

ANU COLLEGE OF SCIENCE

RESEARCH SCHOOL  
OF CHEMISTRY



ANNUAL REPORT 2005





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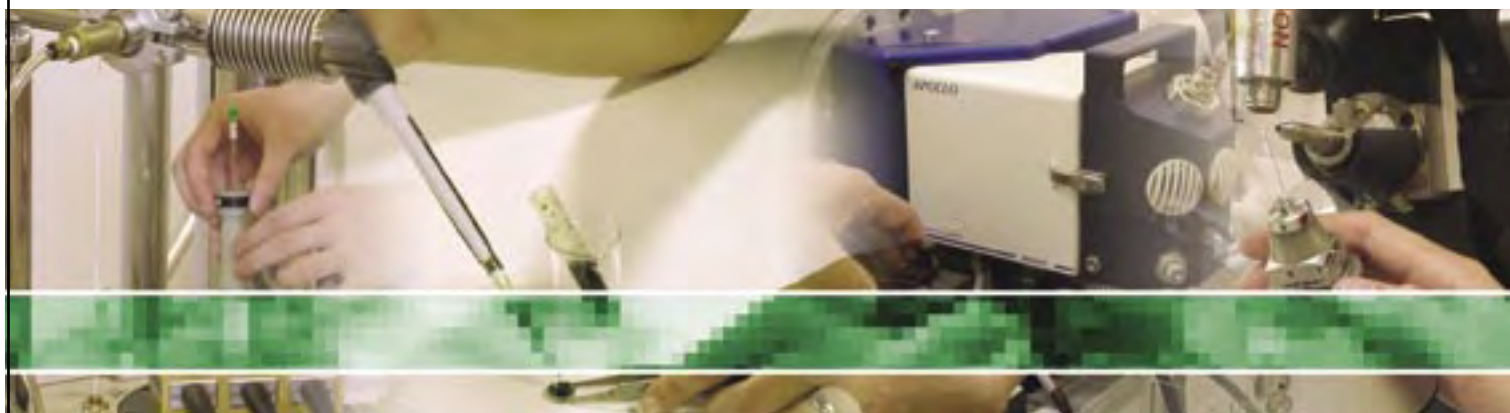


# RESEARCH SCHOOL OF CHEMISTRY

## ANNUAL REPORT 2005

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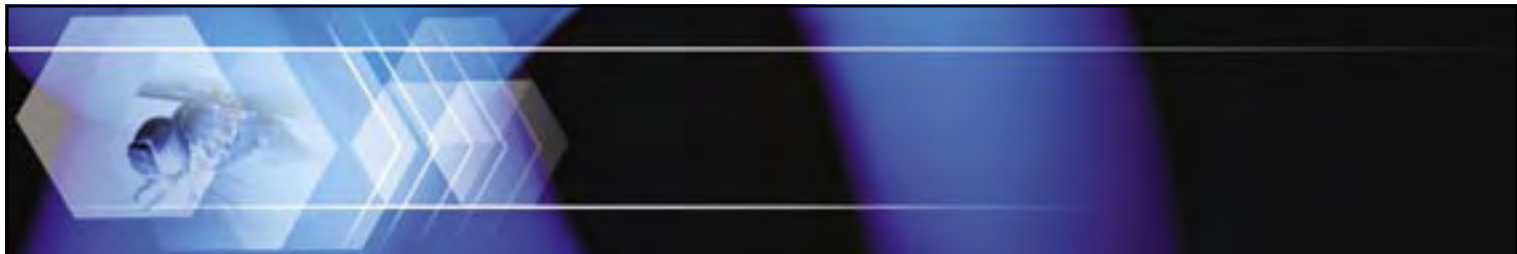


**Editors:** Professor Peter Gill  
Ms Marilyn Holloway  
Ms Christine Sharrad

**Coordinator:** Ms Michelle Baker

### Front Cover:

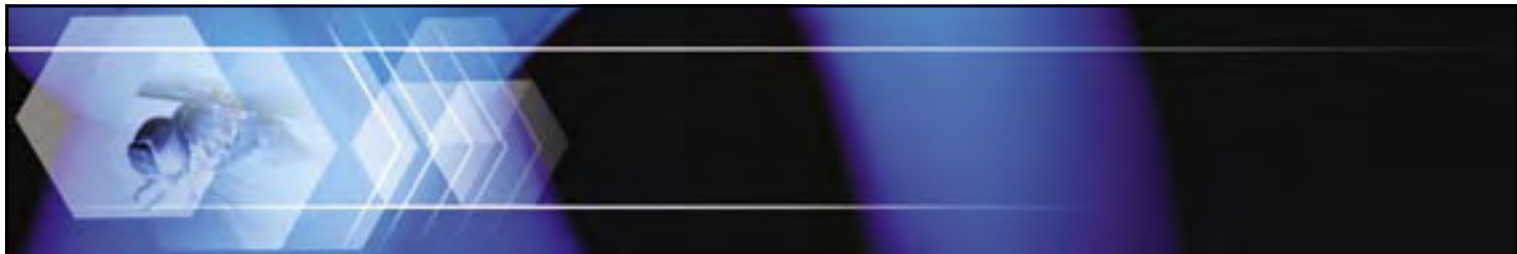
A naturally-fluorescent rubbery cross-linked protein called resilin is found in the wing-hinges of flying insects. In work by a team that included Nick Dixon, and led by Chris Elvin, CSIRO Livestock Industries (formerly a postdoctoral fellow at RSC), the extraordinary properties of natural resilin have been reproduced in a synthetic material. The cover illustration shows a dragonfly and the characteristic fluorescence of a cylinder of synthetic resilin about 1 mm in diameter. *Nature* (2005), 437 (7061), 999-1002, <http://dx.doi.org/10.1038/nature04085>. Artwork by David Merritt (*U Queensland*), David McClenaghan and Nancy Liyou (*CSIRO*), and Ted Hagemeyer.





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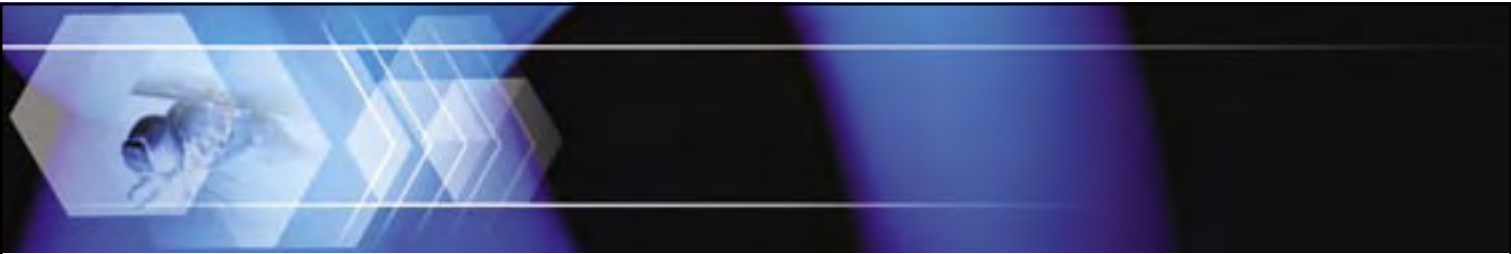
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## DEAN'S REPORT

To say 2005 was eventful would be a gross understatement. In August the School was damaged by an explosion and fire. The School's safety procedures worked extremely well in the immediate aftermath of the fire. Under the leadership of Professor Chris Easton, who was Acting Dean at the time, the performance of our staff was exemplary. Kevin Cooper, Geoff Deeble (who was Acting Laboratory Manager), Chris Tompkins and Lee Welling received special awards from the Vice-Chancellor for their actions during and after the fire. A large number of RSC staff and students did an amazing job during the cleanup after the fire resulting in a return to the building in less than four weeks. As the year progressed demolition of the damaged section of the top floor of the Birch Building commenced and plans were developed for reconstruction.

2005 was a year of considerable change for the Research School of Chemistry and for the Australian National University. During the year the University began to organise itself into ANU Colleges. The Research School of Chemistry is a member of the largest College namely the College of Science (CoS) which by choice is a Federated College with the internal members remaining independent. I was appointed as Convenor of the College of Science and I work closely with the Dean of CoS, Professor Tim Brown, and the College Executive. We aim to improve the efficiency and effectiveness of our education and research programs through better planning and coordination across the Science Faculty and Science Research Schools of the ANU.

One concrete example of the increased coordination afforded by CoS was announced in December. From the beginning of 2006 Professor David Ollis of the RSC will move to a joint appointment as Head of the Department of Chemistry in the Faculty of Science. One of David's aims will be to increase the biochemical content of the undergraduate curriculum. This is a perfect example of one of the main aims of the ANU Colleges. The RSC has a major research program in biological chemistry, which at the moment is not mirrored in the undergraduate teaching program. The CoS will help to facilitate this improved alignment of undergraduate curriculums with our postgraduate research programs.

Late in the year there were two very happy developments in the School. Associate Professor Mick Sherburn was awarded the prestigious Le Fèvre Medal of the Australian Academy of Science. Just after Christmas Dr Michelle Coote was promoted to Fellow and was granted tenure. These events were exceptionally pleasing. I was also delighted to present the 2005 Dean's Award for General Staff Excellence to Bob O'Brien who willingly takes on many and varied tasks, often assigned to him at short notice.

Professor Chris Easton took a leading role in a successful application for an ARC Centre of Excellence – The Centre for Free Radical Chemistry and Biotechnology. Other RSC staff involved in the Centre include Associate Professor Mick Sherburn and Dr Michelle Coote. A second initiative during the year involving Professors Chris Easton, Nick Dixon and David Ollis, was the successful bid for a CSIRO Emerging Science Initiative – Synthetic Enzymes for Synthetic Chemistries – in collaboration with CSIRO Entomology and CSIRO Molecular and Health Technologies.



## 2005 RESEARCH HIGHLIGHTS

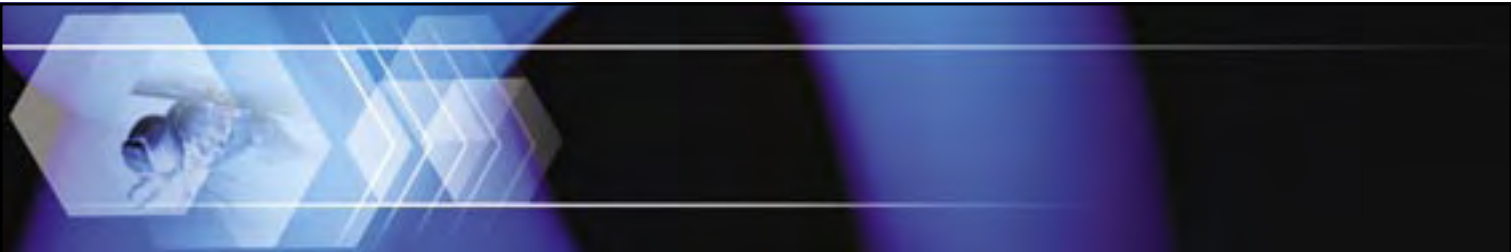
**From Professor Peter Gill's group:** The Hartree–Fock energy of a system is the energy that it would have if each electron felt only the average effect of all of the others. The error of the Hartree–Fock approximation is called the correlation energy  $E_c$  and, in order to predict chemical behaviour from quantum mechanical first principles, it is important to calculate  $E_c$  accurately. Traditionally, this has been very complicated and time-consuming but, recently, we made the radical proposal that  $E_c$  can be found relatively simply from knowledge of the positions and momenta of pairs of electrons in the system. Our first detailed discussion of this was chosen as a "Hot Article" in *Phys. Chem. Chem. Phys.* and was highlighted on the front cover of the first 2006 issue of that journal. As one reviewer wrote, "Since really novel approaches to obtaining molecular energies arise only occasionally (the last one was probably density functional approximations), this is a potentially very exciting development."

**Ms Iris Li from Professor Chris Easton's group** presented her work on the development of enzyme inhibitors to regulate the over-production of mammalian peptide hormones at the Gordon Conference on Free Radicals in New Hampshire, USA, and as a result of that presentation, was invited to present a lecture to the Conference. Gordon Conferences are for the top specialists in the field and only the top few percent of presentations are ever selected for invited lectures – so this was quite an honour for Iris.

**Dr Michelle Coote and her group** used computational chemistry to design the first multipurpose RAFT agents (fluorodithioformates), capable of controlling the polymerisation of monomers with disparate reactivities. Although designed entirely by computer they have subsequently been synthesised by collaborators at UNSW and demonstrated experimentally to control polymerisation. Computer-aided chemical design was also used to design a new route to polyphosphines and a new method for controlling free-radical polymerisation using thioketones as radical spin traps. The illustration (right) featured on the cover of *Chemical Communications* (Ah Toy A, Chaffey-Millar H, Davis T P, Stenzel M H, Izgorodina E I, Coote M L, Barner-Kowollik C, *Chem. Commun.* (2006) (8), 835-837, <http://dx.doi.org/10.1039/b515561d> and signifies their method for controlling free-radical polymerisation using thioketone spin traps.



**A novel NMR spectroscopic technique was developed in the Otting/Keniry groups** that allows the rapid determination of the three-dimensional (3D) structures of protein–protein complexes. The method starts from the known structures of the individual protein molecules (determined by previous X-ray or NMR studies) and uses the effects from paramagnetic lanthanide ions on the  $^1\text{H}$ -NMR spectra to establish the relative orientation and positioning of the protein molecules with respect to each other. The attraction of the method lies in the fact that only a few NMR signals of each protein need to be assigned and that these assignments can be obtained in an automatic manner based on the 3D structures of the proteins and few NMR spectra recorded of selectively  $^{15}\text{N}$ -labelled protein samples. The method was demonstrated with the complex of the  $\epsilon$  and  $\theta$  subunits of DNA polymerase III, whose structures had been determined separately in collaborations among the Keniry, Ollis, Dixon and Otting groups.



## MISSION STATEMENT

Consistent with the **Australian National University Act** and with the Australian National University's aspiration to be one of the world's great research institutions, the Research School of Chemistry has established itself as a national and international centre of excellence. In order to maintain and enhance that position, the School proposes to:

- maintain its research and scholarship in the chemical sciences at the highest international standards
- foster the advancement of fundamental knowledge in chemistry with special reference to research of national importance and activities that not only strengthen the discipline of chemistry in the Australian context, but also contribute to cognate research fields both within and outside the University
- provide the best possible training and education of graduate students and postdoctoral fellows
- nurture the career development of early career academic staff
- encourage links with other Australian universities and cognate research organisations that enable the intellectual and material resources of the School to be broadly utilised by the Australian research community
- develop links that enable the Australian community, industry, and government to benefit from the scholarship and research undertaken in the School
- maintain and enhance international networks that benefit the University and the Australian community



## SENIOR STAFF

<b>Dean:</b>	Professor Denis J Evans
<b>Deputy Dean:</b>	Professor Christopher J Easton
<b>Associate Dean (Students):</b>	Professor Raymond L Withers
<b>Group Leaders:</b>	Professor Martin G Banwell BSc PhD <i>Wellington</i> , FWIF, Hon FRSNZ, FRACI, FAA Professor Michael A Collins BSc PhD <i>Sydney</i> Dr Michelle L Cooté BSc PhD <i>New South Wales</i> Professor Nicholas E Dixon BSc PhD <i>Queensland</i> Professor Christopher J Easton BSc <i>Flinders</i> PhD DSc <i>Adelaide</i> , FRACI, FAA Professor Denis J Evans BSc <i>Sydney</i> PhD <i>ANU</i> , FRACI, FAA Professor Peter M W Gill MSc (Hons) <i>Auckland</i> PhD <i>ANU</i> Dr Graham A Heath BSc PhD <i>Melbourne</i> Professor Anthony F Hill MSc (Hons) <i>Auckland</i> DrRerNat <i>Bayreuth</i> , FRSC Dr Max A Keniry BSc PhD <i>Sydney</i> Professor Elmars R Krausz BSc PhD <i>Sydney</i> , FRACI Professor Emeritus Lewis N Mander (Adjunct) MSc <i>Auckland</i> PhD <i>Sydney</i> , FRACI, FAA, FRS Dr Aaron J Oakley BSc <i>Tasmania</i> PhD <i>St Vincent's IMR Melbourne</i> Professor David L Ollis BSc <i>New South Wales</i> PhD <i>Sydney</i> Professor Gottfried Otting Dipl <i>Freiburg</i> PhD <i>ETH Zürich</i> Associate Professor Edith M Sevick BSE <i>Pittsburgh</i> PhD <i>Massachusetts</i> Associate Professor Michael S Sherburn BSc PhD <i>Nottingham</i> Professor Richard T Welberry MA <i>Cambridge</i> PhD <i>London</i> Professor John W White CMG MSc <i>Sydney</i> MA DPhil <i>Oxford</i> , FAPS, FRACI, FRSC, FAA, FRS Professor S Bruce Wild BSc <i>New South Wales</i> PhD <i>Manchester</i> , FRACI, FRSC, FAA Professor Raymond L Withers BSc PhD <i>Melbourne</i>
<b>Laboratory Manager:</b>	Ms Lesley Harland
<b>Academic Secretary:</b>	Ms Marilyn A Holloway

# PROTEIN STRUCTURE AND FUNCTION

PROFESSOR NICK DIXON



Some proteins are enzymes that promote chemical reactions; others provide molecular switches that control metabolic and developmental processes through precise interactions with other proteins, nucleic acids and other ligands. We aim to understand the chemistry that governs the specificity and strength of interactions of proteins with substrates, inhibitors, nucleic acids, and other proteins.

As a model system, we use the thirty different proteins that collaborate to replicate the DNA of the bacterial chromosome prior to cell division. DNA replication presents a good system to study general aspects of protein–protein and protein–nucleic acid interactions because the proteins act together in a giant nucleoprotein assembly called the replisome, which makes perfect copies of the chromosomes. We use molecular genetics to engineer rich sources of the proteins and to produce mutant derivatives and segments of them, and conventional enzymology, DNA synthesis assays, protein chemistry and biophysical techniques like surface plasmon resonance to study protein function and molecular interactions. This is complemented by structural and spectroscopic studies in collaborating laboratories, using techniques that include protein X-ray crystallography, ESR and high-field NMR spectroscopy, mass spectrometry, electron microscopy and computational methods. This enables us to relate the structures of proteins and complexes to how they work and interact with each other and with DNA. This year, we have focused our efforts on how the interaction of the replicative helicase (DnaB) with the replication terminator protein arrests progress of the replisome. We have also studied interactions among the ten different subunits of the replicative DNA polymerase, DNA polymerase III holoenzyme (Pol III HE).

Many of the replication proteins are also being used for development of a suite of new techniques in protein chemistry, including methods for *in vitro* evolution of new protein functions, *in vitro* synthesis of proteins on a preparative scale, library methods for precise location of boundaries between distinct folded domains in larger proteins, and stabilisation of small protein domains by end-to-end cyclisation of their polypeptide chains. Used together, these techniques are helping to overcome some of the bottlenecks in rapid determination of protein structures and functions, thereby increasing the efficiency of worldwide efforts in structural and functional genomics. They are also being used to study the fundamental chemistry that underpins the relationship between the structure, folding, stability and functions of proteins.

## Intrinsically-unstructured Interaction Domains

The replisome contains two molecular motors that interact with each other. One is Pol III HE, the machine that synthesises the new DNA chains, and the other is the ring-shaped hexameric helicase (DnaB) that drives the replication machinery while separating the two strands of DNA at the apex of the replication fork. Pol III HE contains 10 subunits: a catalytic core ( $\alpha$ ,  $\epsilon$  and  $\theta$ ), a sliding clamp ( $\beta_2$ ), and the six subunits of the clamp loader ( $\delta$ ,  $\delta'$ ,  $\gamma$ ,  $\tau$ ,  $\chi$  and  $\psi$ ). We routinely prepare large quantities of all of the subunits, then mix them to isolate the many sub-complexes for structural studies. A few years ago we proposed that the replisome presents a new paradigm for such flexible, dynamic molecular machines, in particular that many of the protein–protein interactions occur through intrinsically-unstructured regions (domains) that attain their folded forms only when the interactions occur. In work this year, we have shown this to be true, at

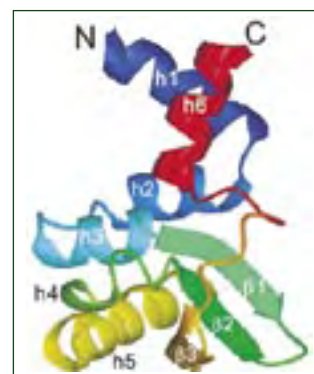


Figure 1: Structure of the folded core of the C-terminal domain of  $\tau$ .



least in some cases. In collaborative work with the Biomolecular NMR group, we determined the molecular structure of the folded domain of the  $\tau$  subunit that distinguishes it from  $\gamma$  (Figure 1). Although this domain contains the regions of  $\tau$  that interact with the  $\alpha$  subunit of Pol III and DnaB, the major sites of interaction are not in its structured region, but in the flexible regions that flank it. In other work, we showed that  $\psi$  interacts with  $\gamma$  through its intrinsically unstructured N-terminal region, and NMR and crystallographic studies of the structure and function of the  $\epsilon$  proofreading exonuclease subunit have continued in collaboration with Professors Gottfried Otting and David Ollis, Drs Max Keniry and Gary Schenk. (With P D Carr, M J Headlam, S Jergic, M John, M A Keniry, K V Loscha, A J Oakley, D L Ollis, G Otting, K Ozawa, A-Y Park, P Prosselkov, P M Schaeffer, X-C Su, N K Williams, P S C Wu, and E Liepinsh [Latvian U, Riga], G Schenk [U Queensland])

## Replication Termination

In the final stage of replication, forks encounter the terminator protein Tus in complex with *Ter*-site DNA, and are arrested in a polar manner – a replisome approaching from the one face of the Tus-*Ter* complex can progress, while another approaching from the other face is blocked. We showed that this process works like a molecular mousetrap that is set by DNA strand separation by DnaB, and sprung to create a structure that is kinetically trapped by unusually stable binding of the *Ter* DNA to Tus. This year, we confirmed the mechanism that determines polarity by solving the structure of the arrested "Tus-*Ter* Lock" complex (Figure 2). (With M Mulcair, A J Oakley, P M Schaeffer, and T M Hill [U North Dakota], C Neylon [U Southampton])

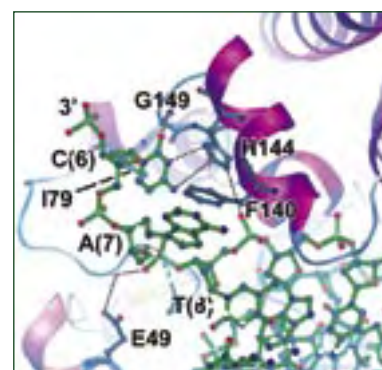


Figure 2: Structure of the arrested "Tus-*Ter* Lock".

## New Protein Technologies



Figure 3: Synthetic resilin. See Elvin *et al.* *Nature* (2005) 437, 999.

In collaboration with several other groups, new methods are being developed for *in vitro* molecular evolution of proteins with new functions, for intein-mediated end-to-end cyclisation of protein domains and peptides, for preparative *in vitro* protein synthesis and labelling for NMR studies, for site-specific incorporation of unnatural amino acids and paramagnetic lanthanide ions into proteins, for the use of library methods for protein domain identification, and for use of mass spectrometry in studies of protein-ligand complexes. A highlight this year was the publication in *Nature* of a method for preparation of a synthetic biopolymer that closely mimics the properties of resilin (Figure 3), the rubbery material that occurs in the wing hinges of insects, the legs of jumping fleas, and the tymbal organs of cicadas. (With M J Headlam, M Mulcair, G Otting, K Ozawa, A-Y Park, P Prosselkov, P M Schaeffer, N K Williams, and K Alexandrov, A Rak [Max-Planck Institute for Molecular Physiology, Dortmund, Germany], J L Beck, M M Sheil [U Wollongong], G Coia [EvoGenix, Melbourne], C M Elvin [CSIRO Livestock Industries, Brisbane], D Spencer, H-X Zhou [Florida State U])



# NUCLEAR MAGNETIC RESONANCE

DR MAX KENIRY

One of the great challenges of contemporary Nuclear Magnetic Resonance (NMR) spectroscopy is the application of the technique to highly complex problems in biology. No other form of spectroscopy can contribute to the elucidation of the structure, function and dynamics of biomacromolecules at the atomic level. Our research is focused on the following three broad areas: the structure of complexes between DNA and anticancer antibiotics; the structure of unusual forms of DNA that have biological significance; and the structure and function of moderately sized proteins with a special focus on proteins that bind to DNA and RNA. Work has just been completed on structural studies of a large protein-protein complex and work is continuing on the structures of two small biologically important human proteins. The investigation of the interaction of spermine and calothrixin with various forms of DNA continues to give surprising results. As our expertise in macromolecular structure determination increases we intend to tackle more demanding structural problems. In the near future, we will attempt the structure determination of the *N*-terminal and *C*-terminal domains of a 42 kDa protein that is over expressed in the cells of early breast cancer tumours and the structure determination of an RNA-binding protein. The ultimate goal of this work is to use the structure of the protein to design drugs that may be used to block the progression of the tumour cells. The major theme of our work is to deduce the function of biological molecules and complexes from knowledge of their structure and dynamics at the atomic level.

