather for ducks, it

was a lovely sunny day for what was probably the slowest race the Cam has ever seen. The river was over-run with ducks, many of which had been decorated in pretty patterns – and some with insane costumes that dramatically affected their ability to float.

The winning duck swam from Jesus Lock to the end of the edge of boat traffic in a record 40 minutes. There was also a prize for the best decorated duck, which won for both an inventive design and the name Quacks and Cheese.

Overall the race raised a total of £900 and drew a large crowd who came out to cheer on the ducks.

The duck race was one of a number of events and activities Rob is holding to help raise the £7,000 to support his mission work in Peru, and he's really grateful to all the people who made the effort to support the race.

P-partying the night away

The annual organic sector postgrad symposium and welcome party in October was once again sponsored by Pfizer. And the theme this year was... the letter P. It inspired plenty of particularly phenomenal costumes – and some pretty pfantastic beer!!



Left: Miles Tackett and Simon Sprague with a spot of police brutality on a penguin; Above: Prize-winning present (or is it parcel?) Cat Tubb with Pfizer's Daf Owen; Below: Picture Siri Kumam, Paddington Catherine Smith and pirate Alex van den Heuvel



Above: Pirate Katy Bridgwood
Below: Pie-muncher Colin Pearson



Above left: pool table Richard Horan; Left: puffin Matthew O'Brien (bet even his mum doesn't recognise him); Below: Pfizer's Tony Wood and Dafydd Owen pfoolishly pforgot their costumes!



Even the drinks got into the P-party mood...



Last issue's winners

Elementary crossword

The elementary crossword we ran in the last issue, set by Graham Quartly, attracted loads of entries – not all of them correct! A number of people were a little confused by 20 down – clue ‘Dung lost in the past’ – and ended up with ‘PATs’ instead of ‘PATs’ (as in ‘cowpats’ and an anagram of ‘past’), giving ‘Narwhals’ instead of ‘Narwhals’. Spelling let a couple of people down, too – so we had

	C	At	Ar	Rh			Ra	In
He	Ra		K	In		Ac	Re	S
Re	Ne	W		O	N	Ce		I
Ti		He	Li	C	O	Pt	Er	S
C		Re	V	Er	Se	S		Te
			Er	Os			Ca	N
Ca	Lu	Mn	Y		P	La	I	Ce
Bi	N			P	At	Te	Rn	
N	Ar	W	H	Al	S		S	Am

‘Catarrh’ with only one ‘R’, and various instances of ‘Insistance’, not ‘Insistence’.

Plenty managed to get it right, though. This issue’s metaphorical hat is a bit of a departure from the norm – rather than a Sheffield Wednesday one, *Chem@Cam*’s getting herself in the mood for the Ashes, which are due to start as we go to press – here’s hoping England aren’t behind in the series once this magazine starts plunking through letterboxes! Anyway, it’s one from the match at Old Trafford last summer which ended in a truly nail-nibbling draw. And the first correct entry out of said mug came from D.M.W. Pascoe of Ickenham in Middlesex. Congratulations – your cheque is on its way.

Other correct entries came from Ian Fletcher, Peter Keefe, Jim Dunn, Michael Aicken (who sent his entry in attached to a rather nice postcard of a pub – much to be encouraged!), J.P. Dickinson, John Salthouse, Bill Collier, T.A. Mather, Helen Stokes, A.J. Wilkinson, Stephanie Walker (with the help of Cris, aged 14), John Carpenter, Roger Duffett, William McFarlane, Susan Sun (the 14-year-old daughter of Li Sun), David Thompson, Derek Palgrave, Peter Farne, Paul Stickland, John Malone, Tessa Ennals (who says ‘Kudos to Graham for coming up with

this one – a lot of fun!), Alan Hart, Pat Lamont Smith, Paul Hickford (who suggested that *CHoCoLaTe* would make a good future prize), Robert Broughton, Martin Stentiford, Donald Stedman and Keith Parsons.

Annette Quartly also sent a correct solution in, although she happens to be married to the puzzle setter, who had most kindly disqualified her.

We shan’t name and shame the nine entrants whose spelling let them down!

One for all

Unsurprisingly, Keith Parsons’ ‘One for all’ card puzzle drew rather fewer entries. However, we did still get quite a few. These come from Annette Quartly, Graham Quartly (I’m sure they weren’t copying!), Robert Broughton, Pat Lamont Smith, Richard Brown, Richard Moss, Roger Duffett, A.J. Wilkinson, T.A. Mather and Ian Fletcher.

And the prize goes to... Richard Moss. Congratulations!

£20 prizes are on offer for both puzzles. Send entries by email to jsh49@cam.ac.uk or by snail mail to *Chem@Cam*, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW

This issue's puzzles

Transmutation

This puzzle is from our regular setter Keith Parsons, which he says he’s called Transmutation for ‘obvious reasons’!

He adds he’s pretty sure that there is only one solution, judging by the difficulty he had in setting the puzzle. Should anyone find an alternative correct solution we will, of course, accept it...

Anyway, here goes. Rearrange all of the letters used to spell the eight elements listed below to transmute them into another eight elements.

Chromium
Indium
Iron
Neptunium
Palladium
Rubidium
Sulfur
Ytterbium

Simple but fiendish! The usual £20 will go to the first correct solution drawn.

Chemdoku

			U			At		
			Rn	Po	Fr	U		
Th	Rn							
	U					Ac	At	
	Ra					Th		
Pa	At					U		
						Pa	Rn	
		Ac	Pa	Fr	Th			
		Fr			Ra			

It’s back! After last issue’s foray into the world of the chemical crossword, *Chem@Cam* is going back to basics and, by popular demand, here’s another fiendish Chemdoku.

This time, we’ve come over all radioactive, and instead of the boring old numbers you find in a Sudoku puzzle the grid needs to be filled with the symbols of the nine naturally-occurring radioactive elements.

Should anyone never have encountered Sudoku (or even Chemdoku!) before, the grid must be filled in with the nine symbols arranged in such a way that each row, column and 3x3 square contains each symbol just once.

The usual £20 prize will go to the first correct solution out of whichever coffee mug *Chem@Cam* happens to have lurking in the office when we do the draw.



Climate change made the journey into the lab a little more challenging



UNIVERSITY OF
CAMBRIDGE

Chem@Cam is written,
edited and produced
by SARAH HOULTON

Printed by Cambridge Printing,
the printing business of
Cambridge University Press