## NMR Studies of the Interaction of Spermine with Oligonucleotides

Spermine, an aliphatic polycationic molecule found in all cells, plays an essential role in cell growth and differentiation. At present, there is no thorough understanding of how polyamines exert their physiological effects. Spermine is known to interact both with DNA and with proteins, yet the details of these interactions and the molecular basis of the biological function of spermine are poorly understood. There is evidence in the literature that spermine interacts with different forms of DNA in distinct and divergent modes. We have confirmed this and have characterised the complexes of spermine with duplex B-DNA and G-DNA using a specifically  $^{13}\text{C}$ -labelled spermine and advanced NMR techniques to take advantage of the specific isotope label on spermine. Quantitative analysis of the field dependence of  $^{13}\text{C}$   $T_1$  and  $T_2$  relaxation times and homonuclear and heteronuclear NOEs have been used to characterise the dynamics of spermine in the presence of different forms of DNA. The fast internal motion of spermine is slowed by two orders of magnitude on binding to all forms of DNA. Only in the case of folded DNA quadruplexes is there evidence of a slower motion associated with overall tumbling of the macromolecular structure and an exchange process between two or more different binding sites. *(With K Clayton)*

## Novel Antibiotics and DNA

Calothrixin A and B are novel pentacyclic metabolites from cyanobacteria that exert growth-inhibitory effects at nanomolar concentrations against rapidly proliferating cell cultures. The binding properties of the calothrixins and their synthetic analogues with various structural forms of DNA are under investigation by NMR, circular dichroism and fluorescence. Calothrixin binds to linear quadruplexes as shown by UV, CD and NMR spectroscopy. *(With E A Owen, R W Rickards, and C Chai, M Waring [Dept Chemistry, ANU], G D Smith [BaMBi, ANU])*

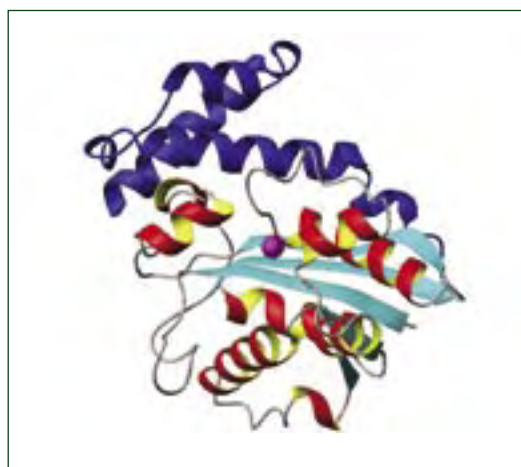


## HuR, a Protein that Modulates the Stability and Lifetime of mRNA

Hu proteins control the post-transcriptional expression of proteins by binding to and modulating the decay rates of mRNA. We have cloned a splice variant of one of these Hu proteins, HuR, with the aim of pursuing structural studies. (With N E Dixon, P Prosselkov, and C C Benz, G Scott [Buck Institute for Age Research, USA])

## Interaction of the $\theta$ -subunit and the $\epsilon$ -subunit of DNA Polymerase III

The catalytic core of *Escherichia coli* DNA polymerase III contains three tightly associated subunits ( $\alpha$ ,  $\epsilon$ , and  $\theta$ ). The refinement of the three-dimensional structure of the  $\theta$ -subunit was completed by the NMR group. The  $\theta$ -subunit has three  $\alpha$ -helices in the *N*-terminal two thirds of the protein that fold to form a three helix bundle. As part of a program aimed at understanding the molecular mechanism of the core, we have set out to investigate the association of the  $\theta$ - and  $\epsilon$ -subunits. The structure of the  $\theta$ -subunit bound to  $\epsilon$  has been refined using an innovative technique that combines NOE restraints with distance and orientation restraints calculated from a paramagnetic centre located in the active site of  $\epsilon$ . We have mapped the binding surface of  $\epsilon$  on  $\theta$  to a hydrophobic patch on  $\theta$  using advanced NMR techniques. The structure of the complex between  $\theta$  and  $\epsilon$  has been assembled using the same paramagnetic restraints that were used to refine the structure of  $\epsilon$ . The final structure and alignment is shown below. (With N E Dixon, S Hamdan, G Otting, A-Y Park, G Pintacuda, T K Ronson, and S E Brown [CSIRO Entomology])



The three-dimensional structure of the  $\theta\epsilon$  complex.  $\theta$  is shown in blue and the lanthanide ion in the catalytic pocket of  $\epsilon$  is shown as a magenta ball located at the  $\epsilon$  active site.

## ESX, a Protein Over Expressed in the Early Stages of Epithelial Breast Cancer

ESX is a protein that belongs to the Ets family of transcription factors. Ets proteins exhibit diverse roles in development, cell-differentiation and tissue-specific gene expression and are implicated in cancers such as acute myeloid leukemia and Ewing's sarcoma. The ESX transcription factor may have a role in the activation of the HER2/neu oncogene, which is over expressed in over 40% of breast tumours. To this end we have over expressed ESX and its *C*-terminus containing the two DNA-binding domains. Attempts will be made to crystallise these proteins. This project is supported, in part, by a Yamagiwa-Yoshida travel grant from the International Union against Cancer. (With N E Dixon, P Prosselkov, and C C Benz, G Scott [Buck Institute for Age Research, USA])





# STRUCTURAL BIOLOGY

DR AARON OAKLEY

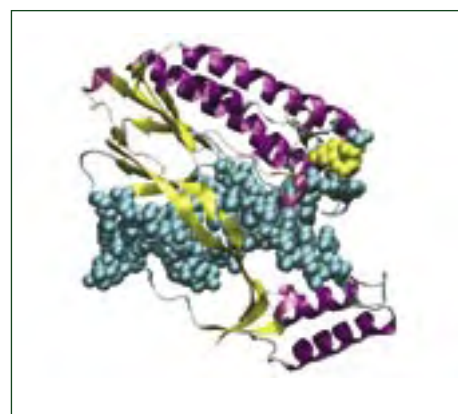
At a fundamental level, living processes are driven by the chemistry of biomolecules such as proteins and DNA. Understanding the chemistry of life requires detailed information about the structures of the molecules involved. Why is this important? Many advances in medicine, biotechnology and industry result from understanding of these processes. Within this broad sphere, my group conducts fundamental and applied research:

## Cofactor Free Oxygenases

Divergent evolution in enzymes is poorly understood. While there are numerous examples of related enzymes catalysing identical chemistries, little is known about how novel chemistries arise. We have crystallised an enzyme called QDO, which is a member of the  $\alpha/\beta$ -hydrolase superfamily. Most members of this very large group of enzymes catalyse hydrolysis reactions. QDO however is a cofactor free oxygenase, catalysing a reaction that is fundamentally different from its close relatives. By solving the structure of this enzyme we hope to gain insight into how the  $\alpha/\beta$ -hydrolase fold has been adapted to cofactor free oxygenase chemistry. *(With R Qi, and S Fetzner [U Oldenburg, Germany])*

## Termination of DNA Replication in Bacteria

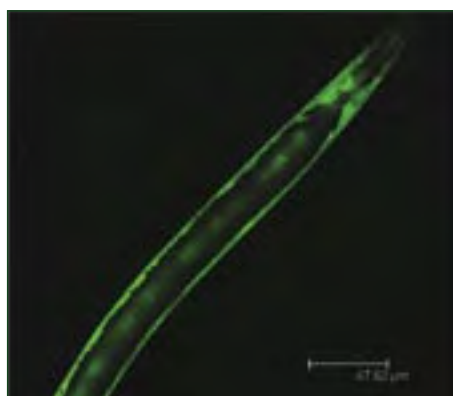
Bacterial DNA replication is halted at specific sites on the chromosome called *Ter* sites. A protein called Tus recognises and binds to these *Ter* sites. Recent work in the Dixon group has shown that by breaking a specific DNA-base-pair interaction, Tus bind more tightly to DNA, preventing the replisome from progressing. We have recently determined the structure of this locked form of the Tus-*Ter* complex. *(With N E Dixon, M D Mulcair, P M Schaeffer)*



Cartoon representation of the "locked" Tus-*Ter* complex.

## Nematode Proteins: Potential Drug Targets

Nematodes, commonly known as round worms, are the most numerous multicellular organisms on earth. There are tens of thousands of different



The nematode *C. elegans*.

species; most are free living and some are significant parasites to animals, humans or plants. As such, there is a need for new drugs against parasitic nematodes. We have identified a number of proteins that are potential drug targets, and are working to solve the structures of these proteins with a view to structure-based drug design. *(With P Lloyd, C Behm [BaMBi])*

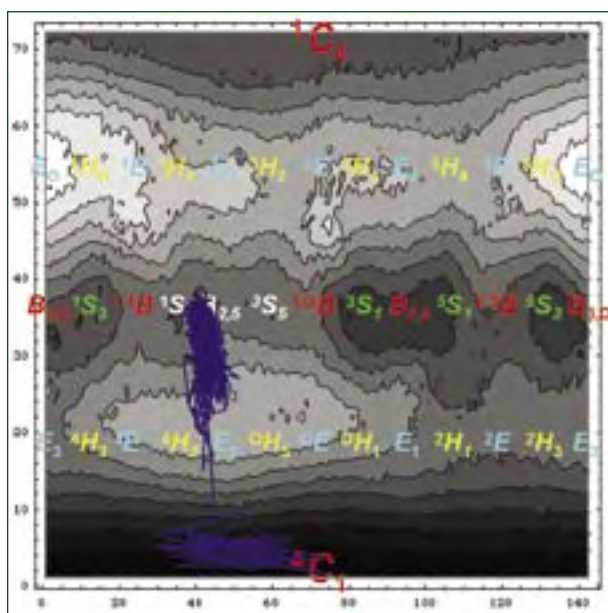


## Human Omega-class Glutathione S-transferases

The omega class glutathione S-transferases (GSTO) play a central role in the metabolism of arsenic and in the recycling of vitamin C in the brain. Genetic polymorphisms may alter their structure and function and cause individual variations in toxicity and response to arsenic. We are examining the structure of GSTO in complex with its substrates as well as the structures of mutants resulting from genetic polymorphisms found in the population. (With P G Board, R Baker [JCSMR, ANU])

## Conformational Changes in Glucopyranose Rings During Catalysis

Sugars and their polymers are of importance to such diverse areas as immunity and paper bleaching. In order to better understand the enzymes that cleave sugars, we have mapped energy landscapes of glucopyranoses commonly found in nature using empirical force fields. We are using these force fields to examine the transitions that sugar rings undergo when bound to enzymes prior to cleavage. Using molecular dynamics simulations, we have mapped the transition of mannoside residues from  ${}^4C_1$  chair-conformation to  ${}^1S_5$  skew-boat conformation in a bacterial *endo*- $\beta$ -mannanase. The conformation degrees of freedom of the sugar can be decomposed into two essential degrees of freedom and plotted (see below).



Conformational mapping of a mannoside residues as it transits from  ${}^4C_1$  chair-conformation to  ${}^1S_5$  skew-boat conformation (blue line). Here, the energy ranges from low (black) to high (white).

<http://rsc.anu.edu.au/research/oakley.php>



# PROTEIN CRYSTALLOGRAPHY AND ENGINEERING

PROFESSOR DAVID OLLIS

The group works at the interface between chemistry and biology. Our major interest is in working out how proteins function and how they might be modified for new and useful purposes. Directed evolution is used to produce mutant proteins that frequently have interesting properties that can be utilised in industrial and environmental applications. These mutants can also be analysed using a variety of techniques, including X-ray crystallography, to further understand the detailed mechanics of protein function.

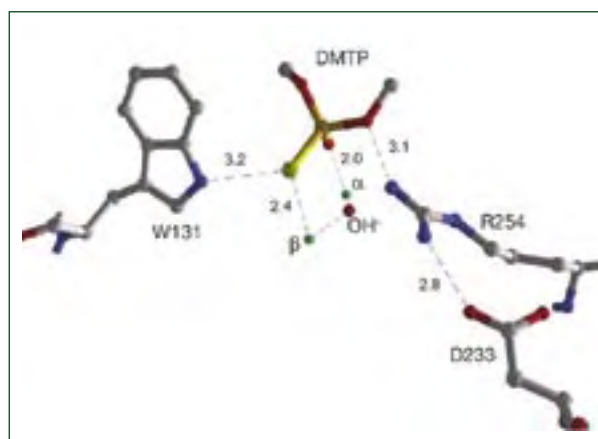
In the past year, we have developed a technique to evolve the proteins to be more soluble. We have also used directed evolution to enhance the expression of an organophosphate degrading enzyme from *Agrobacterium radiobacter* (OPDA). Other papers have focused on the mode action of OPDA – the structure of the protein in the presence of its reaction product has been determined. We have also published the results of a long-term study that involves the evolution and structure analysis of mutant forms of the enzyme dienelactone hydrolase (DLH). The results of this study show how mutations change the way DLH interacts with inhibitors and substrates.

## Improving Protein Solubility

Structure function studies are frequently limited by the availability of large quantities of soluble protein. We have developed a procedure for selecting soluble variants of an insoluble protein. The procedure utilises the enzyme dihydrofolate reductase (DHFR) that is inhibited by the antibiotic trimethoprim (TMP). In our procedure, a mutant library of an insoluble target protein is fused to that of dihydrofolate reductase. Variants of the target protein that have enhanced solubility can be selected on the basis of their ability to overcome the normally lethal effects of TMP. This technique can be used to enhance the solubility of proteins for structural genomics studies. *(With J-W Liu)*

## Enzyme Engineering with an Organophosphate Degrading Enzyme

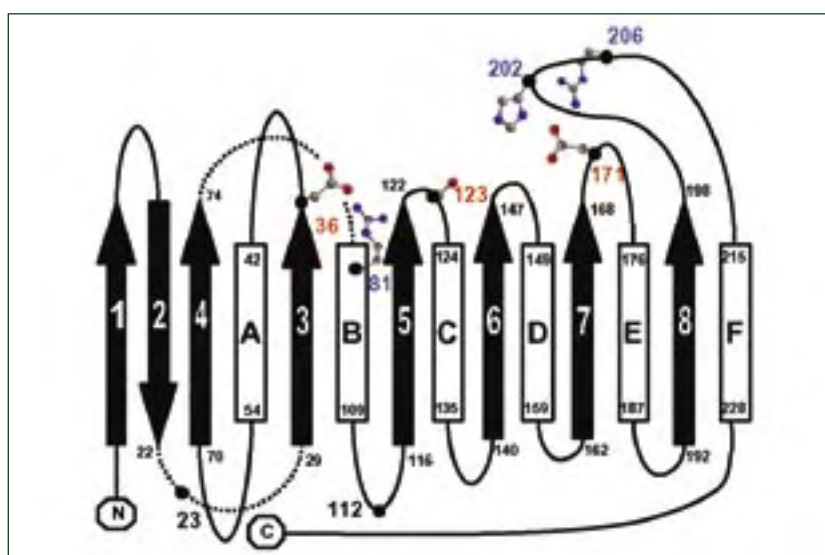
OPDA is a bacterial enzyme that shows considerable utility in bioremediation. The protein was initially discovered in the laboratory of John Oakeshott in the Division of Entomology, CSIRO. In the past years we have obtained the structure of OPDA while more recently our attention has been directed towards evolving the enzyme so that it is more efficiently expressed in *Escherichia coli*. We have also been involved in studies to better understand the mechanism of the protein and to this end we have solved the structure of the protein in the presence of its reaction product. *(With C Jackson, P D Carr, J-W Liu, S Yu-McLoughlin)*



Dimethyl monophosphate (DMMP) in the active site of OPDA. The diagram shows the active site residues that interact with the reaction product.

## The Structure of Evolved Form of Dienelactone Hydrolase

Dienelactone hydrolase (DLH) is a bacterial enzyme involved in the degradation of aromatic compounds. It is the smallest member of the  $\alpha/\beta$  hydrolase fold class of proteins. In previous years, the structure of DLH was obtained, its active site identified, and a catalytic mechanism proposed. More recently, we have altered the enzymatic activity of DLH with directed evolution. We have examined the structure of DLH in the presence and absence of inhibitors so that we can determine how the mutant forms of the enzyme interact with substrates. (With H-K Kim, J-W Liu, P D Carr)



Schematic diagram of DLH with secondary structure elements represented by arrows ( $\beta$  strands) and rectangles ( $\alpha$  helices). The side-chains of key catalytic residues are shown in atomic detail.



# BIOMOLECULAR NMR

PROFESSOR GOTTFRIED OTTING



The group develops novel tools for biomolecular applications of NMR spectroscopy. Emphasis is placed on extending the range of protein targets that can be investigated by NMR in pharmaceutical drug development. Thus, methods are developed for rapid identification and characterisation of ligand binding sites, including protein-protein and protein-DNA interactions. In addition, NMR is used to determine the three-dimensional (3D) structures of proteins and protein domains. This research is supported by an 800 MHz NMR spectrometer with cryoprobe.

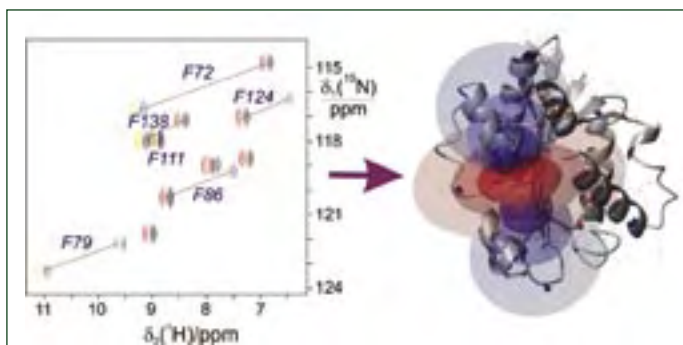


Figure 1: From NMR spectra to resonance assignment, structure determination and interaction studies of proteins. A wealth of structural information is gained by labelling with a paramagnetic ion. Isosurfaces of the anisotropic magnetic susceptibility (blue and red) are superimposed on the structure of the *N*-terminal domain of the proofreading exonuclease epsilon.

We discovered that site-specific labelling of a protein with a lanthanide ion provides access to the 3D structures of protein-protein and protein-ligand complexes with unprecedented ease and speed. Furthermore, if the 3D structures of the individual components in the complex are known, the lanthanide label makes the assignment of NMR spectra straightforward.

We are currently synthesising different compounds that allow the site-specific labelling of proteins with lanthanide ions. These will allow us to attach lanthanide ions to proteins that don't have a natural ion binding site. In particular we are aiming for ways of attaching lanthanide ions to proteins synthesised in cell-free extracts. Cell-free protein synthesis techniques are being refined in collaboration with Professor Nicholas Dixon. It provides fast and inexpensive access to  $^{15}\text{N}$ -labelled proteins that we can analyse by NMR spectroscopy without prior purification.

Labelling proteins with lanthanide tags opens up a wide range of applications that were hitherto difficult or impossible to address by NMR or other methods. For example, they will provide a tool for 3D structure determination of small regions in large proteins, *i.e.* to "zoom" in on a region of a protein and study its structure without having to analyse the rest of the protein. It has long been known that lanthanides confer structural information. The lanthanide tagging approach promises to broaden these applications considerably. As one of the most exciting applications, we are currently evaluating the possibility of using lanthanides to gain information about the orientation of small chemicals (drug candidates) as they bind to protein targets. In a different project, we are investigating the use of lanthanide labels to characterise large amplitude motions of proteins with unprecedented accuracy.

The highlight of the year was the installation of the cryoprobe on the 800 MHz NMR facility. This completed the installation of the system that presents the highest magnetic field available for NMR in Australia. Purchased with support



from the Australian Research Council, ANU, U Sydney, UNSW, U Wollongong, U Newcastle and UNSW College at ADFA, the spectrometer is set up for remote operation so that it can be operated by interstate users from their desktop computers *via* the internet.

Continuing major collaborators are Professor Nicholas Dixon and Dr Max Keniry, Dr Thomas Huber (U Queensland), Drs Edvards Liepinsh, Anatoly Sharipo (Latvian U), Dr Guido Pintacuda (École Normale Supérieure de Lyon) and Dr Laszlo Patthy (Hungarian Academy of Sciences).

## Docking of Proteins of Known 3D Structure Using Paramagnetic NMR

The 3D structure of the 30 kDa  $^{15}\text{N}$ -labelled complex formed between the *E. coli* proteins epsilon and theta was determined. The 3D structures of epsilon and theta were known from crystallography and NMR, respectively, and the paramagnetic NMR data generated by different lanthanide ions bound to epsilon were used to dock the two protein molecules. The structure of the complex was verified by conventional NMR methods. (With N E Dixon, M A Keniry, A-Y Park, and G Pintacuda [École Normale Supérieure de Lyon])

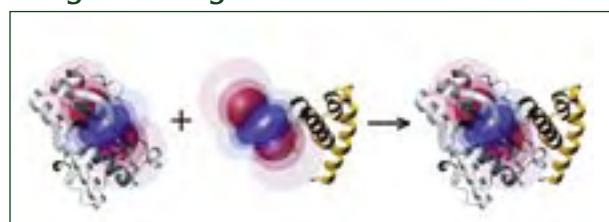


Figure 2: Isosurfaces of the anisotropic magnetic susceptibility (blue and red) are superimposed on the structures of the N-terminal domain of  $\epsilon$  (left) and of  $\theta$  (middle). The isosurfaces originate from the same lanthanide ion, i.e. their superposition yields the complex (right). It's simple!

## Cell-free Synthesis of Residue-selectively Isotope Labelled Proteins

The cell-free expression system available in Professor Nicholas Dixon's laboratory was used to express samples of a number of selectively  $^{15}\text{N}$ -labelled proteins. NMR spectra were recorded straight from the reaction medium.

A combinatorial  $^{15}\text{N}$ -labelling scheme was developed that allows the identification of all  $^{15}\text{N}$ -HSQC cross-peaks by their amino acid type from no more than five samples. In a separate project, the nascent state of the proteins produced *in vitro* was shown to allow the formation of correctly folded complexes with soluble binding partners. This presents access to complexes, where only one partner is isotope labelled. (With N E Dixon, K Ozawa, P S C Wu, M J Headlam, S Jergic)

## Structure Dependent Modulation of Paramagnetic Shifts

Paramagnetic ions bound to proteins weakly align the proteins in the magnetic field. This gives rise to residual dipolar couplings that contain valuable structural information. For nuclear spins with pronounced chemical shift anisotropy (CSA), however, this effect results in paramagnetic shifts that depend not only on their position with respect to the paramagnetic ion (Figure 1), but also on the orientation of their CSA tensor with respect to the alignment tensor. A careful evaluation showed that the CSA correction is noticeable at 800 MHz, but negligible at 600 MHz and lower magnetic fields. (With M John, A-Y Park, N E Dixon, and G Pintacuda [École Normale Supérieure de Lyon])

## Protein Structure Determinations

The 3D structures of the C-terminal domain of the subunit  $\tau$  of the *E. coli* DNA replisome, of the subunit  $\theta$  in complex with the N-terminal domain of the subunit  $\epsilon$  and of the  $\epsilon$ - $\theta$  complex were determined. (With X-C Su, S Jergic, A-Y Park, N E Dixon, M Keniry, and G Pintacuda [École Normale Supérieure de Lyon])



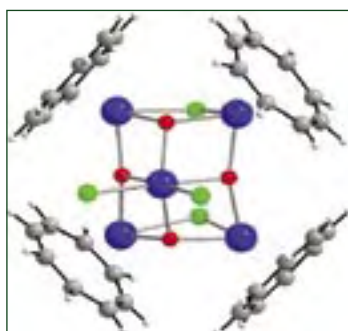
# SYNTHETIC ORGANOMETALLIC AND COORDINATION CHEMISTRY

PROFESSOR ANTHONY HILL

Our work covers a diversity of challenges in coordination and organometallic chemistry. Particular foci include unsaturated ligands involving metal-carbon multiple bonding and the interface of transition and main group chemistries. In attempting to understand and, ideally, control the reactivity of such systems, the nature of the metal centre is of paramount importance; this may be tuned through variations in oxidation state, d-configuration and, most importantly, the nature of the co-ligands. Accordingly, considerable effort is directed towards the synthesis of new co-ligands which themselves do not necessarily take part in the transformations of other ligands but may moderate these indirectly.

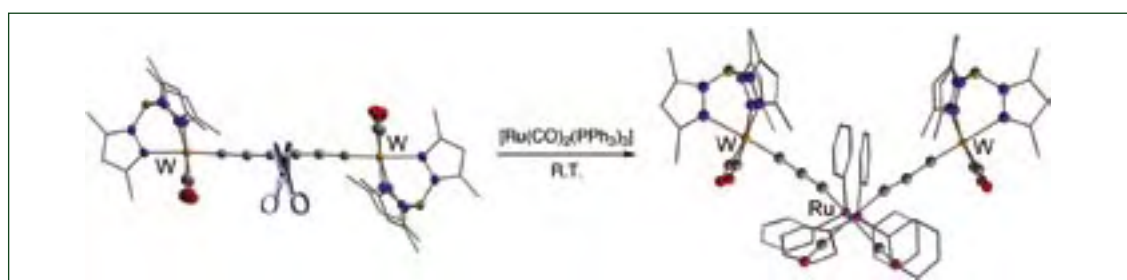
## Cyclooctatetraene ( $C_8H_8$ ) Chemistry

We have initiated a study of the chemistry of coordinated cyclooctatetraene ( $C_8H_8$ ), specifically involving the early transition metals. The key feature of  $C_8H_8$  in an organometallic context is that it may, as a ligand, provide 2, 4, 6 or 8 valence electrons to a metal centre and this is manifest in the adopted geometry. We have thus used the hapticity of  $C_8H_8$  as a 'reporter' to assess the nature of bonding of other co-ligands. Specifically, the facility with which poly(azolyl)borate ligands may enter into 3-centre, 2-electron B-H-Metal interactions has been assessed with respect to the synthesis of a range of complexes of the form  $[ZrCl(C_8H_8)(L)]$  ( $L = H_2B(pz)_2, H_2B(mt)_2, HB(pzMe_2)_3$  etc). Tangential to the systematic chemistry, we have isolated an aesthetically beautiful side product (shown) that comprises a pyramidal array of five zirconium centres bridged by oxide and chloride ligands and encapsulated by four planar cyclooctatetraene ligands. *(With M K Smith)*



## Carbon Wires with Metal Carbon-multiple Bonding

It has long been argued that connecting two metals by a linear chain of carbon atoms would provide a means of electronic communication between the metals - 'a carbon wire'. Reflecting their ease of synthesis, effort has generally focused on poly-yne-diyl carbon chains that bind to the metal centres as simple  $\sigma$ -acetylides with at best modest retrodonation into the unsaturated  $\pi$ -system of the carbon spacer. Our approach has been to turn to the strongest known  $C_1$ - $\pi$ -acid ligands - alkylidynes with metal-carbon triple bonds - on the grounds that metal to ligand charge transfer will be most favoured in such systems. Recent advances within the group have included the first examples of dimetallaocotatetraynes for which a valence-localised bonding description of the form  $L_n W \equiv C-C \equiv C-C \equiv C-WL_n$  has been shown to be appropriate as distinct from the more





common  $L_nM-C\equiv C-C\equiv C-C\equiv C-ML_n$  description for a hexacarbido linkage. Lessons learned from the discovery of such species have now led us to a '3+1' synthetic strategy for the synthesis of both symmetrical and non-symmetrical dimetallahexatriynes of the form  $L_nW\equiv C-C\equiv C-C\equiv ML_n$  ( $M = Mo, W$ ). We have also now considered the functionalisation of carbon wires. One of the most versatile methods for alkyne functionalisation involves hydrometallation of  $-C\equiv C-$  bonds. We have now shown that this may be extended to carbon wires and reported the first such reaction leading to complexes in which two metals are spanned by the 'C<sub>6</sub>H' ligand to which is also appended a third metal, thus paving the way for protocols allowing the decoration of carbon wires with further tangential metal centres. Our synthesis of the first dimetallaooctatetraynes involved the coupling of two tricarbido-metal precursors. In a remarkable reverse of this process we have reported the cleavage of one Csp-Csp bond of a carbon wire to provide complexes in which the third metal is inserted into the carbon chain. (With R D Dewhurst, M K Smith, A C Willis)

### Alkyne-alkylidyne Coupling and Chalcogenolate Migration Process

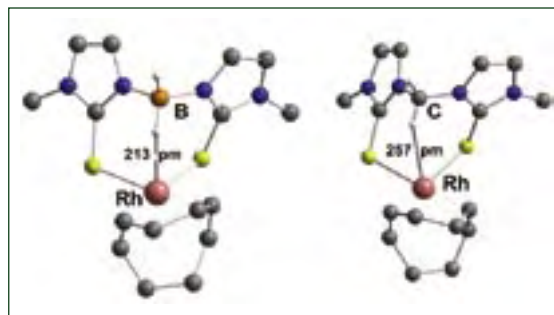
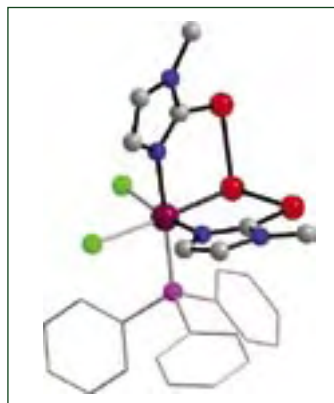
Of relevance to the Fischer Tropsch process is the coupling of small C<sub>1</sub> and C<sub>2</sub> fragments on metal surfaces and such processes have been modelled using bimetallic molecular complexes. Building on our previous studies of intraligand chalcogenolate migration on mononuclear complexes, we have now investigated the coupling of alkylidyne (C<sub>1</sub>) and alkyne (C<sub>2</sub>) units in which the alkyne bears chalcogenolate substituents. In dramatic contrast to simple hydrocarbon chemistry, a far more complex situation arises in which a plethora of novel unsaturated organoselenium ligands have been encountered. (With L M Caldwell, A C Willis)

### Unusual Methimazolyl-derived Ligands

We have in previous years pursued the chemistry of poly(methimazolyl)borates and boranes, however more recent emphasis has turned to alternative polydentate ligands in which the bridgehead boron atom is replaced by other potential donors. Two highlights include the first complexes of bis(methimazolyl)methanes, H<sub>2</sub>C(mt)<sub>2</sub>

(mt = methimazolyl) and bis(imidazolyl)polyselenanes. In the former, it could be shown that the geometry

predisposes the chelate towards incipient agostic C-H-Metal interactions allowing direct comparison with isoelectronic B-H-Metal systems as illustrated above for the complexes [Rh(cod){H<sub>2</sub>X(mt)<sub>2</sub>}] (X = B, C<sup>+</sup>). The coordination chemistry of diorganopolyselenanes 'RSe<sub>n</sub>R', has not previously been explored. We have now synthesised the novel ligand Se<sub>3</sub>(mt)<sub>2</sub> via a templation protocol providing the complex [RuCl<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub>]{Se<sub>3</sub>(mt)<sub>2</sub>} (shown left) in which the ligand coordinates in a tridentate manner through one selenium and two nitrogen donors. (With I R Crossley, E R Humphrey, M K Smith, N Tshabang, A C Willis)



### B-functionalisation of Poly(pyrazolyl)borates

Poly(pyrazolyl)borates H<sub>x</sub>B(pz)<sub>4-x</sub> are renowned as 'innocent' spectator ligands that generally play no direct role in the subsequent chemistry of their complexes. We are currently studying situations in which this is demonstrably not the case. Specifically, the bridgehead borohydride groups have now been shown to enter into metal-mediated methanolysis reactions providing complexes of, for example, the novel (MeO)<sub>2</sub>B(pz)<sub>2</sub> ligand in which one methoxide group also acts as a donor to the metal centre. (With R J Abernethy, M K Smith, A C Willis)

<http://rsc.anu.edu.au/research/hill.php>

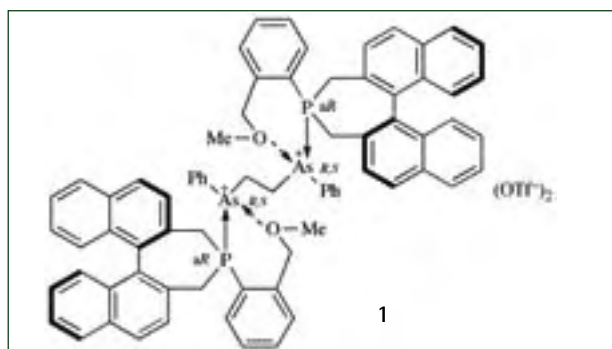


# INORGANIC STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS

PROFESSOR BRUCE WILD

Coordination chemistry has merged with organic and organometallic chemistry and with catalysis such that there are now modifications available for nearly every standard reaction for converting achiral organic precursors into chiral products. Together with modern purification techniques, this has allowed the preparation – in a single step – of compounds in >98% enantiomeric purity for many reaction types. Work in this group is concerned with the synthesis of new types of chiral ligands, especially enantiomerically pure phosphines and arsines, for use as probes of inorganic stereochemistry, rearrangements in metal complexes, and as auxiliaries for asymmetric synthesis.

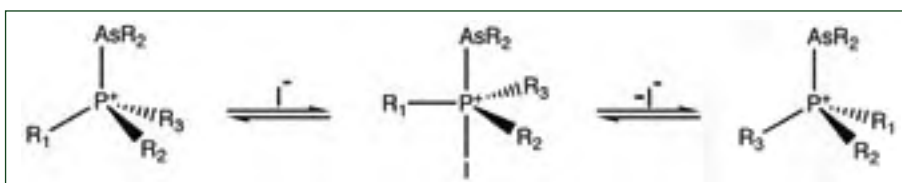
## Phosphine-stabilised Arsenium Salts and the Asymmetric Synthesis of Tertiary Arsines



Our work in this area has been extended to the asymmetric synthesis of ditertiary arsines. Thus, the bis(*aR*)-phosphine-stabilised diarsenium salt **1** has been reacted at low temperature with *n*-butyllithium to give the (*S,S*)-bis(*n*-butylphenyl)diarsine in 88% enantioselectivity, along with 15% of the achiral (*R,S*) compound. The enantioselectivity of the reaction was determined by a novel NMR spectroscopic method involving the use of an enantiomerically pure diphosphineplatinum(II) group as the reference agent. This is the first asymmetric synthesis of a ditertiary arsine containing two chiral arsenic stereocentres. (With M L Coote, E H Krenske, A D Rae, M L Weir, A C Willis, X-T Zhou)

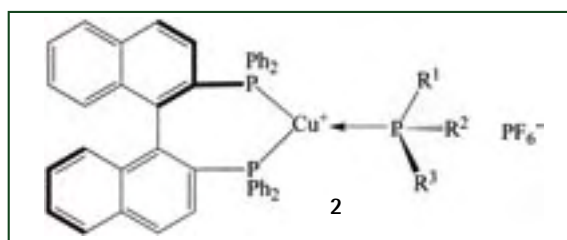
## Deracemisation of Chiral Arsines and Phosphines via Asymmetric Transformation

Chiral phosphines are crucial for many industrial catalysts, but their resolutions are often time consuming and wasteful.



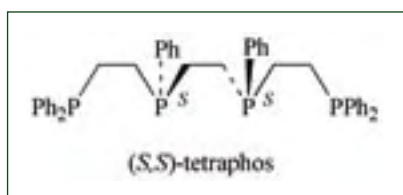
Pyramidal inversion at a phosphine centre results in racemisation, which has been observed for an enantiomerically pure phosphine in the presence of an iodoarsine.

If the arsenium ion is chiral, a shift in the equilibrium towards the most stable diastereomer of the adduct is conceivable via an asymmetric transformation. This deracemisation could allow the isolation of chiral phosphines without the need for traditional resolution. Initial investigations have focused on the synthesis of complexes derived from  $[\text{Cu}(\text{R-BINAP})(\text{NCCH}_3)_2]\text{PF}_6^-$  with tertiary phosphines, viz. **2**. (With N L Kilah)



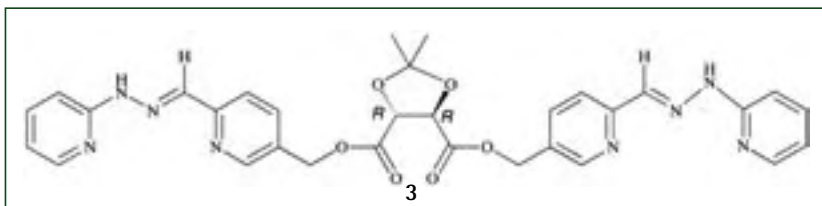
## Polytertiary Phosphine Helicates

The self-assembly of molecules into large supramolecular structures is an important feature in biology and is now readily achieved in inorganic coordination chemistry with appropriate helically ligating ligands and metal ions. Work in our laboratory has shown that (*S,S*)-tetraphos spontaneously self-assembles dinuclear metal helicates of the type of  $(M)_2\{(R,R)\text{-tetraphos}\}_2(PF_6)_2$  upon reaction with univalent silver and gold salts and  $(M)\text{-Pt}_2\{(R,R)\text{-tetraphos}\}_2(OTf)_4$  upon reaction with  $Pt(COD)Cl_2$  in the presence of TMSOTf. The central 10-membered ring in each of these complexes has a chiral twist-boat-chair-boat conformation; the  $\delta$  or  $\lambda$  twist of the ring generates a parallel or double  $\alpha$ -helix conformer of the helicate. Current work is focused on the synthesis of similar complexes involving zero-valent metals and the synthesis of tetraphosphines with substituted backbones that will stabilise the double  $\alpha$ -helix conformer of the helicate over that of the parallel helix conformer. (With H Kitto, A D Rae, A C Willis)



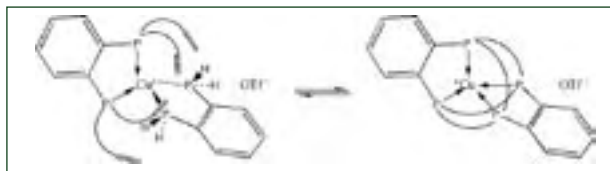
## Asymmetric Synthesis of Two-bladed Propeller Octahedral Metal Complexes

We have embarked on a project aimed at demonstrating that single enantiomers of chiral metal complexes can be prepared by inorganic asymmetric synthesis. The approach being adopted is to transfer chiral information from an auxiliary attached to



appropriate chelating groups, as in **3**, with the auxiliary subsequently being removed to leave the configurationally pure metal complex. For this method to be successful, the product must have sufficient chemical and configurational stability to observe the single enantiomer of the complex produced. For these reasons, we have chosen as targets two-bladed propeller complexes of the type  $(\pm)\text{-}[M(PAPHY)_2]X_2$  and  $(\pm)\text{-}[M(PAPY)_2]$ , which are available for a wide range of metals. Ligand **3** diastereoselectively chelates iron(II) to produce the corresponding mononuclear complexes in >99% diastereoselectivity. Hydrolysis of the ester linkages in the pure diastereomer of the deprotonated iron complex furnishes  $P\text{-}(+)\text{-}[Fe(HOCH_2PAPY)_2]$  with 85% enantioselectivity. This is the first inorganic asymmetric synthesis of a two-bladed propeller metal complex using classical organic methodology. (With A D Rae, R J Warr, A C Willis)

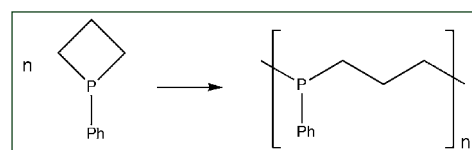
## Tetrahedral Phosphine Cage Ligands and Complexes



Work is in progress concerning the metal-template synthesis of a tetrahedral phosphine cage complex by the route shown below. Molecular modelling and a crystal structure determination of  $[Cu\{1,2\text{-C}_6\text{H}_4(\text{PMe}_2)_2\}_2]OTf$  has established the chain length parameter for the alkylene groups. (With K Wells, A C Willis)

## Quantum Chemical Design of Stereoregular Polyphosphines

Theoretical and synthetic work concerning the free-radical polymerisation of 1-phenylphosphetane and related compounds is underway. (With M L Coote, E H Krenske, J Steinbach)

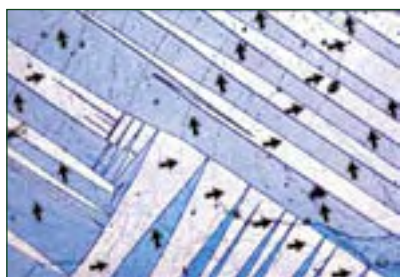




# SOLID STATE INORGANIC CHEMISTRY

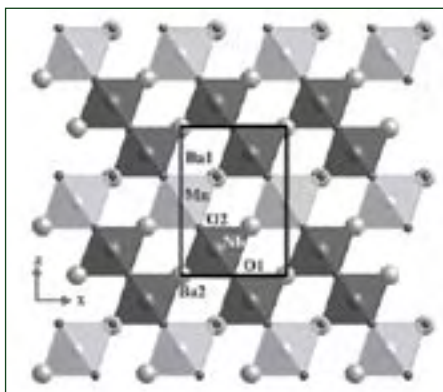
PROFESSOR RAY WITHERS

We aim to understand and exploit the factors that determine structure and function in the crystalline solid state. A major interest is in the balance between local crystal chemistry and longer-range order in a wide range of flexible crystalline phases. The principal experimental research tools used include a wide range of solid state synthesis techniques, transmission and scanning electron microscopy in combination with powder and single crystal diffraction as well as physical properties measurements including resistivity as well as dielectric properties. Crystalline systems investigated include wide range non-stoichiometric solid solutions, displacively flexible framework structures, ferroic phases and phase transitions, solid electrolytes, dielectric materials and incommensurately modulated structures.



## A Structure, Phase Analysis and Dielectric Properties Investigation of Some Complex Perovskites

The "1:1"  $A_2\text{In}^{3+}\text{Nb}^{5+}\text{O}_6$  double perovskites have been the subject of recent interest due to their potential as visible light driven photocatalysts as well as for their microwave dielectric properties in the case of the  $A = \text{Ba}$  and  $\text{Sr}$  compounds. Likewise the 1:2  $\text{Ba}_3\text{Mn}^{2+}\text{Nb}^{5+}_2\text{O}_9$  triple perovskite is of interest for its dielectric properties. A careful investigation has therefore been carried out into the room temperature crystal structures of these complex perovskite materials as well as their



temperature-dependent dielectric properties. In the case of the nominally "1:1"  $A = \text{Ca}$  compound, an extensive  $\text{Ca}_2[(\text{Ca}_{2x/3}\text{In}_{1-x}\text{Nb}_{x/3})\text{Nb}]\text{O}_6$  'solid solution' field spanning compositions virtually the whole way from  $\text{Ca}_4\text{Nb}_2\text{O}_9$  to  $\text{Ca}_2\text{InNbO}_6$  in the  $\text{CaO}-\text{InO}_{3/2}-\text{NbO}_{5/2}$  ternary phase diagram has been shown to exist. In terms of the optimisation of physical properties, the existence of  $B$ -site variable solid solutions fields such as this is of considerable interest as it raises the possibility of being able to continuously tune desired physical characteristics. In the case of the 1:2  $\text{Ba}_3\text{Mn}^{2+}\text{Nb}^{5+}_2\text{O}_9$  triple perovskite, stacking fault disorder appears to play a strong role in the dielectric loss properties of the material. (With Y Liu, L Norén, V Ting, and J Fitz Gerald [RSES, ANU], M James [Bragg Institute, ANSTO])

## Precise Diffraction Studies of Temperature-dependent as well as Composition-induced Structural Phase Transitions in the $\text{Ca}_{1-x}\text{Sr}_x\text{TiO}_3$ System

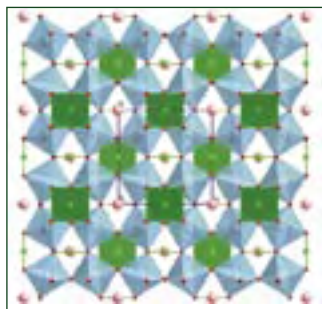
As part of an ongoing ARC-funded project involving precise diffraction studies of structural phase transitions in functional metal oxides, a coupled electron, synchrotron X-ray and neutron diffraction study of temperature-dependent as well as composition induced structural phase transitions in the  $\text{Ca}_{1-x}\text{Sr}_x\text{TiO}_3$  system is under way. The mineral perovskite itself,



$\text{CaTiO}_3$  is a major component of Synroc, a synthetic rock form designed for the immobilisation of radioactive waste. Our interest in the  $\text{Ca}_{1-x}\text{Sr}_x\text{TiO}_3$  system derives from the fact that the  $\text{CaTiO}_3$  acts as a host for fission product Sr. It is therefore of some importance to precisely characterise the polymorphic and phase transition behaviour of this archetypal perovskite system. We are concentrating on regions of the phase diagram where significant disagreements currently exist in the literature. Attention is currently focussed on the  $x = 0.70$  composition where diffraction studies have shown that the room temperature space group symmetry of  $\text{Ca}_{0.3}\text{Sr}_{0.7}\text{TiO}_3$  is  $I4/mcm$  rather than  $Imma$  as recently claimed. Work is also currently underway on the  $x \sim 0.63$  composition where a novel anti-ferroelectric polymorphic form is being carefully investigated. (With C J Howard [ANSTO], B J Kennedy [U Sydney], M Carpenter [U Cambridge, UK])

### Structurally Frustrated Relaxor Ferroelectric Behaviour in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$

Ever since  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  (CCTO) was first reported in 2000 to have a giant dielectric constant at 1 kHz of  $\sim 12,000$  that was nearly constant from room temperature up to  $\sim 600\text{K}$  but which dropped rapidly to less than 100 below 100K, a huge amount of interest and work has been carried out in an attempt to understand the origin of these remarkable



and potentially very useful dielectric properties. Both extrinsic (microstructural) as well as intrinsic mechanisms for the observed dielectric properties have been proposed. Dielectric constants greater than 1000 have traditionally been associated with intrinsic ferroelectric or relaxor ferroelectric (RF) behaviour. We have recently observed a reversible ferroelectric effect in CCTO as well as found direct diffraction evidence for structurally frustrated RF behaviour in the form of 1-d correlated, off-centre displacements of Ti ions within the  $\text{TiO}_6$  octahedra of CCTO. That this incipient ferroelectric behaviour is only correlated along 1-d columns of  $\text{TiO}_6$  octahedra in the absence of an applied electric field offers a crucial insight into the underlying nature of CCTO and suggests the existence of a unique new class of

structurally frustrated, ferroelectric relaxors. As part of a newly funded ARC grant, the correlation between composition, synthesis conditions, structure (both local as well as microstructural) and dielectric properties (dielectric constant as well as dielectric loss) will be carefully investigated in CCTO and related materials. (With Y Liu, L Norén)

### Refinement of Minor Components in Twin-disordered Crystal Structures

The structure determination and refinement of crystalline materials using diffraction techniques is often complicated by the presence of minor components of the scattering density that compromise the accuracy and chemical detail obtainable. Refinement, for example, can be very pathway dependent, especially when twinning occurs. A number of strategies are being pursued to overcome these problems. An in-house program RAELS is currently being rewritten to simplify comparative refinement. Symmetrisation is the description of a structure using irreducible representation theory. Each component of the overall electron density has the true symmetry as a subgroup and is itself a subgroup of an idealised parent space group. The process becomes useful when it reveals symmetrised components which make a limited contribution to the overall intensity of a diffraction pattern. Such components are often poorly defined if standard refinement procedures are used and mechanisms for stacking faulting and twinning are not recognised. There is no correlation between symmetrised components if powder diffraction data is used. The program RAELS allows the combination of structure factors from pseudo-equivalent reflections of an ideally ordered prototype structure to simulate the diffraction pattern. Recent results have shown that robust geometrical parameters can be obtained using this approach. (A D Rae)



# SYNTHESIS AND MECHANISM

PROFESSOR MARTIN BANWELL

The group's activities remain focused on the development of new synthetic strategies and methodologies as well as the application of these in the total synthesis of biologically active natural products and certain analogues. Vinblastine (a binary indole-indoline alkaloid used in the treatment of early childhood leukaemia and bladder cancer) and galanthamine (a plant-derived alkaloid used in the treatment of Alzheimer's disease) remain key targets and have inspired a considerable number of methodological studies. Australian companies have funded a significant portion of our work. For example, Cryptopharma Pty Ltd, a Melbourne-based biotech company, is supporting two PhD candidates who have been working on a very enjoyable collaborative project focused on the identification of non-steroidal compounds capable of treating acute forms of asthma. Another PhD scholar is working on a collaborative project with Biota Holdings that is directed towards the preparation of potent anti-infective agents while a fourth such person is working with Starpharma Pty Ltd on the development of new drug delivery systems. A very productive and longstanding collaboration with the Brisbane-based company Progen has continued throughout the year and involved two postdoctoral co-workers. They have been focused on the preparation of novel classes of anti-angiogenic agents as second-generation analogues of the highly promising drug candidate PI-88 originally developed in Professor Chris Parish's laboratories at the John Curtin School of Medical Research.

Other research highlights include:

- (i) the completion of a chemoenzymatic total synthesis of the triquinane-type natural product (-)-complicatic acid (Figure 1), a fungal metabolite possessing powerful anti-bacterial properties;
- (ii) the completion of a total synthesis of the non-natural enantiomeric form of the alkaloid erythramine (Figure 2);
- (iii) the identification of a new methods for constructing annulated furans;

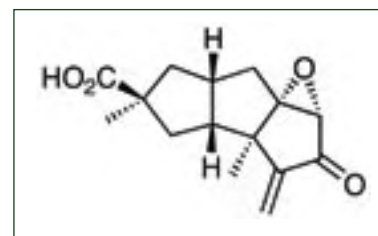


Figure 1: (-)-Complicatic acid, a fungal metabolite possessing anti-bacterial properties.

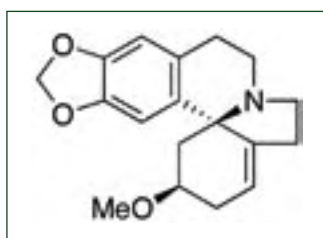


Figure 2: *ent*-Erythramine, the non-natural enantiomeric form of the alkaloid erythramine.

- (iv) the rapid assembly of tetracyclic frameworks related to gibberellins;
- (v) the identification of enzymatic methods for the efficient preparation of enantiomerically pure *gem*-dibromocyclopropanes;
- (vi) the exploitation of the palladium[0]-catalysed Ullmann cross-coupling reaction in the generation of annulated isoquinolines.

During the course of the year, a number of group members reached significant milestones and/or received important recognition for their research efforts. For example, Drs David Lupton and Rebecca Taylor each received their PhD degrees. David was subsequently awarded a Sir Keith Murdoch Fellowship from the American Australian Association and he is now undertaking postdoctoral studies at Stanford University with Professor B Trost in the Department of Chemistry. Former PhD candidate Dr David Loong has been awarded a Ramsay Memorial Fellowship and is now undertaking postdoctoral studies in the Department of Chemistry at Imperial College,

London, with Professor A Barrett. Dr Gwion Harfoot has been awarded a Fellowship from the von Humboldt Foundation and is now undertaking postdoctoral studies in the Department of Chemistry, RWTH-Aachen, Germany and working with Professor C Bolm. Ms Jasmine Jury was the co-recipient of the prize for the best oral presentation by a PhD student within the RACI's Organic Chemistry Division program associated the CONNECT 2005 Conference held in Sydney in July. Ms Kerrie Austin received the prize for the best poster presentation by a PhD student at the RACI's NSW Organic Chemistry Group's 26th Annual One-day Synthesis Symposium held at the University of Wollongong in November.

## Exploitation of *cis*-1,2-Dihydrocatechol Derivatives as Starting Materials for Chemical Synthesis

The title compounds, which can be obtained by enantioselective microbial oxidation of the corresponding arene or through manipulation of the shikimic acid biosynthetic pathway, continue to serve as important starting materials for the preparation of a structurally diverse array of poly-oxygenated natural products and related structures. Methods for the enantiodivergent elaboration of *cis*-1,2-dihydrocatechols, through the application of various pericyclic processes, continue to be a major area of activity and some of the products derived from such reactions have been converted, using photochemically-promoted transformations, into the polycyclic skeleta associated with a diverse range of terpenoid natural products. Other natural products being targeted include the alkaloid brunsvigine and the macrolide tricholomenyn B (a potent anti-mitotic agent). The preparation of various sugar mimetics continues to be another activity in this area and one that has been carried out with commercial partners. The search for synthetic equivalents for the title compounds has started and some promising results have been obtained. (With K A B Austin, M Backes, T Bilski, M Bonnet, L Fearnside, J S Foot, M P Friend, G J Harfoot, J Jury, J Kitching, M Knoke, D T J Loong, D W Lupton, X Ma, J Renner, T Reekie, P Sharpe and R H Don, V Ferro [Progen Industries Ltd, Brisbane], J Lambert [Biota Pty Ltd, Melbourne], G Krippner, T McCarthy [Starpharma Pty Ltd, Melbourne], G Whited [Genencor International Inc, Palo Alto], A Stewart [Cryptopharma Pty Ltd])

## New Synthetic Strategies and Methodologies

The electrocyclic ring-opening of ring-fused *gem*-dibromo- and *gem*-dichloro-cyclopropanes continues to be employed in a wide variety of contexts, with one especially notable activity being focused on the construction of the polycyclic frameworks associated with a range of alkaloids. The exploitation of pyrroles and indoles as nucleophilic scaffolds for the construction of various alkaloids also remains a major activity within the group. Knoevenagel chemistries have been exploited in the construction of the bis-piperidiny core associated with the Australian marine natural product haliclonaclamine A and work is now focused on constructing, using the Ramberg-Bäcklund reaction, the two remaining ring systems associated with this ecologically important compound. (With D A S Beck, A Bissember, D Dauge, S Gross, M J Harvey, K Holden, M Jones, O J Kokas, D A Offermann, D Pinkerton, J Renner, P C Stanislawski, M O Sydnes, R Taylor, and C Burns [Cytopia, Melbourne], R H Don, V Ferro [Progen Industries Ltd, Brisbane], M Garson [U Queensland], C R Parish [JCSMR, ANU])

<http://rsc.anu.edu.au/research/banwell.php>





# BIOCHEMICAL REACTIONS AND MOLECULAR RECOGNITION

PROFESSOR CHRIS EASTON

One aspect of our research involves the manipulation of biochemical reactions. Our objectives in this area are: i) to develop methods to regulate biochemical processes associated with disease states, ii) to produce physiologically active compounds with potential as pharmaceuticals, iii) to develop biomimetic synthetic methods, and iv) to produce enzymes with novel functions and mechanisms of action, to efficiently catalyse classes of chemical processes outside the normal biological range. The other main field of research is in the area of supramolecular chemistry and molecular recognition, and involves the design, synthesis and evaluation of molecular hosts. Applications of this chemistry in the development of catalysts, molecular reactors and devices, and photochemical and thermal switches are being pursued.

Highlights of our recent results include the development of:

- (i) enzyme inhibitors to down-regulate, and prohormones to up-regulate, the biosynthesis of peptide hormones;
- (ii) models to predict the susceptibility of amino acids and peptides towards free radical processes associated with disorders such as Alzheimer's and cardiovascular disease;
- (iii) molecular ratchets, sensors, shuttles, tweezers and switches;
- (iv) molecular reactors to catalyse and control the regioselectivity of carbon-carbon bond forming reactions;
- (v) novel spectroscopic techniques to analyse melamine-urea-formaldehyde and related resins, and improve the manufacture thereof, and
- (vi) compounds to inhibit and stimulate ion-flux through calcium ion channels.

Personnel highlights included the completions of PhD students B Barratt, A Philbrook and M Cieslinski, MPhil student L Chow and BSc(Hons) student R Coulston. I Li presented an invited lecture at the Gordon Conference on Free Radicals, in New Hampshire, and A Philbrook presented an invited lecture at Wood Composites 2005, in San Diego. Professor Gary Weisman of the University of New Hampshire was a welcome visitor for several months.

We were pleased to be part of successful bids for an ARC Centre of Excellence in Free Radical Chemistry and Biotechnology and for a CSIRO Emerging Science Initiative in Synthetic Enzymes for Synthetic Chemistries. Our work on hormone regulation also gained support through the award of a new ARC Discovery Grant, while our research with Orica (Australia) Pty Ltd with wood adhesives attracted an ARC Linkage Grant.

## Free Radical Reactions of Amino Acids, Peptides and Proteins

Free radical reactions of amino acids and their derivatives are associated with a wide variety of disease states, including inflammation, and Alzheimer's and cardiovascular disease. They are also involved in the biosyntheses of many of the hormones that regulate biological activity, and are therefore intimately linked to the associated physiological and pathological conditions. This has prompted us to study aspects of the fundamental free radical reactions that are involved. Through this work we have developed models to predict the susceptibility of amino acids and peptides towards free radical processes associated with physiological disorders, and radical-resistant amino acids and peptides have been designed and

synthesised. We have produced enzyme inhibitors to down-regulate, and prohormones to up-regulate, the biosynthesis of peptide hormones. We are currently evaluating the potential of these compounds as pharmaceutical agents for treating human and animal disease states associated with hormone imbalances. *(With D Brittain, L Y F Chow, M L Coote, A J Herlt, I Li, A J Mortimer, G M Statham, Y-C Tsai, Z I Watts, A Wright, and L Radom [U Sydney], R O'Hair [U Melbourne])*

## Supramolecular Chemistry and Molecular Recognition

This work exploits cyclodextrins as molecular hosts. Our early work in this area resulted in pharmaceutical formulations that are in everyday clinical use worldwide. In more recent studies modified cyclodextrins are being developed and exploited as molecular scaffolds for the construction of catalysts, molecular ratchets, shuttles, tweezers and switches, and photochemical devices. Another application of cyclodextrins involves their use to control the assembly of the components of chemical reactions, to facilitate the reactions and alter the outcomes. The cyclodextrins thereby act as reaction vessels, but at the molecular level. In this regard, we have developed demonstration systems to change the regio- and stereo-selectivity of reactions, and increase their rates by up to 100,000 times. We have also been exploring the synthesis of cyclodextrin rotaxanes, catenanes, knots and daisy chains of various topologies. These form the basis of molecular devices such as ratchets and motors, temperature and light sensors, photochemical frequency switches and molecular tweezers. Solid state and solution studies of cyclodextrin host-guest complexes and rotaxanes show that these assemblies may be designed to exploit the cyclodextrins as insulators of molecular filaments formed by the guests. This has potential, for example, in the development of microelectronic systems. *(With L Barr, S Bowen, M M Cieslinski, R J Coulston, R Dawson, A J Herlt, S Maniam, and M A Buntine, J Gerber, S F Lincoln, B L May, J Patrick [U Adelaide])*

## Other Collaborative Research

Other research involves studies of the structure of melamine-urea-formaldehyde resins, and the search for alternative reagents and improved manufacturing processes. Biochemical molecular recognition processes are also being studied, including the design and development of compounds to inhibit and stimulate ion-flux through calcium ion channels, and the development of novel enzymes. *(With A Buchan, J Khurana, A Philbrook, J K Robinson, M G Teese, and M Casarotto, A Dulhunty, [JCSMR, ANU], N Dunlop, S Earnshaw, N Walker [Orica (Australia) Pty Ltd and the UniChe program], A Ferrante, A Poulos [Adelaide Medical Centre for Women and Children], S Brown, J Oakeshott, R Russell [CSIRO Entomology], G P Savage, G W Simpson [CSIRO Molecular and Health Technologies])*



<http://rsc.anu.edu.au/research/easton.php>



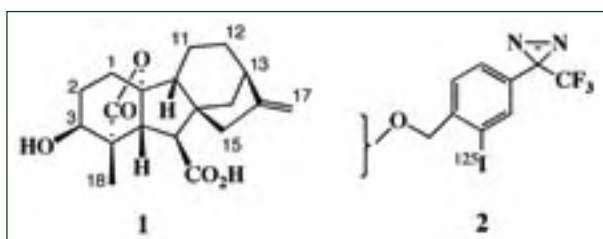
# ORGANIC SYNTHESIS

PROFESSOR LEW MANDER

Our research interests are concerned primarily with methods and strategies for the synthesis of complex natural products that have interesting biological properties. Within this context, members of the group have successfully completed syntheses of numerous complex natural products and developed a number of useful synthetic procedures. We are also interested in the molecular basis of plant growth regulation, using organic synthesis as an enabling technology, with special reference to the gibberellins (GAs). GAs affect numerous aspects of plant growth and development, including for example, germination, induction of stem growth and flowering, and there are several commercially valuable applications. Studies pursued in collaboration with groups in the CSIRO and the University of Calgary have led to the discovery of semi-synthetic derivatives that interfere with the plant's natural production of phytohormones, thereby inhibiting growth.

## Preparation of Photo-affinity Probes for Labelling of Gibberellin Receptors

In order to understand more fully the molecular basis of gibberellin bioactivity, we are presently undertaking the synthesis of gibberellins with attached groups designed to crosslink to binding sites in receptors and other gibberellin ("GA")-binding proteins. Trifluoromethyl aryl diazirines have been shown to be some of the most effective auxiliaries for photo-affinity labelling, but their steric bulk may interfere with binding. Before attempting to prepare a fully elaborated probe, we have made and tested a series of benzyloxy substituted GAs and evaluated their bioactivity. Substituents at C-1, C-2, C-11, C-12,

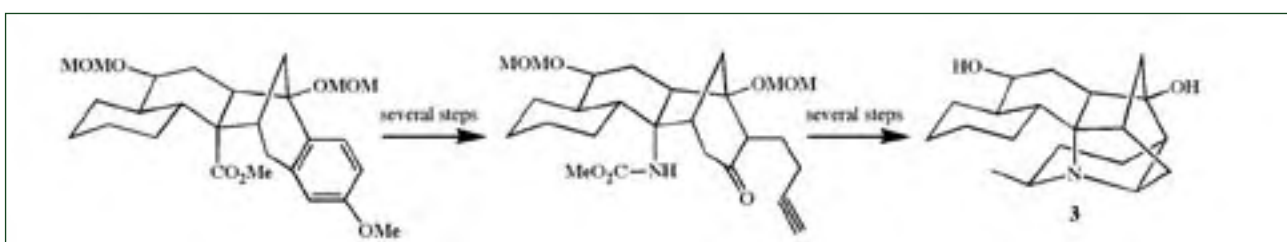


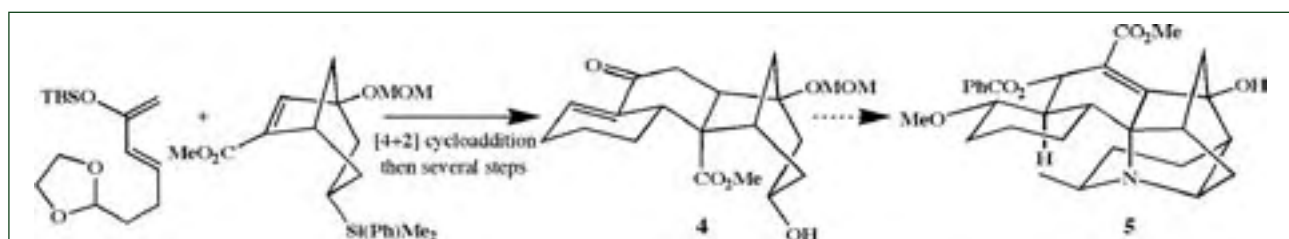
C-13, C-15, C-17 and C-18 (see structure 1 for numbering) have been screened in leaf-growth and barley endosperm bioassays with those substituted at C-2 $\alpha$ , C-11 and C-12 shown to retain acceptable levels of bioactivity. However, when the benzyl group was substituted with iodine and the diazirine photophore (as in part structure 2), biological activity dropped to <1% of the corresponding parent gibberellin. We have therefore directed recent endeavours to gibberellin derivatives

that have the substituted benzyl group attached *via* an extended linker based on tetraethylene glycol. (With J R Crow, M J McDonough, S M McAteer, L C Axford)

## Total Synthesis of Natural Products

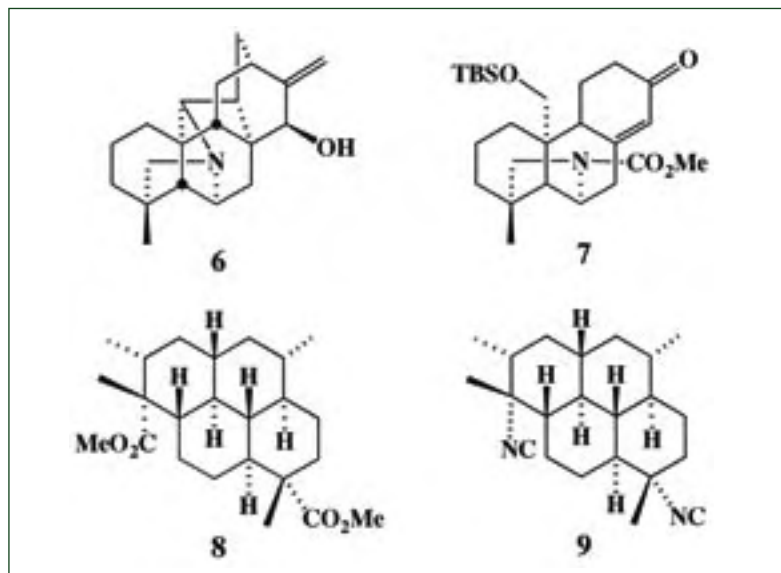
Synthetic studies are being directed towards the assembly of several highly caged natural products. They include members of a group of 28 novel alkaloids isolated from the Northern Australian rain forest species, *Galbulimima belgraveana*. Recent studies have culminated in the assembly of the hexacyclic skeleton 3, which was envisaged as an advanced intermediate





for the preparation of the alkaloid himandrine 5. However, difficulties with the logistics of continuing with this plan have prompted us to take a more direct approach, proceeding *via* 4, the preparation of which is outlined in the following scheme.

Preliminary studies on the construction of the heptacyclic family of diterpenoid alkaloids typified by nominine 6 have been undertaken. A number of promising leads have been developed, culminating in the assembly of the tetracyclic intermediate 7, while the diester 8 has been prepared with complete stereocontrol of all ten stereocentres *en route* to the total synthesis of the potent anti-malarial diterpenoid, diisocyanoadociane 9. All that remains to be done in this last sequence is the conversion of the ester functionality to isonitrile through means of a Curtius rearrangement. (With G Del Signore, O E Hutt, K A Fairweather, A C Willis)







# ORGANIC SYNTHESIS, METHODOLOGY AND HOST-GUEST CHEMISTRY

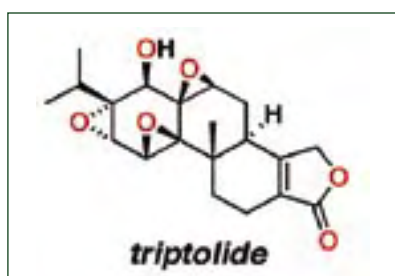
ASSOCIATE PROFESSOR MICK SHERBURN

Domino reactions are spectacular events in which many bonds are made and broken in a single step. These reactions hold much promise for achieving more efficient syntheses: a pressing need in times of increasing production costs and given the importance of protecting the environment by reducing waste. Our research program involves the design and implementation of sequences of cycloaddition reactions, free radical reactions and transition metal-mediated reactions to prepare polycyclic molecules with important biological properties. This program also targets new ways to achieve molecular recognition, complexation and catalysis. Overall, the primary goal is to synthesise such complex molecules in a practical manner.

## Efficient Total Synthesis: Anti-tumour and Anti-Alzheimer's Natural Products

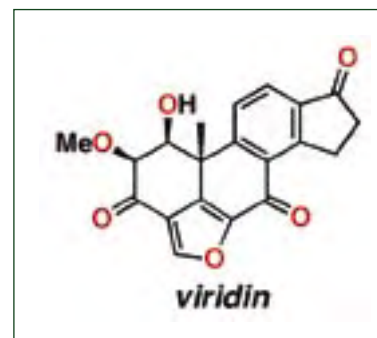
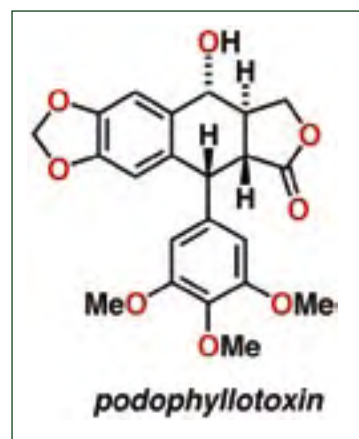
Lignans like podophyllotoxin have cancer-fighting properties and are used in chemotherapy. An efficient and highly modular approach for the synthesis of lignan natural products has been developed, culminating in several total syntheses, including that of podophyllotoxin. This strategy has several advantages over previous syntheses, the most significant being that it allows a high level of convergency at the end of the synthetic route.

We have developed a novel, efficient and very general way to produce complex polycyclic molecules with useful biological properties from simple, unsaturated, acyclic precursors



using sequences of Diels–Alder reactions. Major advances this year in this area include the first practical synthesis of [4]dendralene and a demonstration of its use in the rapid formation of different polycyclic frameworks.

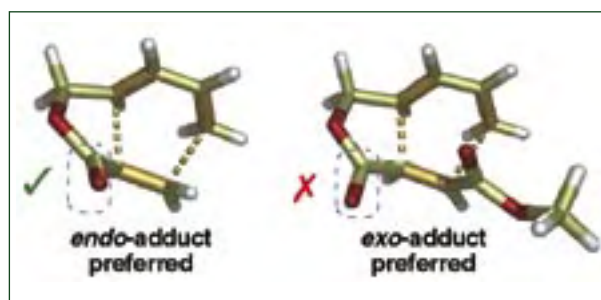
This work was featured as a news item in the influential magazine *Chemical and Engineering News* [*Chem. Eng. News* (2005), 83(34), 38]. These methods are being applied in the total synthesis of the biologically important compounds triptolide and viridin. Significant progress has been made this year on these projects. (With GBojase-Moleta, TBradford, LCarpinelli, SKGoodwin, LCHKwan, NAMiller, ADPayne, D Robinson)





## A Deeper Understanding of the Most Important Organic Reaction

The Diels–Alder reaction is one of the most powerful and most commonly used reactions in synthetic organic chemistry. Predicting, controlling and explaining the stereochemical outcome of this reaction continues to be a major activity within the group. The location of transition structures at high levels of theory is providing stimulating new insights into the reaction. Our better understanding of the Diels–Alder reaction is driving the development of new methodology. (With *T N Cayzer, W Lording, E L Pearson, R J-P Tripoli, C I Turner, and M N Paddon-Row [UNSW]*)



## Host-guest Chemistry

Research in this area is concerned with the design and synthesis of host molecules for molecular recognition, complexation and catalysis. Investigations into uses of these intriguing hosts as molecule-sized devices are underway. A major achievement

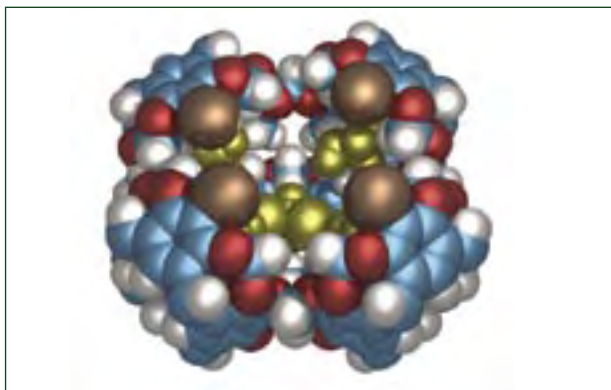


Figure 1: Crystal structure of a "superbowl" host molecule binding one chloroform and four ethanol molecules (bronzed). This new type of host can encapsulate molecules up to 100 atoms, *i.e.* the size of small medicinal agents.

includes the synthesis of the superbowl container molecules, a new class of synthetic hosts with non-collapsible interiors which encapsulate molecules of the size of medicinal agents (Figure 1). This paper was the subject of press releases by the ANU and the American Chemical Society (ACS) in February 2005 and was featured in *The Sydney Morning Herald/The Age, The Canberra Times*, ABC radio, Channels 9 and 7, newspapers around the world and on TV in the USA. The superbowl molecule was named "molecule of the week" on the ACS website, featured as a highlight article in the journal *Angewandte Chemie* [*Angew. Chem. Int. Ed.* (2005), 44(24), 3652–3654], and in a news item in the journal *Drug Discovery Today* [*DDT* (2005), 10(7), 454]. A Google search using the terms "superbowl" with "molecule" or "sherburn" will provide the interested reader with a large number of relevant documents. We have also demonstrated for the first time that molecules imprisoned in separate cells of a "cell-block" host molecule "communicate" with each other (Figure 2). (With *E S Barrett, M W Carland, A J Edwards, N Kanizaj, D J Sinclair*)

This paper was the subject of press releases by the ANU and the American Chemical Society (ACS) in February 2005 and was featured in *The Sydney Morning Herald/The Age, The Canberra Times*, ABC radio, Channels 9 and 7, newspapers around the world and on TV in the USA. The superbowl molecule was named "molecule of the week" on the ACS website, featured as a highlight article in the journal *Angewandte Chemie* [*Angew. Chem. Int. Ed.* (2005), 44(24), 3652–3654], and in a

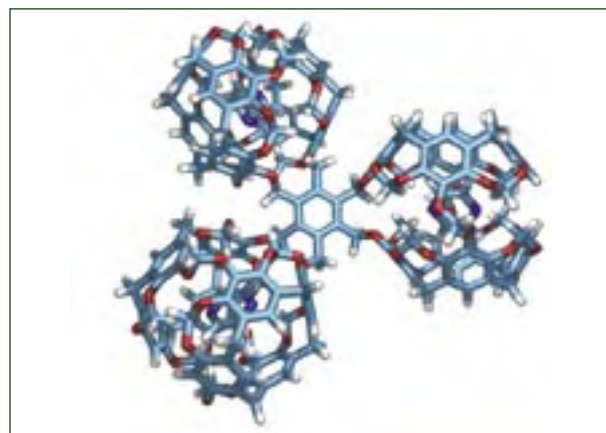


Figure 2: Energy minimised structure of a triple cage, single molecule host molecule. One pyrazine molecule is encapsulated within each cage. These encapsulated molecules "sense" one another.



# THEORETICAL CHEMICAL PHYSICS

PROFESSOR MICHAEL COLLINS

The group's main interest is in understanding the mechanisms of chemical reactions. This pursuit involves the development of methods for constructing potential energy surfaces for chemical reactions and the reaction dynamics on these surfaces.

*Ab initio* quantum chemistry provides accurate information about the energetics of chemical reactions. The potential energy surfaces (PESs) are constructed as an interpolation of this *ab initio* data evaluated at a relatively small number of relevant molecular geometries. Significant progress has now been achieved for moderate sized molecules, so that many different chemical reactions have been investigated. Most of these reactions involve competing mechanisms or reaction pathways and could not be treated using simpler approximate methods. The end result of this work should be a much clearer understanding of the mechanisms of reaction at the molecular level. Our current work is concentrated in two main areas.

We are developing methods to study chemical reactions which take place in multiple electronic states; such processes are dominant factors in photochemistry, for example. The idea is to use *ab initio* quantum chemistry to supply information on both the energies of the electronic states and the coupling between these states which is caused by the motion of the atoms. This data is then transformed in a potential energy matrix, which can be used to simulate the chemical dynamics.

We are also pursuing a rather new avenue of research into "approximate *ab initio* quantum chemistry". We have devised methods for estimating the energies of quite large molecules from the energies of small molecular fragments (which are very much easier to calculate). In this way, we hope to make the first principles study of chemical reactions feasible for large molecules.

The group's work has been enhanced through collaborations with overseas scientists including the dynamics group of Associate Professor Dong Hui Zhang at the National University of Singapore, Professor David Yarkony, Johns Hopkins University (nonadiabatic dynamics), Professor Geert-Jan Kroes, University of Leiden (reaction at surfaces), Professor Mark Gordon, Iowa State University, and Assistant Professor Ryan Bettens, National University of Singapore.

## Hydrogen Abstraction in $\text{H}\bullet + \text{CH}_4$

The abstraction reactions,  $\text{H}\bullet + \text{RH} \leftrightarrow \text{H}_2 + \text{R}\bullet$ , have been observed to yield an unusual distribution of rotation-vibration states in the  $\text{H}_2$  product. To investigate the mechanism of this class of important combustion reactions, we have continued to pursue accurate PESs for the simplest example,  $\text{H}\bullet + \text{CH}_4$ . Quantum scattering calculations of the reaction cross sections and their dependence on the initial state of the reactants can be performed in at most eight dimensions at present. To facilitate high dimensional quantum scattering calculations of this reaction, new algorithms for evaluating the PES in an eight dimensional subspace of the molecular coordinates has been developed and is now being applied. (With D H Zhang [National U Singapore])

## Nonadiabatic Chemical Reactions

Many reactions, particularly in photochemistry, combustion and atmospheric chemistry, take place in more than one electronic state. The PES for these electronic states can intersect, and new methods have been developed to describe all the energy surfaces involved and their "interactions". The methods and computer code to construct two intersecting electronic energy surfaces were completed and applied to the benchmark  $H + H_2$  reaction. The quantum scattering on these surfaces revealed the subtle effect of the surface intersection on the differential reaction cross sections.

The code development for the general multi-state case is nearing completion, and is currently being tested on model systems. *(With C Evenhuis, O Godsi, and D H Zhang [National U Singapore], D Yarkony [Johns Hopkins U, USA])*

## Hydrogen-deuterium Exchange

Deuterium takes an active part in interstellar chemistry, leading to an enhancement of the abundances of deuterated molecules. In interstellar clouds, such processes are known as deuterium fractionation. Gas phase ion-molecule reactions, specifically the reactions involving H and D atoms with  $HOC^+/DOC^+$  play an important role in deuterium fractionation. An accurate molecular potential energy surface for these systems has been evaluated, so that accurate theoretical rate coefficients can be evaluated. *(With G Moyano)*

## Approximate *Ab Initio* Quantum Chemistry

*Ab initio* electronic structure theory provides the practical means to calculate the total electronic energy of moderate-sized molecules. From such data one can calculate thermochemical properties and, in principle, the complete potential energy surface which governs the motion of the atomic nuclei. Hence, chemical reaction dynamics, rate coefficients, and other observables may be evaluated. However, the computational time required to calculate the total electronic energy increases rapidly with the number of electrons in the molecule, and with the level of *ab initio* theory employed. We have developed a systematic hierarchy of methods for decomposing a molecule into fragments to obtain a series of approximations to the total electronic energy, at relatively low computational expense. This year has seen the development of a general computer code to implement this approach to evaluate molecular energies and energy gradients (and higher derivatives in some cases) and perform geometry optimisation. Extensive testing of the method is underway. Further development of the methodology has concentrated on the approximation of the relatively weak long-range interactions between well-separated segments of molecules. *(With V Deev)*

## Approximate *Ab Initio* Quantum Chemistry of Crystals

The method we have developed to approximate molecular energies might be applied to estimating the energies (and free energies) of crystals. To achieve this, we are producing a new approach which fragments a crystal structure into relatively small components under periodic boundary conditions applicable to crystals. *(With H Netzloff)*

<http://rsc.anu.edu.au/research/collins.php>



# COMPUTATIONAL QUANTUM CHEMISTRY, POLYMER CHEMISTRY

DR MICHELLE COOTE

We use computer calculations to determine the structure of molecules and to help understand how molecules react with one another. Using the laws of quantum mechanics, we can calculate from first principles the geometries of molecules, their vibrational frequencies and their energies. This provides detailed information on the mechanisms of reactions, as well as calculations of their kinetics and thermodynamics. Much of this information is very difficult to obtain experimentally, particularly for very reactive or hazardous compounds. Quantum chemistry provides a viable alternative approach for studying these compounds, and is thus an important complement to experimental procedures.

Our main interest is using quantum chemistry to solve practical problems in the polymer field. Polymers are long chain molecules and they can be used in a wide variety of applications, ranging from paints and adhesives, to artificial hips and contact lenses. The suitability of a polymer for a particular application depends not only upon its overall chemical composition, but also on its end-group composition, its chain length and its molecular architecture (*i.e.* whether it is linear, branched, star-shaped, *etc.*). These properties depend, in turn, upon the kinetics and mechanism of the polymerisation process – that is, what reactions occur and how they compete with one another. We use quantum chemistry to obtain this information and then use it to design better methods for controlling polymerisation processes and producing designer polymers. We work with leading experimental groups, both in Australia and internationally, who put our theoretical designs into practice. Our research highlights in 2005 include the design of a new radical route to polyphosphines and a new class of multipurpose RAFT agent for controlling free-radical polymerisation. These computer-designed chemical processes are now showing great promise in experimental testing by collaborators and highlight the growing potential of computational chemistry as a practical tool for the polymer field.

## Accurate Computational Methods

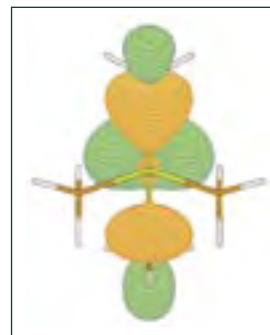
Applying quantum-chemical methods to polymeric systems poses a major challenge. Not only do accurate methods require significant computer power, the computational cost of a method scales exponentially with the size of the molecule. In order to adapt quantum chemistry to the study of polymerisation processes we have been evaluating the accuracy of computational methods and identifying reliable low-cost procedures. We also design small model reactions that effectively mimic the behaviour of real polymer systems. During 2005 we published the first chemically accurate computational predictions of propagation rate coefficients, and designed a computationally efficient approach to the study of addition-fragmentation rate coefficients in RAFT. We also commenced collaborative work with Dr Mansoor Namazian to tackle the important problem of modelling solvent effects on reaction rates. (*With D B R Brittain, E I Izgorodina, and M N Namazian [Yazd U, Iran]*)

## Free Radical Chemistry

To understand the mechanism of complicated radical-based processes (like polymerisation) it is important to study the prototypical systems first. During 2005, we became interested in the unusual behaviour of phosphoranyl radicals. According to textbooks, these radicals should be highly stabilised; however, we found that this notion was inconsistent with the low reactivity of dithiophosphinate esters in certain radical addition reactions. Moreover their stabilities followed very different



structure-reactivity trends to their carbon-centred counterparts, which we explained using qualitative molecular orbital arguments. An important practical implication of our findings is that phosphoranyl radicals should make excellent chain carriers for organic synthesis, and we are looking forward to developing improved reagents in collaboration with fellow members of the new ARC Centre of Excellence in Free Radical Chemistry and Biotechnology. *(With K L Goh, K A Green, J L Hodgson, E H Krenske)*



## Controlled Radical Polymerisation

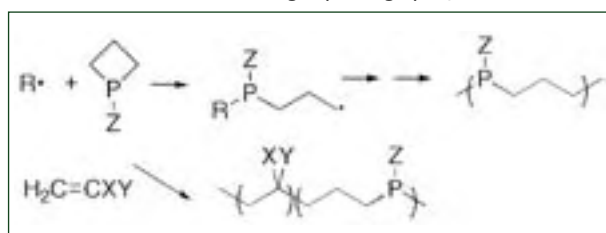
The Australian-invented RAFT process was developed to control the molecular weight and architecture of polymers resulting from free radical polymerisation. We have been using quantum chemistry to build a detailed mechanistic picture of this important process with a view to designing improved RAFT agents for 'difficult' monomers, such as ethylene. In 2005, this culminated in the development and patenting of the first multipurpose agent, capable of controlling monomers with disparate reactivities. Although designed entirely by computer, subsequent experimental testing by collaborators (led by Dr Christopher Barner-Kowollik at the UNSW) has demonstrated it to be capable of controlling free-radical polymerisation. Together, we have also designed an entirely new method for controlling free-radical polymerisation using thioketones as radical spin traps. In 2006, we look forward to applying our computational approach to the atom transfer radical polymerisation process in collaboration with Professors Kris Matyjaszewski (Carnegie-Mellon) and Rinaldo Poli (Toulouse). *(With G E Cavigliasso, E I Izgorodina, E H Krenske, and V Musgrove, D J Henry [RMIT U], A Ah Toy, C Barner-Kowollik, H Chaffey-Millar, T P Davis, M H Stenzel, A Theis [UNSW])*

## Degradation-resistant PVC

The thermal and photochemical stability of poly(vinyl chloride) (PVC) is much lower than it should be on the basis of its chemical structure due to the presence of structural defects, formed by side reactions during the free radical polymerisation process. If these side reactions could be minimised, the inherent stability of PVC would be improved and it would be possible to minimise the use of heavy metal stabilisers in the resulting polymer. To this end, we have been working with the group of Professor Arend Shouten (Groningen) to determine the origin of the structural defects in PVC, and their dependence on polymerisation process conditions. The information will ultimately be used to suggest (and test) improvements to the PVC polymerisation process. *(With A J Schouten, J Purmova, K F D Pauwels, W van Zoelen, J E Vorenkamp [U Groningen, The Netherlands])*

## Polyphosphines

Putting phosphorus into the backbones of polymers can help to impart a range of useful properties including increased polarity, metal ion binding characteristics and fire retardancy. In 2005, we designed a new synthetic method for achieving this, the free radical ring-opening polymerisation of phosphetanes. We showed computationally that these small phosphorus heterocycles would undergo facile ring opening polymerisation *via* substitution of a carbon-centred radical at phosphorus, and that free-radical copolymerisation with normal polyolefins should also be possible. The process is now being tested experimentally in the group of Professor Bruce Wild as part of our larger ARC-funded project to design stereoregular polyphosphines. *(With J L Hodgson, E H Krenske, S B Wild)*







# LIQUID STATE CHEMICAL PHYSICS

PROFESSOR DENIS EVANS

Our research interests include nonequilibrium statistical mechanics and thermodynamics. We have been involved in the development of nearly all of the computer simulation algorithms used for the calculation of transport properties of classical atomic, molecular and short-chain polymeric fluids and lubricants. Algorithms that we have proposed are used to compute the viscosities, thermal conductivities, and diffusion coefficients for molecular fluids and fluid mixtures.

These practical applications are based on the theory of nonequilibrium steady states, also developed by our group. Our theory of such systems provides a framework within which exact relationships between nonequilibrium fluctuations and measurable thermophysical properties have been proved.

We derived the first exact, practical link between the theory of chaos, dynamical systems theory, and thermophysical properties. This link shows that a transport coefficient, like shear viscosity, is related in a direct, quantitative way to the stability of molecular trajectories. Later we derived the so-called Fluctuation Theorem (FT). This remarkable theorem gives an analytic expression for the probability that in a nonequilibrium system of finite size, observed for a finite time, the dissipative flux flows in the reverse direction to that required by the Second Law of Thermodynamics. Close to equilibrium the FT can be used to derive both Einstein and Green-Kubo relations for transport coefficients. In collaboration with members of the Polymers and Soft Condensed Matter Group, the FT has been verified experimentally.

## Unified Description of Recent Theorems in Nonequilibrium Statistical Mechanics

The understanding of thermodynamics is largely confined to equilibrium states. The field of "nonequilibrium thermodynamics" represents an extension of the 19th century concepts of equilibrium thermodynamics to systems that are close to, or at equilibrium. Moreover, these traditional concepts are limited in application to large systems; this restriction is referred to as the "thermodynamic limit". However, in the last decade, two new theorems have revolutionised the field of thermodynamics and its application to modern systems. These new theorems firstly, lift the restriction of the thermodynamic limit, allowing thermodynamic concepts to be applied to small systems, and secondly, apply to systems that may be far-from-equilibrium. The first of these theorems, the Fluctuation Theorem (FT) generalises the Second Law of Thermodynamics so that it applies to small systems, including those far from equilibrium. The second, the Work Relation (WR) (also known as the Jarzynski equality or the nonequilibrium free energy theorem), provides a method of predicting equilibrium free energy differences from experimental trajectories along far-from-equilibrium paths. Previously the FT and WR have been treated as independent theorems. However, in 2005, we proved that these theorems, when expressed as general relations of thermodynamic systems, are related by an additional fluctuation theorem, which we have named the conjugate Fluctuation Theorem (cFT). Each of these theorems describes the distribution of energies along nonequilibrium trajectories. *(With J C Reid, E M Sevick)*



## Experimental Confirmation of Fluctuation Theorems and Nonequilibrium Work Theorems

Associate Professor Sevick and Professor Evans have a joint ARC research grant to work on this subject. See the research summary by Associate Professor Sevick for a description of all the experimental work in this area. *(With E M Sevick, D C Carberry, G Wang, and D J Searles [Griffith U])*

### Gallavotti–Cohen Fluctuation Theorem (FT)

Work has continued on our proof that the so-called Gallavotti–Cohen FT (which only applies to steady states), in fact applies only to constant energy steady states. We now understand why changing from ergostatted to thermostatted dynamics has such a profound effect on the Gallavotti–Cohen FT and the Sinai–Ruelle–Bowen measure. The corresponding Evans–Searles theorems are valid for all kinds of thermostat or ergostat. *(With D J Searles [Griffith U], L Rondoni [Turin Polytechnic])*

### Deterministic Fluctuation Theorem (FT) Applied to Glassy Systems

We applied the FT to glassy systems. Our work on the Gallavotti–Cohen FT has provided a theoretical basis for understanding the limits to the linear response regime in thermal systems. It has been claimed in the past that as the glass transition is approached both the Fluctuation Dissipation Theorem (due to Einstein) and the Evans–Searles Fluctuation Theorem (ESFT) break down. We have shown that these claims are false. Using a combination of theory and nonequilibrium molecular dynamics simulations we have shown that the Fluctuation Dissipation Theorem (FDT) does not fail, but rather as the glass transition is approached the range of field strengths over which linear response can be expected, shrinks to zero. Inside the linear response domain the FDT always works. Outside this domain the FDT does not apply. The previous claims that the ESFT fails as the glass transition is approached was simply due to sampling problems as the glass transition is approached. When sampling is carried out with sufficient care the ESFT always works – as expected from theory.

### Second Law Inequality in Viscoelastic Materials

Linear irreversible thermodynamics asserts that the instantaneous local spontaneous entropy production must always be non-negative. However for a viscoelastic fluid this is not always the case. Given the fundamental status of the Second Law, this presents a problem. Recently we have derived the Second Law Inequality from first principles *via* the Fluctuation Theorem. This derivation proves that the time average of the entropy production is non-negative. The distinction between time averages and instantaneous values has not previously been appreciated. This provides the first known macroscopic consequence of the Fluctuation Theorem. We present a new derivation of the Second Law Inequality from the nonequilibrium Work Relation which has a different domain of validity than that from the Fluctuation Theorem derivation. We tested the Second Law Inequality using molecular dynamics simulations of oscillatory shear in the linear regime. After the decay of the initial transients the Second Law Inequality is valid for time averaged entropy production. We observe that the instantaneous entropy production is negative for various ranges of times.

<http://rsc.anu.edu.au/research/evans.php>

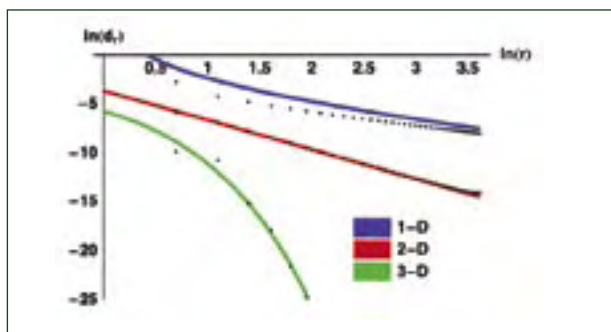


# THEORETICAL QUANTUM CHEMISTRY

PROFESSOR PETER GILL

Quantum chemistry is the discipline in which the laws of quantum mechanics are applied to understand and predict molecular behaviour and, as we enter the 21st century, one of the scientific "grand challenges" is to find ways to extend quantum chemistry's realm to the study of large systems, especially those of biological interest, without using impracticable amounts of computer time. We are contributing to this exhilarating field in several ways.

## Decay Behaviour of Least-squares Expansion Coefficients



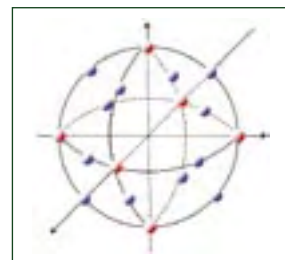
Although it is common to approximate the electron density by a linear combination of expansion functions, little was known about the rate at which the expansion coefficients  $d_r$  decay with distance  $r$ . We found empirically, and then proved rigorously, that the decay is slow ( $1/r$ ) if the expansion basis is one-dimensional (1D), moderate ( $1/r^2$ ) in the 2D case, but surprisingly fast ( $e^{-\alpha r}$ ) in the 3D case. (With A T Gilbert, and M Head-Gordon [U Berkeley, USA], S Taylor [U Auckland, NZ], G Friesecke [U Warwick, UK])

## Electron Correlation in Hookium and Small Molecules

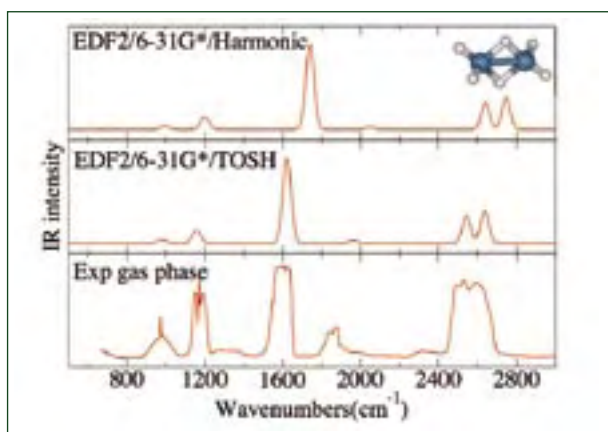
In order to develop better methods for computing molecular energies, it is desirable to have a set of benchmark molecules for which the true correlation energies are known. It was curious, therefore, that such a dataset did not appear to have been tabulated in the literature. However, by judiciously combining high-quality experimental and computational data, we were able to determine the correlation energies of a set of 56 small molecules and a "model atom" called hookium. These results should be useful for the assessment of new quantum chemical methodologies. (With D P O'Neill)

## High-speed Density Functional Calculations

Traditional DFT calculations use quadrature (numerical integration) to compute the exchange-correlation energy and the challenge is to design quadrature grids that are as small as possible (to maximise speed) but as accurate as possible (to minimise numerical errors). We have developed a new grid, SG-0, that employs approximately 1500 points around each nucleus and consumes only half as much CPU time as the SG-1 grid. It is less accurate than SG-1 but, on balance, offers an attractive compromise that is particularly suitable for preliminary investigations of moderately large biochemical systems. It is the default grid within the new Q-Chem 3.0 software package. (With S H Chien)



## Anharmonic Vibrational Frequencies



We have extended our earlier work on the calculation of accurate harmonic frequencies by testing the performance of a number of anharmonic algorithms and developing a new one called TOSH. This enables us to make more accurate predictions of vibrational (i.e. infra-red or Raman) spectra, without recourse to empirical scale factors. In collaboration with various experimental groups, we have computed the spectra of *p*-fluorotoluene, 2-aminopurine,  $\alpha$ -tocopherol and diborane. (With C Y Lin, R D Webster, and K L Reid, M W George [U Nottingham, UK])

## Multipole-derived Atomic Charges

Atomic charges in molecules are not observable quantities but chemists nonetheless find them valuable for interpretive purposes. Many methods have been proposed for calculating these ill-defined quantities, none is entirely satisfactory. We have developed the necessary theory to compute the charges that reproduce as many of the low-order multipole moments of the system as possible. (With A T B Gilbert, and A C Simmonett [U Nottingham, UK])

## Intracules and the Correlation Problem

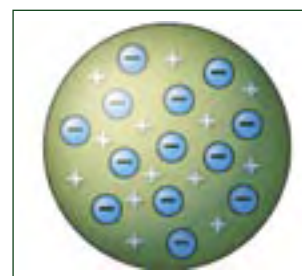
We have extended our earlier work by introducing the Omega intracule  $\Omega(u,v,\omega)$ , a function that gives the probability of finding two electrons whose interelectronic position and momentum vectors have magnitudes  $u$  and  $v$ , respectively, and which subtend an angle  $\omega$ . This provides a more detailed picture of the motion of pairs of electrons than had been available previously and we have conjectured that the correlation energy is given by

$$E_{\text{corr}} = \int_0^{\infty} \int_0^{\infty} \int_0^{\pi} \Omega(u,v,\omega) G(u,v,\omega) d\omega dv du$$

where  $G(u,v,\omega)$  is a universal (but as yet unknown) function that we call the correlation kernel. Omega intracules are mathematically troublesome but we can now generate them for small molecules with sp basis sets and we have begun an assessment of their properties. (With D L Crittenden, D P O'Neill, and N A Besley [U Nottingham, UK])

## The n-Electrons-in-a-box Problem

Density functional theory (DFT) is based on a hypothetical infinite box containing an infinite number of electrons. In order to improve our understanding of this model (which is usually called jellium), we have performed restricted Hartree-Fock calculations on finite analogues of it, containing up to  $n = 174$  electrons. (With S Ghosh [U Nottingham, UK])





# LASER AND OPTICAL SPECTROSCOPY

PROFESSOR ELMARS KRAUSZ

Light, chemistry and photophysics are the most natural and cooperative of partners, dancing together and enabling life on earth. The energy in a photon of visible light is just that needed to perform many chemical transformations. Photosynthesis, the most important chemical process on Earth, is an amazingly efficient and delicately balanced process. Photosynthesis captures light from the sun and converts it to chemical energy. The Earth's chemical storehouse of oil and coal, that we burn so freely and thoughtlessly, has been accumulated through millennia of photosynthetic activity.

Spectroscopy is our passion. We are fascinated by the subtle and utterly distinctive interactions of light with solids and liquids. Light, after hitting a sample, is usually absorbed, converted to fluorescence or just bounced off (scattered). Lasers, through such amazing characteristics as great intensity, purity and coherence, can drive far less familiar processes such as harmonic generation. By combining conventional and laser techniques, a truly impressive range of spectroscopic techniques becomes available. Even a single molecule can be detected and analysed.

Spectroscopy probes the innermost secrets of chemical and physical transformations. It maps out the detailed electronic structure of the different forms of matter: crystals, liquids, glasses, proteins *etc.* For each case, information can be gained on how constituents bind together, how they interact with their environment and how they transform.

Our group performs a wide range of spectroscopic measurements: absorption, dichroism, emission, Raman, excitation, hole-burning and line-narrowing. The systems we study may be organic or inorganic, molecular, ionic, amorphous, crystalline or biological. Our strength lies in our ability to design, develop and construct specialised experiments and apparatus to target fundamentally important questions in an area of interest. A persistent theme we have is that molecules can behave quite differently in solution to when they are 'trapped' or enclosed in a protein or crystal. Such environmental influences are ideally probed *via* laser-selective spectroscopy.

Over the last few years our group has made spectacular progress in identifying the true charge separating state of Photosystem II (PSII), the engine room of life. PSII is unique in its ability to oxidise water and provides virtually all the bioenergetic electrons on Earth. In 2005, aspects of this discovery were presented at the AIP meeting in Canberra, the RACI meeting in Sydney, international conferences in Beijing and Shanghai, and culminated in Elmars Krausz being invited to talk about these dramatic developments at a special symposium in Amsterdam in October.

This year our group hosted internationally renowned researcher in photosynthesis, Bill Rutherford, as the Craig lecturer. During his month-long stay at the RSC, he presented a series of energetic and exciting talks and was actively involved in experimentation in our labs. Also visiting during the year were Mark Riley and ARC Linkage PhD student Andrew Dick who further developed our new MCD spectrometer system. Sindra Peterson Årsköld, of Lund University, came last summer to perform further magneto-optical measurements on cytochrome  $b_6/f$ . Felix Ho, a former RSC summer scholar, currently a postdoctoral fellow in Uppsala, Sweden, spent an exciting month investigating some optical consequences of redox processes in PSII.



## The PSII Saga

Following our utterly unexpected discovery that the charge separating state of PSII lies at far lower energy than thought, we have now firmly established a spectral and photophysical characteristic of this most critical state. Charge separation occurs with wavelengths as long as 730 nm, even at the lowest temperatures, and this 'red tail' phenomenon is general, occurring in both plants and cyanobacteria. Our efforts are attracting increasing attention and the significance of the phenomenon, particularly with respect to primary charge separation and the overall function of PSII, is being widely addressed. Significant discoveries have also been made with respect to secondary redox processes in PSII, again challenging long-held beliefs. *(With J Hughes, L Debono, and R Pace, P Smith [Dept Chemistry, ANU], A W Rutherford [Saclay, France], S Styring, K Sigfridsson, F Ho [Uppsala U, Sweden])*

## The ANU and University of Queensland Magneto-enzyme Spectrometers

Faults in the superconducting magnet cryostats purchased for the ARC LEIF- and MEC-funded spectrometers for the ANU and the University of Queensland have been repaired, and both systems are now functional. The spectrometer interface, based on LabView software development, is proceeding at the University of Queensland and specialised sample handling and detector systems are being developed and refined at the ANU. *(With M Riley, A Dick [U Queensland], Lastek Pty Ltd [Adelaide])*

## Multidimensional Spectral Characterisation of Art Works

Art objects are both unique and priceless. Consequently they cannot be extensively sampled or taken apart for analysis. We have developed a portable, powerful and remarkably cost effective imaging system based on a high sensitivity cooled CCD sensor, which accumulates spatially resolved fluorescence and reflectance spectra of art works *in situ*, with minimal impact on the object studied. The multidimensional optical characterisation of art works provided, also serves as a powerful tool for conservation, preservation and forgery detection. *(With M Kubik, and D Creagh [U Canberra])*



<http://rsc.anu.edu.au/research/krausz.php>



# POLYMERS AND SOFT CONDENSED MATTER

ASSOCIATE PROFESSOR EDITH SEVICK

In the last decade, Atomic Force Microscopy (AFM) and Optical Tweezers (OT) have revolutionised molecular science by measuring piconewton forces over lengthscales from 1 to  $10^4$  Å. Our research focuses upon experiments using the technique of OT, but we are also involved in theory and simulation that is complementary to these OT measurements. The OT apparatus is based upon a focused laser beam that is refracted through a micron-sized, transparent bead. The refracted rays differ in intensity over the volume of the colloidal bead and exert a force on the bead, drawing it towards the region of highest light intensity. The optical trap is harmonic near the focal point: the optical force acting on a colloidal particle positioned at  $x$  from the trap centre is  $F_{\text{opt}} = -kx$ , where  $k$  is the trapping constant which can be tuned by adjusting the laser power. In this way, the optical trap generated by the OT serves to both localise a colloidal particle and to measure the small, sub-piconewton scale forces acting on the particle. These measurements are central to our overall aim to probe and develop new understandings of the energetics and dynamics of small systems, including polymers and colloids.

## Design and Construction of a New Holographic Optical Tweezers Apparatus

With funding from ARC-LIEF and ANU-MEC, we designed and constructed a flexible optical tweezers apparatus that provides a wider range of manipulations on small objects. Using a single light beam passing through a hologram (which is effectively a phase-only diffractive beam splitter), it is possible to construct an array of traps in 2 or 3 dimensions. Depending upon the hologram, traps can be generated with different trapping characteristics, e.g. a combination of forces and twist-like torques. If the hologram is replaced with a computer-addressed SLM or spatial light modulator, a component that dynamically controls the phase-shift and intensity at individual pixel elements, then we create an array of traps that can move or "dance" in 2 or 3 dimensions and dynamically alter the trapping characteristics of each trap. These advances can potentially make difficult OT force measurements far simpler; but more importantly, they also increase the vista of explorations available. This new apparatus will be used to study the stretching of synthetic and biological single polymer chains, to investigate colloidal interactions, to measure the micro-rheology of various solutions, and to demonstrate new theorems in nonequilibrium physics. (With G M Wang, D M Carberry, D J Evans, and T J Senden, D R M Williams [RSPHYSSE, ANU], H R Brown, G M Spinks [U Wollongong])

## Demonstrations of the Fluctuation Theorem using Complex Systems

The puzzle of how time-irreversible microscopic equations of mechanics lead to the time-irreversible macroscopic equations of thermodynamics has been a paradox since the days of Boltzmann. Boltzmann simply sidestepped this enigma by stating, *as soon as one looks at bodies of such small dimension that they contain only very few molecules, the validity of this theorem [the Second Law of Thermodynamics and its description of irreversibility] must cease*. Today we can state that the Fluctuation Theorem (FT), first proposed by Denis Evans and colleagues in 1993, is a generalised, Second-Law-like theorem that bridges the microscopic and macroscopic domains and links the time-reversible and irreversible descriptions. The predictions of the FT should be relevant to many nanotechnological applications, and our experimental demonstration of the FT in 2002 received considerable attention in the popular press, science journals, and other media primarily because of its implications to nanotechnology. However, to date the FT has been confirmed only with exceptionally simplified systems that are fully describable using deterministic or stochastic dynamics, such as a single optically-trapped colloidal particle

in a Newtonian fluid, or a computational sea of Lennard–Jones particles. Our premise is that the FT holds for any general system, including more complex systems that currently defy exact description, such as biological or molecular motors. To test the application of the FT to more relevant nanosystems, we need to address systems of increasing complexity. Our approach is to increase complexity one-step-at-a-time and a strategic system to investigate is, therefore, a single colloidal bead, optically-trapped in a viscoelastic solution. While an optically-trapped particle in a Newtonian fluid is perfectly describable using Langevin dynamics, the dynamics of the same particle in a viscoelastic solution is far more difficult to describe. Our experiments demonstrate that the particle's trajectories in viscoelastic solution obey the FT. *(With D M Carberry, G M Wang, D J Evans)*

### Experimental Demonstrations and Stochastic Description of the Work Relation using a Colloidal Particle in an Optical Trap

The Work Relation (WR) predicts that the free energy difference between two equilibrium systems can be determined by measuring the work done along dynamical paths that connect the two states. These paths may be traversed at arbitrary rates, so that the intervening path may not be in true thermodynamic equilibrium. This is a complete anathema to our understanding of conventional thermodynamics: conventional thermodynamics states that the free energy difference is the work done along a path that is traversed so slowly that the intermediate states are all in thermodynamic equilibrium, *i.e.*, a "quasi-static" pathway. The potential importance of the WR has both theoretical and practical aspects. One could theoretically calculate the free energy difference between states using fictitious paths that "morph" between two states on a computationally convenient (not necessarily realistic) energy surface. On the practical side, the WR suggests that measuring work on small microscopic processes could yield thermodynamic quantities that are traditionally inferred from bulk calorimetric measurements. This is particularly interesting, as measurements of the work done by small colloidal/polymeric/biological systems are possible with techniques such as OT, and the WR then translates these nonequilibrium measurements into thermodynamic information. We investigated both theoretically and experimentally, the work done along the trajectory of a single colloidal particle weakly held by an optical trap whose strength was changed. *(With G M Wang, D M Carberry, J C Reid, P Ranganathan, D J Evans)*

### Collapse Dynamics of Semi-flexible Polymer Chains using Brownian Simulations with Hydrodynamic Interactions

Many linear biopolymers such as actin and DNA have backbones that are much stiffer than, say, polystyrene. These stiff polymers cannot easily bend, much like a garden hose, and are called semi-flexible. When flexible polymers are placed in a poor solvent, where strong attractive monomer-monomer interactions dominate, surface tension drives the chain into a compact, globule shape. However, for semi-flexible chains, the backbone stiffness impedes this compaction and favours conformations with minimal bending along the contour, in particular, very few tight bends. Instead of a collapsed globule, a semi-flexible chain in poor solvent folds into a torus. This toroidal configuration is often seen in experiments. To biologists the toroidal conformation is useful, as it allows one to introduce foreign pieces of compact DNA into cell nuclei. The final folded state of the chain depends sensitively upon the dynamics of the system, including the solvent that mediates forces between distant segments of the chain. However, efficient algorithms that account for hydrodynamic interactions in long polymeric chains were only recently developed. We initiated a simulation study of the dynamics of the collapse of flexible and semi-flexible chains in poor solvent. We use Brownian dynamics simulations that incorporate hydrodynamic interactions to explore and to develop a better understanding of the dynamics of the coil-to-globule transitions of single polymer chains in poor solvents. Understanding the process of single chain collapse is important in predicting the behaviour of DNA and proteins, which form folded and highly compact structures. *(With P Ranganathan, and D R M Williams [RSPHysSE, ANU])*

<http://rsc.anu.edu.au/research/sevick.php>

# MOLECULAR ELECTROCHEMISTRY

DR RICHARD WEBSTER

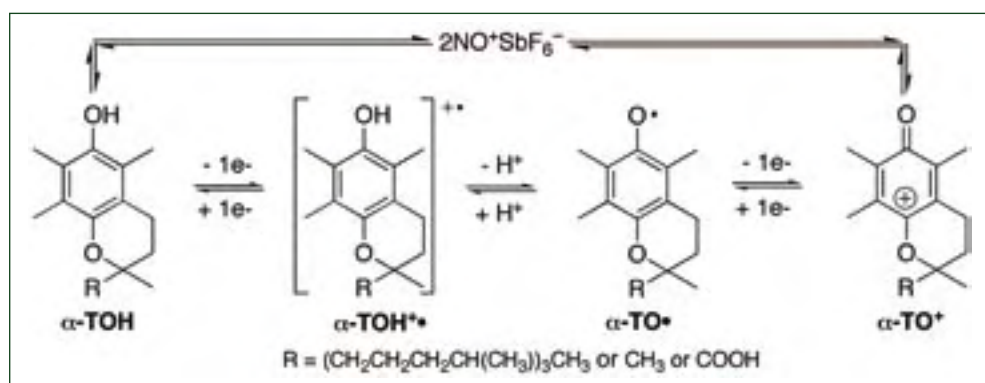


The electrochemical control of oxidation and reduction processes in organic and inorganic systems is an area of extensive research in both academia and industry. Electrochemical techniques are extremely useful in generating interesting species in unusual oxidation states, or for producing reactive intermediates (for example in the reductive dimerisation of vinyl cyanide in the Monsanto manufacture of Nylon 66), but provide little intrinsic structural information. To overcome this limitation, spectroscopic methods have frequently been used in conjunction with electrochemical methods in order to monitor the progress of a reaction and to obtain more detailed structural and mechanistic information. The *in situ* alliance of electrochemistry/spectroscopy is particularly valuable in situations where the species undergoing the redox process would not survive the transfer from an electrochemical to a spectroscopic cell, or in situations where it is essential that the spectroscopic analysis occur concurrently with the electrochemical generation, such as in kinetic studies. The focus of this research is developing and utilising spectroscopic techniques, including EPR, UV-VIS, FTIR and NMR, to study processes involving electron transfer in organic and inorganic systems.

## The Redox Chemistry of Vitamin E

Vitamin E refers to a collection of naturally occurring compounds produced by plants that are based on 6-chromanol with an extended alkyl (phytyl) chain in the 2-position.  $\alpha$ -Tocopherol ( $\alpha$ -TOH), the fully methylated tocopherol is by far the most biologically active and abundant of all the components of vitamin E found in mammalian tissues. Work recently conducted in our laboratories has proven the existence of several intriguing and new oxidised forms of  $\alpha$ -TOH, which are reversibly linked to the starting material through a series of proton and electron transfers. Of particular interest is the phenoxonium cation ( $\alpha$ -TO<sup>+</sup>) that can be produced by chemical oxidation with NO<sup>+</sup> and is remarkably stable in solution with a lifetime of at least several hours in dry organic solvents.

Phenoxonium cations have for a long time been postulated as intermediates produced during the oxidation of phenolic compounds, but were generally thought to be stable for only short times (<1 s). Therefore, it is an extraordinary observation that the phenoxonium cation derived from a naturally occurring compound is stable in solution. Furthermore, the stability is directly attributable to the specific molecular structure that "nature" has assigned to vitamin E. <sup>13</sup>C NMR spectroscopy experiments and theoretical calculations performed on  $\alpha$ -TO<sup>+</sup> indicate that the positive charge is shared between the

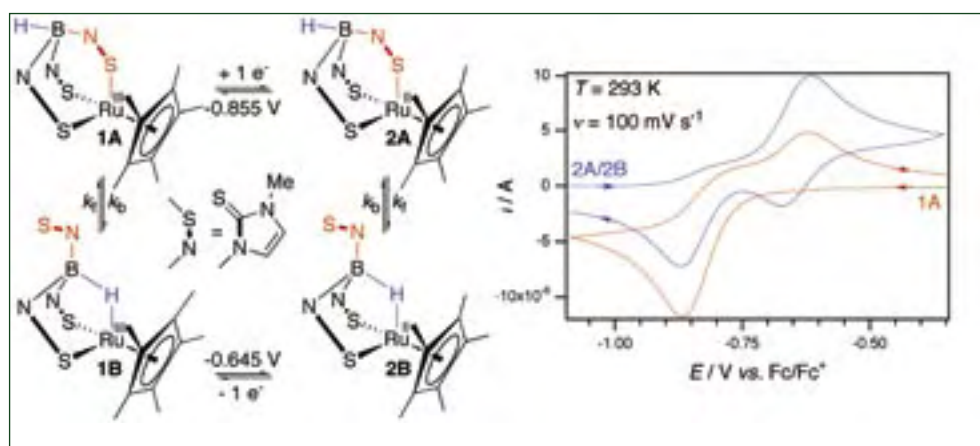




carbon atoms bonded to oxygen atoms and on the quaternary carbon in the chromanol ring. While the phenoxonium cation is reactive towards nucleophiles such as water, it may be moderately stable in the hydrophobic (lipophilic) environment where vitamin E is known to occur naturally. (With S B Lee, C Y Lin, P M W Gill)

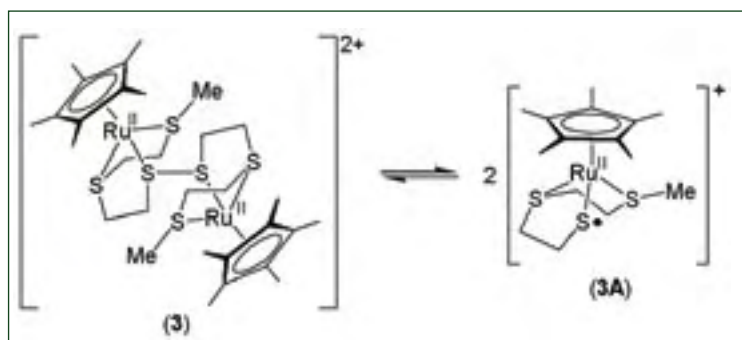
## Electrochemically Induced Transformations of Organometallic Ru Compounds

$[\text{Cp}^*\text{Ru}^{\text{III}}\{\text{HB}(\text{mt})_3\}]\text{X}$  (1A) ( $\text{X} = \text{Cl}, \text{PF}_6$ ) and  $[\text{Cp}^*\text{Ru}^{\text{II}}\{\text{HB}(\text{mt})_3\}](2\text{A})$  ( $\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$ ,  $\text{mt} = N$ -methyl-2-mercaptoimidazol-1-yl) were synthesised by the reactions of  $\text{K}[\text{HB}(\text{mt})_3]$  with  $[\text{Cp}^*\text{Ru}^{\text{III}}\text{Cl}_2]_2$  and  $[\text{Cp}^*\text{Ru}^{\text{II}}(\text{OMe})_2]_2$ , respectively. 1A and 2A exist in the solid state in  $\kappa^3\text{-S,S',S''}$  coordination, so that the sulfur atom in each mt group coordinates to the central Ru ion producing the normal tripodal geometry of the  $[\text{HB}(\text{mt})_3]$  ligand. Both compounds, however, undergo an isomerisation reaction in solution



where the sulfur on one mt group is displaced in favour of coordination to the hydrogen that is bonded to the boron (an agostic B–H–Ru interaction) resulting in  $\kappa^3\text{-H,S,S'}$  coordination about the Ru (an electrochemical “square scheme” mechanism). Variable temperature NMR spectroscopic and cyclic voltammetry experiments were used to obtain the rate and equilibrium constants for the  $\kappa^3\text{-S,S',S''}$  and  $\kappa^3\text{-H,S,S'}$  coordination exchange.

Alkylation of  $[\text{Cp}^*\text{Ru}^{\text{II}}(\text{tpdt})]$  ( $\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$ ,  $\text{tpdt} = \eta^3\text{-S}(\text{CH}_2\text{CH}_2\text{S}^-)_2$ ) with MeI or  $\text{Me}_3\text{OBF}_4$  resulted in the formation of a trans  $\mu\text{-}\eta^1\text{-}\eta^1\text{-S}_2$  coupled species,  $[\{\text{Cp}^*\text{Ru}^{\text{II}}\}_2\{\mu\text{-}\eta^6\text{-S}(\text{CH}_2)_2\text{S}(\text{CH}_2)_2\text{SMe}_2\}]^{2+}$  (3) as the predominant product. A combination of electrochemical, EPR, UV-VIS and NMR experiments indicated that the solution phase chemistry of 3 is governed by its reversible dissociation into the mononuclear cation radical (3A).



The facile alkylation-induced S–S bond coupling and the ease of reversible homolytic S–S bond scission appear to be unique to this Ru(II) system. (With L Y Goh, [National U Singapore])





## DISORDERED MATERIALS

PROFESSOR RICHARD WELBERRY

This group combines diffuse X-ray scattering methods with computer simulation to deduce the arrangement of atoms and molecules in disordered crystals. Conventional crystal structure determination reveals only averaged arrangements, inadequate to explain some of the basic properties of many minerals, inorganic compounds, organic compounds and alloys that exhibit crystalline disorder. Diffuse scattering gives information on how neighbouring atoms or molecules interact with each other. Quantitative studies of diffuse scattering are, however, still rare because of the intrinsically very low intensities involved.

The group uses dedicated diffuse-scattering diffractometer systems based on curved position-sensitive wire detectors. These allow high quality diffuse scattering data to be efficiently recorded over large regions of diffraction space and provide a unique facility for tackling a whole range of complex structural problems. The group also has access to the most advanced synchrotron radiation and neutron source facilities in the world and methods are being developed to utilise these for diffuse scattering measurements.

The group's interests span a wide range of fields, each presenting problems for which this specialised technique can give unique information. Areas in which we have applied the techniques include: disordered molecular crystals, guest/host systems such as urea inclusion compounds, non-stoichiometric inorganic materials and minerals (for example, the cubic stabilised zirconias, mullite and wüstite), flexible framework structures such as silica polymorphs and their analogues, alloys, and quasicrystal phases.

Much of the current effort of the group is concerned with the further development and exploitation of the least-squares method, which was developed in the group for directly fitting a Monte Carlo (MC) simulation to observed X-ray diffraction data.

### Refinement of Monte Carlo Models of Disordered Molecular Crystals



PhD student Andrew Beasley helps Dr Matthias Gutmann with a neutron experiment at ISIS.

We have now extended the automatic refinement method to use neutron diffuse scattering data in addition to X-ray data. Deuterated benzil,  $C_{14}D_{10}O_2$ , has been studied. The neutron data, collected using the SXD instrument at the ISIS facility in the UK, has the advantages of being sensitive to light atoms, such as hydrogen (although to reduce absorption of the neutron beam, deuterium is used instead) and of giving three dimensional data over a very wide region of reciprocal space. The neutron data successfully constrained the magnitudes of the displacements of the atoms in a way that the X-ray data had failed to do. The first simultaneous refinement of neutron and X-ray diffuse scattering data showed that the two techniques can be as successfully combined in the study of diffuse scattering as they are, routinely, in conventional crystallography. *(With D J Goossens, A Beasley, A P Heerdegen, and M J Gutmann [ISIS, Oxon, UK])*

## Diffuse Neutron Scattering from Crystals

We have carried out experiments using the time-of-flight (tof) Laue technique instrument, SXD, at ISIS in order to collect diffuse scattering data for the molecular crystal d-benzil,  $C_{14}D_{10}O_2$  from a complete 3D volume of reciprocal space out to very high  $Q$  ( $30 \text{ \AA}^{-1}$ ). The aim in this work is to obtain a PDF (pair distribution function) in three dimensions. PDFs in 1D have recently become accepted as a valuable tool for probing local structure in materials from powder diffraction data and the thesis of our work is that a 3D PDF that is obtainable from single crystal data should provide a much more detailed view of this local structure, since there is no orientational averaging. Our work on neutron diffuse scattering has featured as a 'Science Highlight' in the ISIS Annual Reports for 2004 and 2005.

Neutron diffuse scattering data have also been collected at ISIS for deuterated *para*-terphenyl at temperatures above and below the structural phase transition near 200K. The study reveals details about the phase transition and is our first example of using neutron data on a molecular system containing static disorder. Below the phase transition temperature the static disorder vanishes and only the thermal motion remains. (With D J Goossens, A Beasley, A P Heerdegen, and M J Gutmann [ISIS, Oxon, UK], Th Proffen, [LANL, Los Alamos, USA])

## The Influence of Disorder on Polymorphism

Polymorphism is of key importance in the pharmaceutical industry since the properties of different polymorphs of the same compound may differ considerably e.g. the rate of uptake of pharmaceutical molecules by the human body is often strongly dependent on which polymorphic form of the material is present. There are many patenting issues that arise from this. The aim of the study is to use diffuse scattering methods to investigate the crystal structures of polymorphic systems in a level of detail that goes beyond the average structures that are revealed by conventional crystallography. A particular aim is to investigate the role that molecular flexibility plays in determining crystal packing and the conformations and dynamics of the molecule that occur in different polymorphs.

As a first step we are studying the model compound *p*-(*N*-methylbenzylidene)-*p*-methylaniline (MeMe), which is known to crystallise in at least three polymorphic forms. Two of these have orientational disorder in which the molecules are "flipped" either end-to-end and/or side-to-side, but the third appears, in conventional crystallographic studies, to be completely ordered. We have collected three-dimensional diffuse scattering data from all three polymorphs at the Advanced Photon Source (APS), and are now attempting to model the features in their diffuse diffraction patterns. Even the 'ordered' polymorph II shows highly structured diffuse scattering, which should reveal a wealth of detail of the local structure and dynamics. (With A Beasley, D J Goossens, A P Heerdegen, and P L Lee [APS, Argonne, USA])



From left to right, the (*h*0*l*) sections of the three polymorphs I, II and III of MeMe.



# SOLID STATE MOLECULAR SCIENCE

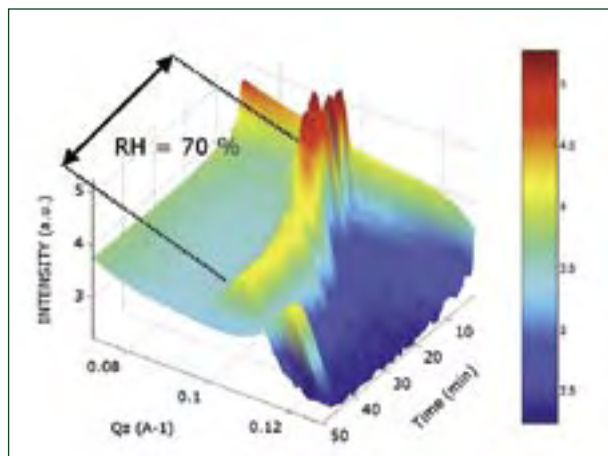
PROFESSOR JOHN WHITE

Neutron and X-ray scattering methods, developed by this research group, are used to study the structure and dynamics on nanometre and picosecond space/time scales. Adsorption, self-assembly at interfaces, polymers, the imitation of biomineralisation phenomena using "template" molecules and, most recently, the structure and denaturation of proteins at interfaces are current areas of interest. The insights gained are used to guide chemical synthesis in making new materials with interesting physicochemical properties. One recent highlight has been the first determination of the thermodynamic parameters for protein denaturation in the 50 Å surface layer of a protein solution. By comparison with denaturation in the bulk, the contribution of the surface forces can be measured quantitatively. Another highlight is the first measurement of the interfacial structure of an emulsion surface by neutron reflectivity and the extension of this program to new surfactant design.

Our collaboration with Orica Ltd and Food Science Australia on the structure and stability of emulsions has produced scientifically interesting and useful practical information. We continue to show that structural relationships at the nanoscale have importance for rheological and other properties.

## Titanium Oxide Films for Solar Energy Capture

Titanium dioxide is an inexpensive and stable semiconductor material. Its wide bandgap, however, (ca. 3.2 eV) allows



Time resolved X-ray reflectivity of a growing titanium oxide film showing quick de-swelling at (ca. 40 minutes) when humidity was changed from 70% RH to 30% RH.

for the capture of only 2–8% of the solar photon flux. A shift in the optical response of  $\text{TiO}_2$  from the UV to the visible spectral range will increase the effect on the photocatalytic efficiency of the material. Our work concerns the preparation of thin mesoporous  $\text{TiO}_2$  films (800 – 3000 Å) doped to provide a shift in the optical response. The films have been prepared by a surfactant template route using evaporative induced self-assembly (EISA). During the year the collaboration identified the conditions required to form well structured films reproducibly; characterised the film structure at each step of the process with reflectometry using X-rays and neutrons; nitrogen doped the oxide framework; and removed the surfactant template with an ethanol rinsing treatment prior to calcination at 400 °C to help prevent collapse of the oxide structure. (With M J Henderson, and A Gibaud [Laboratoire de Physique de l'Etat Condense, Le Mans, France], A R Rennie [Uppsala U, Sweden])

## Solvent Effects in High Internal Phase Emulsions (SANS and USANS Analysis)

Previous work using small angle neutron scattering (SANS) and ultra small angle neutron scattering (USANS) focused on high internal phase emulsions (90% aqueous phase/10% oil phase) in which surfactant nature, concentration and molecular weight have been varied. This year we have completed a comprehensive study on the effects of variation in the oil phase on the emulsion structure. The oil-phase consisted of mixtures of hexadecane and toluene in different ratios. The research



has been supplemented by small angle X-ray scattering data and viscometry on surfactant solutions in the corresponding hexadecane/toluene mixtures. The combination of USANS, SANS (various neutron contrasts) and optical microscopy enabled us to develop a complete structural description of the emulsion system. The polyisobutylene-based surfactant stabilises the droplets within the emulsion by monolayer formation at the aqueous/oil interface, and by formation of nanometer-scale reverse micelles within the oil phase. The obtained data have been fitted to a model of linked micron scale surfactant-rich blocks, whose number, size and dimensionality of linkages vary systematically with the surfactant-oil interaction. The model results reveal that the compatibility of surfactant with oil is the major factor in the type, size and relative amounts of observed emulsion structures. *(With K Baranyai, A J Jackson, P A Reynolds, A J Scott, J Zank, and J Barker [NIST, Gaithersburg, USA])*

### Synthesis and Characterisation of Novel Surfactants

A plethora of novel surfactants for a potential application in high internal phase emulsion systems have been synthesised. Access to a large variety of monomers enabled us to prepare block oligomers with defined properties. The compounds have been characterised by Gel Permeation Chromatography (GPC) and Modulated Differential Scanning Calorimetry (MDSC). In order to understand and predict the behaviour of the surfactant molecules at the water-oil interface, the behavior at the water-air interface (Langmuir Trough) served as a model. The aim of our work is to investigate the stabilisation mechanism of these amphiphiles when used at lower concentration, for the preparation of high internal phase emulsions. *(With J Zank, A J Scott)*

### Denaturation of Proteins at Interfaces at the Nanometre Scale

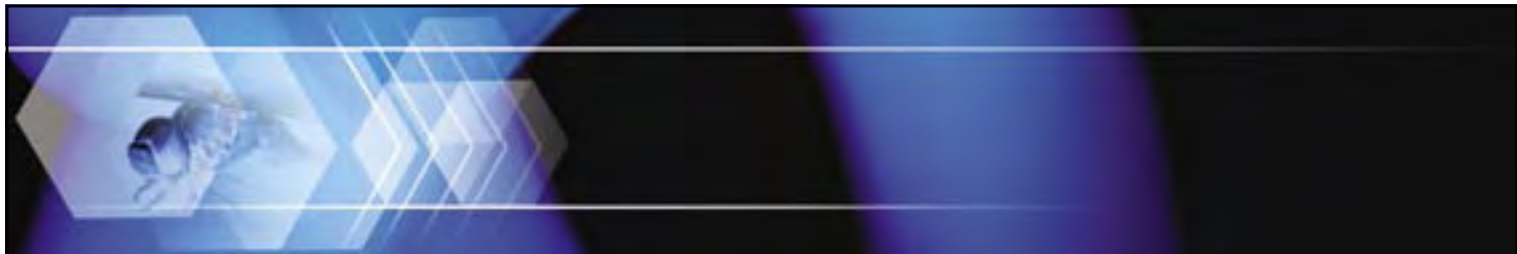
Dried dairy ingredients are an important segment of the Australian dairy market. In the case of high protein content powders a loss of functionality (e.g. solubility) is observed on drying. We are employing scattering techniques (neutron and X-ray) to examine the nanoscale structural changes that occur on dehydration. Our aim is to relate these changes to the observed loss of functionality and propose methods to restore that functionality. *(With A J Jackson, and M A Augustin [Food Science Australia])*

### Kinetics of Adsorption of Lysozyme at the Air/water Interface

The adsorption kinetics of Hen Egg White Lysozyme at the air/water interface has been studied using specular neutron reflectometry. Experiments were performed at a number of pH values to examine the effect of charge on the rate of protein adsorption. Solutions of Hen Egg White Lysozyme in Air Contrast Matched Water at 1 mg/mL were made. These allow direct determination of the surface excess of protein. High repetition experiments with short collection times were used to accurately determine only the surface excess, derived from the product of the film thickness and the scattering length density of the layer. The kinetic traces at pH values where the protein is charged, are well fitted by a first order rate equation with two linear regions, where the change in the gradient occurs as the surface concentration reaches a steady state. This behaviour is characteristic of the transport and distortion of protein molecules, followed by rearrangement in the surface layer. The equilibrium concentration is a function of protein charge with steady state surface concentrations reaching 1.4 mg m<sup>-2</sup> at pH 4 and 3 mg m<sup>-2</sup> at pH 11. Protein charge is inversely related to the rate of adsorption. This dependency has been explored through use of thermodynamic analysis. *(With A W Perriman)*

<http://rsc.anu.edu.au/research/white.php>





## VISITING FELLOWS (POST-RETIREMENT)

Seven of the retired staff members, appointed by invitation of the Dean, have continued independent research programs:

**Emeritus Professor Athelstan L J Beckwith AO BSc WA DPhil Oxford, FRACI, FAA, FRS** (retired 1996) is continuing his work on the structure, stability and reactions of organic free radicals. The ESR spectrometer previously housed in the Birch Building has been moved to a new laboratory and recommissioned. Cooperative work involving ESR spectrometry has been established with other researchers both within the RSC and other Australian Universities. The factors that underlie the high diastereoselectivity of various radical reactions are being studied, as is the utility of ESR spectroscopy for the estimation of radical stability. A major collection of ESR data for organic radicals is in the hands of the publisher. Two major papers on radical stability and the kinetics of reactions involving persistent radical intermediates are nearing completion.

**Emeritus Professor Martin A Bennett BSc PhD DIC DSc London, ARCS, FRACI, FAA, FRS** (retired 2000). During 2005 Professor Bennett has continued collaboration with Professor Suresh Bhargava at RMIT University and has co-supervised a postdoctoral fellow (Matthew Byrnes, a former PhD student at RSC), a research assistant (Steven Privér), and two PhD students working at RMIT on the chemistry of cyclometallated complexes of gold and palladium. A second full paper on Steven Privér's PhD work has appeared in *Inorg. Chem.* Two reviews have been completed during the year: one is a joint work with the RMIT group for *Coord. Chem. Rev.* on cyclometallated tertiary phosphine complexes, the other results from the PhD work of Joanne Adams, his last ANU PhD student,

on tethered arene complexes, and will be published in *Advances in Organometallic Chemistry*. He also continues to referee extensively for international journals, including *Organometallics*, *Dalton Trans.*, *Inorg. Chem.*, *New J. Chem.*, *J. Organomet. Chem.*, and *Inorg. Chim. Acta*.

**Dr Richard Bramley MSc Sydney, PhD London, MRACI** (retired 1997). During the year, Dr Bramley has continued consultations with the Laser Physics Group, RSPHysSE, ANU, particularly on microwave safety issues concerning unshielded loop-gap resonators. He has also consulted with the Faculty of Engineering and Information Technology on aspects of EPR spectroscopy, similarly with the EPR Dating Laboratory of RSES, and with academic staff in the School of Environmental and Mathematical Sciences at University College, ADFA, on low radiation, digital X-ray imaging. Consultations last year with staff at Caltech in their attempts to pursue zero-field EPR spectroscopy have been rewarded with their successful construction and operation this year of a zero-field EPR spectrometer. He continues a major collaboration with University College, ADFA, and indirectly with the Quantum Computing group at UNSW, extending this year to the University of Melbourne, all ultimately aiming to use implanted silicon as a quantum computing material. Work has continued on electric field rather than magnetic field readout in P doped silicon, and EPR has been successfully detected photoelectrically in such materials. The transfer of an electromagnet to ADFA will facilitate their construction of a millikelvin pulsed EPR spectrometer, a unique facility to which the RSC will have access.



Dr Desmond J Brown BSc MSc Sydney PhD DSc London (retired 1986), formerly of the JCSMR, has begun a detailed critical review of research on the six naphthyridine systems. This will be the first book on naphthyridines in over a century and will be his eleventh book on diazabenzenes and di- or polyazaphthalenes within the Wiley series *The Chemistry of Heterocyclic Compounds*.

Dr John K MacLeod BSc PhD Queensland, FRACI (retired in 1999) continued to be involved in writing papers resulting from work carried out by two of his former PhD students and from a collaborative project with Dr Murali Nayudu, Division of Botany and Zoology (BoZo), School of Life Sciences, ANU.

**Emeritus Professor Rodney W Rickards BSc Sydney FRACI, FAA** (retired in 1999) is also a Visiting Scientist at CSIRO Entomology. Collaboration continued with Dr Geoffrey Smith in the Division of Biochemistry and Molecular Biology (BaMBi), Faculty of Science, ANU, on biologically-active cyanobacterial metabolites, in particular the calothrixins, pentacyclic indoloquinone heterocycles from the genus *Calothrix*. These structurally unique natural products possess potent antimalarial activity and cytotoxic activity, which is selective for tumour cells. Under an agreement with the ANU, and with a view to possible human application, an international pharmaceutical company has screened the calothrixins and several derivatives against tumour cell lines *in vitro*, and will now synthesise larger amounts of selected compounds for *in vivo* testing in animals. Research on a possible aggregation pheromone of the unusual velvet worm *Onychophora* continues in conjunction with Drs David Rowell of BaMBi and Judith Reinhard of the RSBS, ANU. This material is

available only at mass spectrometric levels, and presents a major structural challenge. Professor Rickards' research, in collaboration with Dr Stephen Trowell at CSIRO, is directed towards the discovery of new antibiotics for human use from novel natural sources such as termites, sawflies, and other insects and terrestrial invertebrates selected from Australia's unique biodiversity. The four million species of insects that exist on Earth constitute a virtually untapped pharmaceutical resource, in contrast to the plants and microorganisms which have long been the conventional areas for drug discovery, but which are now failing to provide the structural novelty required in new antibiotics. Work to date has established the value of this new approach to antibiotic discovery, and has resulted in two international patent applications.

**Emeritus Professor Alan M Sargeson BSc PhD DipEd Sydney, FRACI, FAA, FRS** (retired in 1996) is collaborating with Dr S V Smith, ANSTO, and with Professor B T Golding, University of Newcastle-upon-Tyne, UK, on the development of detecting therapeutic agents for cancer. In this past year, collaborations have continued with Addenbrook's Hospital of Cambridge University, UK, for detecting breast cancer with the SarAr technology. The project with the Boston Children's Hospital, Harvard Medical School, to label a humanised antibody and target neuroblastoma is also progressing. Recently, Dr Suzanne Smith has also made batches of the cage complex, SarAr, for other research groups in the UK and USA and advertised its advantages at the PacifiChem Meeting in Honolulu.

**Publications arising from work conducted by these Fellows and their groups are listed in the Publications Section.**



## HONOURS AND AWARDS

**Ms Kerry Austin** received the prize for the best poster presentation by a PhD student at the RACI NSW Organic Chemistry Group's 26th Annual One-day Synthesis Symposium held at the University of Wollongong in November.

### **Professor Martin G Banwell**

- was awarded a Merck (UK) 2005 Lectureship;
- was awarded a 2005 Erskine Fellowship at the University of Canterbury, NZ;
- was elected to the Fellowship of the World Innovation Foundation;
- was appointed as Australian Representative to the International Advisory Board of the major new journal *Chemistry – an Asian Journal* to be published from early 2006 by Wiley-VCH in Germany;
- was appointed to the ARC College of Experts;
- was appointed to the Physical Sciences Peer Review Panel of New Zealand's Performance-based Research Fund (PBRF); and
- was appointed to the United Kingdom's EPSRC Peer Review College.

**Emeritus Professor Martin Bennett** was elected to the Bavarian Academy of Sciences as a corresponding member.

**Professor Peter Gill** received the Pople Medal awarded by the Asian Pacific Association of Theoretical and Computational Chemists.

**Dr Gwion Harfoot** was awarded a Fellowship from the von Humboldt Foundation and is now undertaking postdoctoral studies with Professor Bolm in the Department of Chemistry, RWTH-Aachen, Germany.

**Dr Michael John** was awarded a Feodor Lynen Research Scholarship by the Alexander von Humboldt Foundation for a research project in collaboration with the ANU.

**Ms Jasmine C Jury** was the co-recipient of the prize for the best oral presentation by a PhD student within the RACI's Organic Chemistry Division program associated with the CONNECT 2005 Conference, Sydney in July.

**Dr D T J Loong** was awarded a Ramsay Memorial Fellowship and is now undertaking postdoctoral studies with Professor A Barrett in the Department of Chemistry at Imperial College, London.

**Dr David W Lupton** was awarded the Sir Keith Murdoch Fellowship, and was one of seven young Australians who shared over AUD270,000 (USD200,000) in fellowship grants announced by the American Australian Association, the largest national not-for-profit group in the US devoted to American and Australian and New Zealand relations. David is now undertaking postdoctoral studies with Professor B Trost in the Department of Chemistry, Stanford University.

**Ms Natalie Miller** won a IUPAC Poster Prize at the ICOS-15, Nagoya, Japan in August.

**Mr Mark Mulcair** won a student poster prize at the 30th Annual Lorne Conference on Protein Structure and Function (Phillip Island) for his poster entitled *Replication termination: the end of the story?*

**Mr Bob O'Brien** was awarded the 2005 Dean's Prize for General Staff Excellence.

**Professor Gottfried Otting** was elected as a Fellow of the Latvian Academy of Sciences.

**Dr Kiyoshi Ozawa** won a travel award for young scientists at the 1st Asia-Pacific NMR symposium in Japan, 8–11 November. He was invited to present the talk entitled *Cell-free synthesis of selectively isotope-labeled proteins for NMR studies*.

**Ms Emma Pearson** won a prize for best student lecture entitled *A computational and experimental investigation into the intramolecular Diels–Alder reaction* at the Halpern Symposium, University of Wollongong, in November.

**Associate Professor Michael S Sherburn** was awarded the Le Fèvre Prize of the Australian Academy of Science. This prestigious prize is awarded for fundamental research in chemistry, carried out by a researcher who is normally under the age of forty.

### **Professor John W White**

- was awarded the 2005 Craig Medal of the Australian Academy of Science; and
- was awarded the 2006 Leighton Medal of the Royal Australian Chemical Institute. This is the Institute's most prestigious medal and is awarded *in recognition of eminent services to chemistry in Australia in the broadest sense*.

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### Protein Structure and Function

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## Single Crystal X-ray Diffraction Unit (External Collaborations)

Dalton G T, Viau L, Waterman S M, Humphrey M G, Bruce M I, Low P J, Roberts R L, Willis A C, Koutsantonis G A, Skelton B W, White A H Mixed-metal cluster chemistry. 28. Core enlargement of tungsten–iridium clusters with alkynyl, ethynyl, and butadiynyl reagents. *Inorg. Chem.* (2005), 44(9), 3261–3269. <http://dx.doi.org/10.1021/ic050040+>

Graham B, Spiccia L, Skelton B W, White A H, Hockless D C R Imidazole derivatives of binuclear copper (II) and nickel (II) complexes incorporating bis(1,4,7-triazacyclononan-1-yl) ligands. *Inorg. Chim. Acta* (2005), 358(13), 3974–3982. <http://dx.doi.org/10.1016/j.ica.2005.06.053>

Jackson W G, Dickie A J, McKeon J A, Spiccia L, Brudenell S J, Hockless D C R, Willis A C Synthesis, structure, and kinetics and stereochemistry of base-catalysed hydrolysis of *meso*- and *rac*-[Co<sub>2</sub>(tmpdtne)Cl<sub>2</sub>]<sup>4+</sup>, bis(pentaamine) complexes devoid of deprotonatable NH centers. *Inorg. Chem.* (2005), 44(2), 401–409. <http://dx.doi.org/10.1021/ic0400888>

Lucas N T, Humphrey M G, Willis A C [ $\mu_8$ - $\eta^4$ -2,5-Bis (oct-1-ynyl)thiophene]bis[octacarbonylbis ( $\eta^5$ -methylcyclopentadienyl)-tetrahedro-diiridiumdimolybdenum] dichloromethane hemisolvate. *Acta Crystallogr., Sect. E* (2005), 61(3), m463–m464. <http://scripts.iucr.org/cgi-bin/paper?S160053680500214X>

Willis A C, Mahdi W K, Humphrey M G Bis( $\mu_3$ -4-bromophenylimido)tris(tricarbonylruthenium)(2 *Ru*–*Ru*). *Acta Crystallogr., Sect. E* (2005), 61(11), m2335–m2337. <http://dx.doi.org/10.1107/S1600536805032885>

Zhou X, Day A I, Edwards A J, Willis A C, Jackson W G Facile C–H bond activation: synthesis of the  $N_4C$  donor set pentadentate ligand 1,4-bis(2-pyridylmethyl)-1,4-diazacyclononane (dmpdacn) and a structural study of its alkyl-cobalt(III) complex [Co(dmpdacn-C)(OH<sub>2</sub>)](ClO<sub>4</sub>)<sub>2</sub>•H<sub>2</sub>O and its hydroxylated derivative [Co(dmpdacnOH-O)Cl](ClO<sub>4</sub>)<sub>2</sub>•C<sub>3</sub>H<sub>6</sub>O. *Inorg. Chem.* (2005), 44(2), 452–460. <http://dx.doi.org/10.1021/ic040081q>

Zhou X, Hockless D C R, Willis A C, Jackson W G Oxidative condensation reactions of (diethylenetriamine)cobalt(III) complexes with substituted bis(pyridin-2-yl)methane ligands. *J. Mol. Struct.* (2005), 740(1–3), 91–100. <http://dx.doi.org/10.1016/j.molstruc.2004.12.035>

## Bioinorganic and Medicinal Chemistry

Fry F H, Dougan B A, McCann N, Ziegler C J, Brasch N E Characterisation of novel vanadium(III)/acetate clusters formed in aqueous solution. *Inorg. Chem.* (2005), 44(15), 5197–5199. <http://dx.doi.org/10.1021/ic050336f>

## Adjunct Professors

Haworth N L, Sullivan M B, Wilson A K, Martin J M L, Radom L Structures and thermochemistry of calcium-containing molecules. *J. Phys. Chem. A* (2005), 109(40), 9156–9168. <http://dx.doi.org/10.1021/jp052889h>

Izgorodina E I, Coote M L, Radom L Trends in R–X bond dissociation energies (R = Me, Et, *i*-Pr, *t*-Bu; X = H, CH<sub>3</sub>, OCH<sub>3</sub>, OH, F): a surprising shortcoming of density functional theory. *J. Phys. Chem. A* (2005), 109(33), 7558–7566. <http://dx.doi.org/10.1021/jp052021r>

James V, Corino G, Robertson T, Dutton N, Halas D, Boyd A, Bentel J, Papadimitriou J Early diagnosis of breast cancer by hair diffraction. *Int. J. Cancer* (2005), 114(6), 969–972. <http://dx.doi.org/10.1002/ijc.20824>

James V J, Richardson J C, Robertson T A, Papadimitriou J M, Dutton N S, Maley M A L, Berstein L M, Lantseva O E, Martins R N Fibre diffraction of hair can provide a screening test for Alzheimer's disease: a human and animal model study. *Med. Sci. Monit.* (2005), 11(2), CR53–57. [http://www.MedSciMonit.com/pub/vol\\_11/no\\_2/5873.pdf](http://www.MedSciMonit.com/pub/vol_11/no_2/5873.pdf)

Sandala G M, Smith D M, Radom L Divergent mechanisms of suicide inactivation for ethanolamine ammonia-lyase. *J. Am. Chem. Soc.* (2005), 127(24), 8856–8864. <http://dx.doi.org/10.1021/ja051527k>

Wood G P F, Moran D, Jacob R, Radom L Bond dissociation energies and radical stabilisation energies associated with model peptide-backbone radicals. *J. Phys. Chem. A* (2005), 109(28), 6318–6325. <http://dx.doi.org/10.1021/jp051860a>

Wood G P F, Rauk A, Radom L Modeling  $\beta$ -scission reactions of peptide backbone alkoxy radicals: backbone C–C bond fission. *J. Chem. Theory Comput.* (2005), 1(5), 889–899. <http://dx.doi.org/10.1021/ct050133g>

## Visiting Fellows (Post-retirement)

Barfod R, Eriksen J, Golding B T, Hammershøi A, Jacobsen T A, Langkilde A, Larsen S, Mønsted O, Sargeson A M, Sørensen H O Facile cobalt(III) template synthesis of novel branched hexadentate polyamine monocarboxylates. *Dalton Trans.* (2005), (3), 491–500. <http://dx.doi.org/10.1039/b416994h>

Bennett M A, Bhargava S K, Boas J F, Boeré R T, Bond A M, Edwards A J, Guo S-X, Hammerl A, Pilbrow J R, Privér S H, Schwerdtfeger P Electrochemically informed synthesis and characterisation of salts of the  $[\text{Pt}_2(\mu-\kappa\text{As},\kappa\text{C}-\text{C}_6\text{H}_3-5-\text{Me}-2-\text{AsPh}_2)_4]^+$  lantern complex containing a Pt–Pt bond of order  $\frac{1}{2}$ . *Inorg. Chem.* (2005), 44(7), 2472–2482. <http://dx.doi.org/10.1021/ic048660i>

Bennett M A, Byrnes M J, Chung G, Edwards A J, Willis A C Bis(acetylacetonato)ruthenium(II) complexes containing bulky tertiary phosphines. Formation and redox behaviour of  $\text{Ru}(\text{acac})_2(\text{PR}_3)$  (R = 'Pr, Cy) complexes with ethene, carbon monoxide, and bridging dinitrogen. *Inorg. Chim. Acta* (2005), 358(5), 1692–1708. <http://dx.doi.org/10.1016/j.ica.2004.07.062>

Brown D J Cinnolines and Phthalazines: Supplement II. *The Chemistry of Heterocyclic Compounds, Vol. 64*, Taylor E C, Wipf P, eds. John Wiley & Sons: New York (2005), pp. xvii–481.

Rickards R Biosynthesis in insects by E. David Morgan. *Aust. J. Chem.* (2005), 58(2), 152. [http://dx.doi.org/10.1071/CH0409\\_BR](http://dx.doi.org/10.1071/CH0409_BR)

Wijesekera R D, Sargeson A M Reactivities of coordinated phosphodiesteres. *J. Coord. Chem.* (2005), 58(1), 3–19. <http://dx.doi.org/10.1080/00958970512331327393>

## Technical Services

Townsend B J, Poole A, Blake C J, Llewellyn D J Antisense suppression of a (+)- $\delta$ -cadinene synthase gene in cotton prevents the induction of this defense response gene during bacterial blight infection but not its constitutive expression. *Plant Physiol.* (2005), 138(1), 516–528. <http://dx.doi.org/10.1104/pp.104.056010>



## NATIONAL AND INTERNATIONAL LINKS

### Collaborative Research Projects with Universities, CSIRO and Other Institutions

#### BIOLOGICAL CHEMISTRY

##### *Protein Structure and Function – N E Dixon*

Carbohydrate binding by C-type lectins. (With J E Gready, M Hulett, Y-M Hyun [JCSMR, ANU])

Evolution of new protein functions. (With P M Schaeffer, and G Coia [Evogenix Pty Ltd, Melbourne])

*In vitro* protein synthesis. (With G Otting, M J Headlam, K Ozawa, and A V Kralicek [HortResearch, Auckland, NZ], M Pavlov, M Ehrenberg [U Uppsala, Sweden])

Mass spectrometry of protein-protein and protein-DNA complexes. (With M J Headlam, P Prosselkov, P M Schaeffer, S Jergic, K V Loscha, A-Y Park, and J L Beck, S J Watt, T Urathamakul, M M Sheil [U Wollongong])

Mechanisms of termination of DNA replication. (With P M Schaeffer, A J Oakley, M D Mulcair, and D C Neylon [U Southampton, UK], A V Kralicek [HortResearch, Auckland, NZ], T M Hill [U North Dakota, USA], I G Duggin, R G Wake [U Sydney])

Near-perfect rubber. (With C M Elvin [CSIRO Livestock Industries, Brisbane])

Properties and structures of proteins circularised by intein-mediated reactions. (With D L Ollis, G Otting, P Prosselkov, N K Williams, P D Carr, A-Y Park, and J M Matthews [U Sydney], J L Beck, S J Watt, M M Sheil [U Wollongong], E Liepinsh [Karolinska Institute, Stockholm], D Spencer, H-X Zhou [Florida State U, USA], A Rak, K Alexandrov [Max-Planck-Institute for Molecular Physiology, Dortmund, Germany])

Spectroscopic studies of the proofreading exonuclease subunit of DNA polymerase III. (With M J Headlam, A-Y Park, and G Schenk, G R Hanson [U Queensland])

Structural genomics of integron proteins. (With G Otting, P M Schaeffer, P S-C Wu, and B Mabbutt, H Stokes, A Robinson [Macquarie U], Z Dosztányi [Institute of Enzymology, Budapest])

Structure and mechanism of action of proline aminopeptidase. (With P M Schaeffer, P E Lilley, and S C Graham, J M Guss [U Sydney])

Structures and functions of the *Escherichia coli* replicase. (With G Otting, A J Oakley, K Ozawa, P Prosselkov, X-C Su, S Jergic, P S-C Wu, A-Y Park, and K Kongsuwan, G Wijffels [CSIRO Livestock Industries, Brisbane], R Rothnagel, B Hankamer [U Queensland])

Structures of complexes of the proofreading exonuclease subunit of DNA polymerase III. (With G Otting, M John, M A Keniry, A-Y Park, and G Pintacuda [École Normale Supérieure de Lyon, France], T Huber [U Queensland], E Liepinsh [Karolinska Institute, Stockholm])

Structures of domains of DnaB helicase and DnaG primase. (With G Otting, A J Oakley, P M Schaeffer, K V Loscha, and M C J Wilce [U Western Australia], E Liepinsh [Karolinska Institute, Stockholm])

Structures of the *Bacillus subtilis* DnaC helicase and DnaI proteins. (With G Otting, P M Schaeffer, X-C Su, K V Loscha, and R G Wake, J M Guss [U Sydney], P Sultanas [U Nottingham, UK])

Structures of the *Escherichia coli* DnaB helicase protein and the DnaB•DnaC complex. (With P M Schaeffer, K V Loscha, and J-M Carazo, L E Donate, M Bárcena, Y Robledo [Nacional de Biotecnología, Universidad Autónoma, Madrid])



### Nuclear Magnetic Resonance – M A Keniry

Defining the structure of a proteins involved in the onset of breast cancer. (With C C Benz, G Scott [Buck Institute for Age Research, USA]. Supported by a travel grant from the International Union Against Cancer)

The association of calothrixin with DNA. (With E A Owen, R W Rickards, and C Chai [Dept Chemistry, ANU], G D Smith [BaMBi, ANU])

### Structural Biology – A J Oakley

Glutathione transferases from the malaria vector *anopheles dirus*. (With A Ketterman [Mahidol U, Thailand])

Structural studies of nematode proteins as targets for drug design. (With C Behm [BaMBi, ANU])

Structure and evolution of haloalkane dehalogenases. (With J Damborsky [Masaryk U, Czech Republic])

Structures of coenzyme-A biosynthetic enzymes from the malaria parasite: targets for structure-based drug design. (With K Kirk, K Saliba [BaMBi, ANU])

### Protein Crystallography and Engineering – D L Ollis

Structural studies of the  $\beta$  IL5 receptor. (With P D Carr, and I Young [JCSMR, ANU])

Structural studies of the PII and GlnK proteins. (With P D Carr, and S G Vasudevan, Y Xu [James Cook U])

Structure function studies with esterases. (With J Oakeshott [CSIRO Entomology, Canberra])

### Biomolecular NMR – G Otting

Development of a program for automatic  $\chi$ -tensor determination from the  $^{15}\text{N}$ -HSQC spectrum of a lanthanide-labelled protein with known 3D structure. (With M John, N E Dixon, A-Y Park, and T Huber [U Queensland], C Schmitz [Institut National de Recherche en Informatique et en Automatique, France], G Pintacuda [École Normale Supérieure de Lyon, France])

Integron proteins. (With N E Dixon, P M Schaeffer, P S-C Wu, and H W Stokes, B C Mabbutt, M R Gillings, A J Holmes, K M H Nevalainen, A Robinson [Macquarie U], P M G Curmi, S J Harrop [UNSW], Z Dosztányi [Institute of Enzymology, Budapest])

NMR spectroscopy of replication terminator protein of *B. subtilis* with DNA. (With J A Wilce, M C J Wilce [Monash U], G A Wake, A F Hastings, I G Duggin [U Sydney], R H A Folmer [Astra-Zeneca, Sweden])

Oligomerisation of the PYRIN domain of ASC. (With P S-C Wu, and J Sagara, M Moriya, S Taniguchi [Shinshu U, Japan], E Liepinsh [U Latvia])

Sortase applications. (With A Sharipo, E Liepinsh [U Latvia])

Synthesis of  $^{19}\text{F}$ -labelled amino acids. (With M Headlam, D Padmakshan, and D Fairlie, G Le [U Queensland])

3D protein structure determination with paramagnetic restraints. (With M John, X-C Su, S Simonsen, and G Pintacuda [École Normale Supérieure de Lyon, France])

## INORGANIC CHEMISTRY

### Synthetic Organometallic and Coordination Chemistry – A F Hill

Towards nano-circuits: 2- and 3-dimensional carbon-wired nano-architectures. (With M I Bruce [U Adelaide])

### Inorganic Stereochemistry and Asymmetric Synthesis – S B Wild

Tertiary arsine adducts of iodoarsines: a structural and theoretical investigation. (With A D Rae, A C Willis, X-T Zhou, and R Stranger, S Petrie [Dept Chemistry, ANU])

### Solid State Inorganic Chemistry – R L Withers

A coupled electron diffraction and Fermi Surface study of structural disorder and its relationship to the Kondo effect in UAsSe and ThAsSe. (With J Schoenes [Technical U Braunschweig, Germany], R Vincent [U Bristol, UK], A Prodan, H van Midden [Jozef Stefan Institute, Ljubljana, Slovenia])



A phase analysis investigation of the  $(\text{Sr}_{1-x}\text{Ca}_x)\text{TiO}_3$  system. (With C J Howard [ANSTO, NSW], B J Kennedy [Sydney U], M Carpenter [U Cambridge, UK])

Infra-red and diffuse scattering studies of the effects of strain on the crystal chemistry of Fe-bearing sphalerites. (With Y Liu, and A Pring, C Tenailleau [South Australian Museum], M Carpenter [U Cambridge, UK])

The structural characterisation and properties design of Bi-containing dielectric materials. (With Y Liu, and H Wang, X Yao [Xian Jiaotong U, China])

## ORGANIC CHEMISTRY

### *Synthesis and Mechanism – M G Banwell*

Anti-tumour immunity and tumour immunotherapy support studies. (With D A Offermann, and J Altin [BaMBi, ANU and Lipotek Pty Ltd, Adelaide])

Biotransformations. (With D W Lupton, and G M Whited [Genencor International Inc, Palo Alto, California])

Chemoenzymatic routes to novel dendritic architectures suitable for pharmaceutical applications. (With L Fearnside, and G Krippner, T McCarthy [Starpharma Ltd, Melbourne])

Studies in biologically active alkaloid analogue synthesis. (With M O Sydnes, and C Burns [Cytopia Pty Ltd, Melbourne], C Parish [JCSMR, ANU])

The development of chemoenzymatic methods for the selective elaboration of polyfunctionalised therapeutic agents to oligomers with improved efficacy. (With M P Friend, and J Lambert [Biota Chemistry Laboratories, Melbourne])

The development of new, non-steroidal anti-asthma drugs with novel modes of action. (With J Kitching, T Bilski, and A Stewart [Cryptopharma Pty Ltd, Melbourne])

The development of novel carbohydrate-like drugs. (With M Bonnet, A Kreipl, D A Offermann, and R H Don, V Ferro [Progen Industries Ltd, Brisbane])

The total synthesis of biologically active marine alkaloids from the Great Barrier Reef. (With M Backes, D Dauge, and M J Garson [U Queensland])

### *Biochemical Reactions and Molecular Recognition – C J Easton*

Activators and inhibitors of ryanodine receptor calcium ion channels. (With J K Robinson, and A Dulhunty, M Casarotto [JCSMR, ANU], M Miller [Biotron Ltd, Canberra])

Cycloaddition reactions of nitrile oxides. (With G P Savage, G W Simpson [CSIRO Molecular Health and Technologies, Melbourne])

Free radical chemistry and biotechnology. (With D Brittain, A J Herlt, I Li, A J Mortimer, G M Statham, Y-C Tsai, Z I Watts, A Wright, M L Coote, M S Sherburn, and CH Schiesser, JA Angus, RA J O'Hair, U Wille [U Melbourne], L Radom, M J Davies [U Sydney], P J Scammels, WR Jackson [Monash U], S E Bottle [Queensland U Technology], P J Barker [BlueScope Steel], E Rizzardo [CSIRO Molecular Health and Technologies, Melbourne], B Jarrott [Howard Florey Institute, Melbourne], C H Such [Orica Australia Pty Ltd], P Rogers [Carlton and United Breweries])

Lipid chemistry. (With A Ferrante, Adelaide Medical Centre for Women and Children, SA)

Supramolecular chemistry of cyclodextrins. (With L Barr, S K Bowen, M M Cieslinski, R J Coulston, R E Dawson, A J Herlt, S Maniam, and S F Lincoln, M A Buntine, J Gerber, B L May, J Patrick [U Adelaide])

Synthetic enzymes for synthetic chemistries. (With A Buchan, J Khurana, M G Teese, and S Brown, J Oakeshott, R Russell [CSIRO Entomology, Canberra], G W Simpson [CSIRO Molecular Health and Technologies, Melbourne])

Towards improved melamine-urea-formaldehyde resins. (With A Philbrook, and N Dunlop, S Earnshaw, N Walker [Orica Adhesives and Resins, Melbourne])

### Organic Synthesis – L N Mander

Biosynthetic, structural and metabolic studies on gibberellins. (With B Twitchin, and R P Pharis [U Calgary, Canada], M Koshioka, M Nakayama [National Institute of Floricultural Science, Tsukuba, Japan], S Yamaguchi [RIKEN, Wako-Shi, Japan])

Structural and biosynthetic studies on antheridiogens from fern gametophytes. (With J Banks [U Purdue, USA], J Nester [Sam Houston State U, Texas, USA])

Studies on gibberellin receptors. (With M J McDonough, S M McAteer, L C Axford, and P M Chandler [CSIRO Plant Industry, Canberra])

Studies on growth inhibition and flowering. (With B Twitchin, and L T Evans, R W King [CSIRO Plant Industry, Canberra], R P Pharis [U Calgary, Canada])

### Organic Synthesis, Methodology and Host-guest Chemistry – M S Sherburn

Cavitand boronic acids. (With E S Barrett, and P Duggan [CSIRO Molecular and Health Technologies, Melbourne])

Cavitand coordination cages. (With D J Sinclair, and P J Stang, H Jude [U Utah, USA])

New horizons in Diels–Alder chemistry. (With R Tripoli, D Robinson, T N Cayzer, W Lording, and M N Paddon-Row [UNSW])

## PHYSICAL AND THEORETICAL CHEMISTRY

### Theoretical Chemical Physics – M A Collins

Approximate *ab initio* quantum chemistry. (With R Bettens [National U Singapore])

Chemical reaction dynamics. (With D H Zhang [National U Singapore], R Valero, G-J Kroes [U Leiden, The Netherlands])

Construction of the energy surfaces for multiple electronic states. (With M Gordon, H Netzloff [Iowa State U, USA])

Nonadiabatic dynamics and coupled potential energy surfaces. (With D Yarkony [Johns Hopkins U, USA], D H Zhang [National U Singapore])

### Computational Quantum Chemistry, Polymer Chemistry – M L Coote

Combined experimental/theoretical studies of RAFT polymerisation. (With G E Cavigliasso, E I Izgorodina, E H Krenske, V Musgrove, and D J Henry [RMIT U], A Ah Toy, C Barner-Kowollik, H Chaffey-Millar, T P Davis, M H Stenzel, A Theis [UNSW])

Structure-reactivity in ATRP polymerisation. (With B Viswanathan, and K Matyjaszewski [Carnegie Mellon U, Pittsburgh], R Poli [Toulouse U, France])

Degradation resistant PVC. (With A J Schouten, J Purmova, K F D Pauwels, W van Zoelen, J E Vorenkamp [U Groningen, The Netherlands])

Modelling solvation in chemical reactions. (With E I Izgorodina, and M Namazian [Yazd U, Iran])

Computational predictions of  $pK_a$  values and two electron reduction potentials. (With M Namazian, S Siahrostami, H A Almodarresieh, F Kalantary, M R Noorbala [Yazd U, Iran], D J Searles [Griffith U])

Reactions catalysed by vitamin B<sub>12</sub>. (With L Radom, G Sandala, and D Smith [Rudjer Boskovic Institute, Zagreb, Croatia], B T Golding [U Newcastle upon Tyne, UK])

### Liquid State Chemical Physics – D J Evans

Chaos and nonequilibrium statistical mechanics. (With L Rondoni [Politecnico di Torino, Italy])

Fluctuation theorem. (With E M Sevick, E Mittag, G M Wang, and D J Searles [Griffith U])

### Theoretical Quantum Chemistry – P M W Gill

Research into the decay behaviour of least-squares expansion coefficients. (With M Head-Gordon [UC Berkeley, USA], S W Taylor [U Auckland, NZ], G Friesecke [U Warwick, UK])

### Laser and Optical Spectroscopy – E Krausz

Development of the new generation MCD metallo-enzyme spectrometer. (With M Riley [U Queensland], A Stanco [Lastek Pty Ltd, Adelaide])

EPR and optical spectroscopy of thermophilic PSII from *synechococcus vulcanus*. (With R Pace [Dept Chemistry, ANU], J-R Shen [Riken Institute, Hyogo, Japan], S Peterson Årksöld [U Lund, Sweden])

Light induced changes in single crystals of *Rhodospseudomonas viridis*. (With J Norris, R Baxter [U Chicago, USA])

Magneto-optical spectroscopy of cytochrome  $b_6f$ . (With S Peterson Årksöld, J F Allen, J Ström [U Lund, Sweden])

Spectroscopy of mutants of the *Rhodospseudomonas viridis* bacterial reaction centre. (With J Norris, R Baxter, N Ponomarenko [U Chicago, USA])

Spectroscopy of PSII protein sub-assemblies. (With R Pace [Dept Chemistry, ANU], M Seibert [National Renewable Energy Laboratory, Colorado, USA])

### Polymers and Soft Condensed Matter – E M Sevick

A pico-Newton force measurement apparatus for polymer physics and nonequilibrium statistical mechanics. (With D J Evans, and G M Spinks, H R Brown [U Wollongong], T J Senden, D R M Williams [RSPHysSE, ANU])

Collapse dynamics of semi-flexible polymer chains using Brownian simulations with hydrodynamic interactions. (With D R M Williams [RSPHysSE, ANU])

### Disordered Materials – T R Welberry

A structure, conductivity and dielectric properties investigation of  $A_3\text{CoNb}_2\text{O}_9$  ( $A = \text{Ca}^{2+}, \text{Sr}^{2+}, \text{Ba}^{2+}$ ) triple perovskites. (With V Ting, Y Liu, L Norén, R L Withers, D J Goossens, and M James [Bragg Institute, ANSTO], C Ferraris [NTU, Singapore])

Deformed model sets and distorted Penrose tilings. (With B Sing [U Bielefeld, Germany])

Diffuse neutron scattering and structural phase transition in *p*-terphenyl. (With D J Goossens, and M J Gutmann [ISIS, UK])

Problems in measuring diffuse X-ray scattering. (With D J Goossens, A P Heerdegen, and P L Lee [Advanced Photon Source, Argonne, USA])

Single-crystal neutron diffuse scattering and Monte Carlo study of the relaxor ferroelectric  $\text{PbZn}_{(1/3)}\text{Nb}_{(2/3)}\text{O}_{(3)}$  PZN. (With D J Goossens, and M J Gutmann [ISIS, UK], H Woo, G Y Xu [Brookhaven National Laboratory, NY, USA], C Stock [U Toronto, Canada], W Chen, Z G Ye [Simon Fraser U, Canada])

Structural phase transition in *d*-benzil characterised by capacitance measurements and neutron powder diffraction. (With D J Goossens, and X D Wu [Monash U], M Prior [ANSTO])

The structural phase transition in deuterated benzil,  $\text{C}_{14}\text{D}_{10}\text{O}_2$ . (With D J Goossens, and M E Hagen, J A Fernandez-Baca [SNS, Oak Ridge National Laboratory USA])

Structure and magnetism in  $\text{Ho}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$ . (With D J Goossens, and K F Wilson [Dept Physics, ANU], M James [Bragg Institute, ANSTO])

Structure and magnetism in the oxygen-deficient perovskites  $\text{Ce}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$  ( $x \geq 0.90$ ). (With R L Withers, D J Goossens, and M James, K S Wallwork, M Colella [ANSTO], K F Wilson [Dept Physics, ANU], J Horvat, X L Wang [U Wollongong])

Total neutron scattering from single crystals of benzil,  $\text{C}_{14}\text{D}_{10}\text{O}_2$  and  $\text{C}_{14}\text{H}_{10}\text{O}_2$ . (With D J Goossens, and Th Proffen [Los Alamos National Laboratory, USA], M J Gutmann [ISIS, UK], R Neder [Ludwigs Maximilians U, München, Germany])

### Solid State Molecular Science – J W White

Conformation of proteins at interfaces. (With M J Henderson, and S A Holt [Rutherford Appleton Laboratory, Oxford, UK])

Making film stars – nanocomposite films for solar energy capture. *(With M J Henderson, and A Gibaud, J-F Bardeau [Laboratoire de Physique de l'Etat Condensé, Le Mans, France], A R Rennie [Uppsala, Sweden])*

Nanostructure of milk membrane and proteins. *(With S A Holt [Rutherford Appleton Laboratory, UK], B Cox [Dairy Research Corporation, Melbourne])*

Structure of high internal phase emulsions. *(With P A Reynolds, M J Henderson, J Zank, K Baranyai, and R Goodridge, C Such [Orica Ltd, Australia], A Fontaine [FIUPSO, France])*

Structure of polymer composites. *(With D Martin [U Queensland])*

The interface between complex fluids and solids. *(With P A Reynolds, M J Henderson, J Zank, K Baranyai, and S A Holt [Rutherford Appleton Laboratory, Oxford, UK], D Tunaley [Orica Ltd, Australia])*

X-ray small angle scattering from whole blood and haemoglobin. *(With C Garvey [U Sydney])*

### **Molecular Electrochemistry – R D Webster**

Electrochemistry and EPR spectroscopy of organometallic ruthenium complexes. *(With L Y Goh [National U Singapore])*

## **Academic Visitors**

### **The Birch Lecturer**

Tsien, Professor Roger Y, BSc *Harvard*, PhD *Cambridge UK*, Howard Hughes Medical Institute Investigator, Department of Pharmacology, University of California, San Diego

### **The David Craig Lecturer**

Rutherford, Professor A W, BSc *Liverpool*, PhD *University College, London*, Research Director CNRS and Head of Section of Bioenergetics CEA, France

### **Visiting Fellows**

The following were appointed to visiting positions in the School. They worked on collaborative research projects and presented invited lectures and research seminars for staff and students:

Beck, Dr Jennifer, University of Wollongong

Brink, Dr Franciscus, formerly of the Research School of Chemistry

Brown, Dr Susan, CSIRO Entomology (Biotechnology), ACT

Creagh, Professor Dudley, Cultural Heritage Research Centre, University of Canberra

Gibaud, Professor Alain, Université du Maine, France

Gilbert, Dr Elliot, Neutron Scattering Group, ANSTO

Goodwin, Professor Thomas, Hendrix College, Conway, Arkansas, USA

Hanley, Professor Howard, NIST, Colorado, USA

Ho, Dr Felix, Molecular Biomimetics, Uppsala University, Sweden

Hoffman, Dr Christina, Oak Ridge National Laboratory, Tennessee, USA

Ingold, Dr Keith, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa

Kralicek, Dr Andrew, HortResearch, Mt Albert, Auckland, NZ

Larese, Professor John, University of Tennessee, USA

Lechner, Dr Ruep, Hahn-Meitner-Institut, Berlin, Germany

Meurig Thomas, Sir John, The Royal Institute of Great Britain, London and University of Cambridge, UK

Namazian, Dr Mansoor, Yazd University, Iran

Neylon, Dr Cameron, University of Southampton, UK

Padwa, Dr Albert, Emory University, USA. Currently Wilsmore Fellow, School of Chemistry, University of Melbourne

Rennie, Dr Adrian, Uppsala University, Sweden.





Perkins, Dr Michael, School of Chemistry, Physics and Earth Sciences, Flinders University

Peterson Årsköld, Dr Sindra, Center for Chemistry and Chemical Engineering, Lund University, Sweden

Prodan, Dr Albert, Condensed Matter Physics Department, Jozef Stefan Institute, Ljubljana, Slovenia

Soni, Dr Saurabh, Laboratoire de Physique de l'Etat Condensé, Université du Maine, France

Srinivasan, Dr Madhavi, School of Materials Sciences and Engineering, Nanyang Technical University, Singapore

Stachurski, Dr Zbigniew, Department of Engineering, Faculty of Engineering and Information Technology, ANU

Taylor, Dr Andrew, ISIS, Rutherford Laboratory, UK

Thomas, Dr R K, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK

Van Well, Dr Adrianus, Delft University of Technology, The Netherlands

Weisman, Professor Gary, University of New Hampshire, Durham NH, USA

### *Research Seminar Speakers*

The following presented invited lectures or research seminars and held discussions with academic staff and students:

Addicoat, Ms Magdalene, School of Chemistry and Physics, University of Adelaide

Bain, Dr Colin, Dept Chemistry, Chemical Research Laboratory, University of Oxford, UK

Ball, Dr Graham, NMR Facility and School of Chemistry, University of New South Wales

Bernhardt, Dr Paul, University of Queensland

Blair, Professor Ian, University of Pennsylvania, USA

Borden, Professor Weston, University of Washington, USA

Brocks, Dr Jochen, Research School of Earth Sciences, ANU

Buckingham, Professor David, University of Cambridge, UK

Carver, Professor John, School of Chemistry and Physics, University of Adelaide

Chaffey-Millar, Mr Hugh, University of New South Wales

Chen, Dr David, Institute of Chemical and Engineering Sciences, Singapore

Cisneros, Dr Gerardo, SGI (Silicon Graphics)

Clayden, Professor Jonathan, School of Chemistry, University of Manchester, UK

Constable, Professor Ed, Department of Chemistry, University of Basel, Switzerland

Cowden, Dr Cameron, Merck Research Laboratories, UK

Crittenden, Ms Deborah, Department of Chemistry, University of Sydney

Elvin, Dr Chris, CSIRO Livestock Industries, Queensland Bioscience Precinct

Furneaux, Dr Richard, Crown Research Institute, NZ

Gelb, Dr William, Microcal Northampton, MA, USA

Ghiggino, Dr Ken, University of Melbourne

Grimes, Professor Robin, Imperial College of Science, Technology and Medicine, London, UK

Hanson, Professor Graeme, Centre for Magnetic Resonance, University of Queensland

Herges, Professor Rainer, Institut für Organische Chemie, Kiel, Germany

Holmes, Professor Andrew, Bio21 Institute and CSIRO Molecular and Health Technologies, University of Melbourne

Houk, Professor Kendall, University of California, Los Angeles, USA

Hursthouse, Professor Mike, School of Chemistry, University of Southampton, UK

Isobe, Professor Minoru, Nagoya University, School of Bioagricultural Sciences, Nagoya, Japan

Jaindl, Dr Martina, Institute for Theoretical Chemistry, University of Vienna, Austria



Kappe, Professor C Oliver, Institute of Chemistry, Karl-Franzens University, Austria

Karuso, Assoc. Professor Peter, Macquarie University

Kim, Professor Kimoon, Pohang University of Science and Technology, Pohang, Republic of Korea

Kobayashi, Dr Rika, ANUSF/APAC National Facility

Kramer, Professor Ed, University of California, Santa Barbara, USA

Kessler, Professor Horst, Munich Technical University, Garching, Germany

Lorenz, Professor Ingo, Department of Chemistry, LMU, Munich, Germany

Luning, Professor Ulrich, Institut für Organische Chemie, Kiel, Germany

Macgregor, Dr Stuart, Heriot-Watt University, Edinburgh, UK

McKenzie, Dr Ross, University of Queensland

Migaud, Dr Marie, Queen's University, Belfast, UK

Möller, Dr Angela, University of Köln, Germany

Moriya, Assoc. Professor Shigeki, University for the Biotechnology of Infectious Disease (IBID), University of Technology, Sydney

Morokuma, Professor Keiji, Emory University, Atlanta, USA

Mueller, Professor Axel, University of Bayreuth, Germany

Nair, Dr Vijay, University of Trivandrum, India

Nelson, Assoc. Professor Scott, University of Pittsburgh, USA

Nolte, Professor R J M Radboud, University Nijmegen, The Netherlands

Ogilvie, Professor John F Simon, Fraser University, British Columbia, Canada

Penner-Hahn, Dr James, Department of Chemistry and the Biophysics Research Division, University of Michigan, USA

Smith, David, Rudjer Boskovic Institute, Zagreb, Croatia

Wallace (Cowden), Dr Debra, Merck Research Laboratories, UK

Wouterse, Dr Alan, Van't Hoff Laboratory, Utrecht University, The Netherlands

## Conference Presentations

### *Biological Chemistry*

**XXI International Conference on Magnetic Resonance in Biological Systems (XXI ICMRBS)**, Hyderabad, India, 16–21 January. The following invited lecture was presented:

G Otting, G Pintacuda, T Huber, M A Keniry, X-C Su, A-Y Park, N E Dixon, A Moshref, A Leonchiks, A Sharipo and A Kaikkonen: *Paramagnetic labelling of proteins for biomolecular NMR*

**20th Conference of the Australian and New Zealand Society for Mass Spectrometry (ANZMS 20)**, Glenelg, South Australia, 30 January–3 February. The following invited lecture was presented:

S J Watt, P M Schaeffer, N E Dixon, M M Sheil and J L Beck: *Probing interactions of the E. coli helicase (DnaB) and its loading partner (DnaC) by electrospray ionisation mass spectrometry*

**10th Annual Lorne Proteomics Symposium**, Phillip Island, Victoria, 4–6 February. The following posters were presented:

T Urathamakul, A-Y Park, N E Dixon, M M Sheil and J L Beck: *Formation of lanthanide–protein complexes monitored by mass spectrometry*

S J Watt, N K Williams, P Prosselkov, G Otting, N E Dixon, M M Sheil and J L Beck: *Coupling  $^1\text{H}$ – $^2\text{H}$  exchange and electrospray ionisation mass spectrometry to probe protein conformations of linear and cyclised DnaB–N*

**30th Lorne Conference on Protein Structure and Function**, Phillip Island, Victoria, 6–10 February. The following posters were presented:

M D Mulcair, P M Schaeffer, A J Oakley and N E Dixon: *Replication termination: the end of the story? for which M D Mulcair was awarded a student poster prize*

A Robinson, K A Vincent, S J Harrop, Y Boucher, P S Wu, P M Schaeffer, N E Dixon, G Otting, H W Stokes, P M G Curmi and B C Mabbutt: *Structure-led definition of the mobile metagenome for which A Robinson was awarded a student poster prize*

N Williams, E Liepinsh, S J Watt, P Prosselkov, J M Matthews, P Attard, J L Beck, N E Dixon and G Otting: *Stabilisation of native protein fold by intein-mediated covalent cyclisation*

**CRYSTAL 24 Conference (SCANZ)**, Marysville, Victoria, 29 March–1 April. The following invited lecture was presented:

P D Carr, D L Ollis, P Prosselkov, N E Dixon, Y Xu, A Rak, O Pylyprnko and K Alexandrov: *Proteins within proteins – the X-ray structure of the protein splicing intein from the DnaB protein of Synechocystis sp.*

**53rd ASMS Conference on Mass Spectrometry**, San Antonio, Texas, USA, 5–9 June. The following invited lecture was presented:

S J Watt, P M Schaeffer, N E Dixon, M M Sheil and J L Beck: *Using an extended mass range electrospray ionisation mass spectrometer to probe the non-covalent interactions of the E. coli helicase (DnaB) and its loading partner (DnaC)*

**30th FEBS Congress and 9th IUBMB Conference**, Budapest, Hungary, 2–7 July. The following poster was presented:

M D Mulcair, P M Schaeffer, A J Oakley and N E Dixon: *Replication termination in Escherichia coli: the end of the story?*

**Conference on Helicases and NTP Driven Nucleic Acid Machines**, Arolla, Switzerland, 5–10 July. The following invited lecture was presented:

N E Dixon, M D Mulcair, P M Schaeffer and A J Oakley: *How helicase action determines polarity of replication fork arrest by Tus-Ter sites in E. coli*

The following poster was also presented:

P M Schaeffer, N K Williams, P Prosselkov, K V Loscha and N E Dixon: *The interaction of DnaB helicase with DnaG primase is abolished by a single mutation in the dimer interface of the DnaB N-terminal domain*

**ComBio2005**, Adelaide, South Australia, 25–29 September. The following invited lectures were presented:

J L Beck, S J Watt, M M Sheil, S Jergic, P M Schaeffer and N E Dixon: *Stoichiometries and stabilities of very large non-covalent complexes studied by ESI-mass spectrometry*

M D Mulcair, P M Schaeffer, A J Oakley and N E Dixon: *A molecular mousetrap determines polarity of replication fork arrest at Tus-bound Ter sites in E. coli*

D L Ollis: *Evolving enzymes with directed evolution: implications for structure/function studies*

K Ozawa, S Jergic, M J Headlam, G Otting and N E Dixon: *Cell-free synthesis of selectively <sup>15</sup>N-labelled proteins for NMR studies*

The following posters were also presented:

K Ozawa, S Jergic, M J Headlam, G Otting and N E Dixon: *Cell-free synthesis of selectively <sup>15</sup>N-labelled proteins for NMR studies*

A-Y Park, S Hamdan, M J Headlam, P Prosselkov, P D Carr, D L Ollis and N E Dixon: *Deoxyribonucleotides or ribonucleotides: how does Pol III 3'→5' exonuclease discriminate?*

**4th East Coast Bacillus Meeting**, ANU, Canberra, 14 October. The conference was organised by the group, and the following lectures were presented:

N E Dixon: *Overview of DNA replication in E. coli*

K Ozawa: *NMR applications of cell-free protein synthesis*

M D Mulcair: *Polarity determination in replication termination*

A-Y Park: *The exonucleolytic proofreader: structure and assays*

Wood Adhesives 2005, San Diego, USA, 2–4 November. The following invited lecture was presented:

A Philbrook, N Dunlop, C J Easton and M A Keniry: *Demonstration of cross-linking in melamine-urea-formaldehyde and cellulose-urea-formaldehyde reactions using <sup>15</sup>N NMR correlation spectroscopy*

44th Annual Meeting of the NMR Society of Japan and 1st Asia-Pacific NMR Symposium, Yokohama, Japan, 8–11 November. The following invited lecture was presented:

K Ozawa, P S-C Wu, M J Headlam, D Padmakshan, S Jergic, N E Dixon and G Otting: *Cell-free synthesis of selectively isotope-labelled proteins for NMR studies*

Halpern Symposium – 2005. Frontiers of Mass Spectrometry, Drug Design and Synthesis, University of Wollongong, 28–30 November. The following invited lecture was presented:

T Urathamakul, L L Jessop, A-Y Park, N E Dixon, M M Sheil and J L Beck: *Protein-metal interactions in the E. coli replisome using electrospray ionisation mass spectrometry (ESI-MS)*

The following poster was also presented:

S J Watt, T Urathamakul, P M Schaeffer, N E Dixon, M M Sheil and J L Beck: *Probing structural properties of the DnaB helicase by electrospray ionisation mass spectrometry*

Bringing Bioscience Together 2005 – 3rd Annual Postgraduate and Postdoctoral Symposium, ANU, Canberra, 8 December. The following lectures were presented:

C Jackson, J-W Liu, M Coote and D L Ollis: *The effects of substrate orientation on the mechanism of a phosphotriesterase*

M John, A-Y Park, N E Dixon and G Otting: *Transferred pseudo contact shifts: a new tool for studying protein-ligand interactions*

P Lloyd, C Behm and A J Oakley: *Structural analysis of nematode specific proteins*

K Ozawa, G Otting and N E Dixon: *Cell-free protein synthesis for structural biology*

X-C Su, S Jergic, N E Dixon and G Otting: *Solution structure of C-Terminal 14 kDa Domain to the subunit from Escherichia coli DNA Polymerase III*

The following posters were presented:

M D Mulcair, P M Schaeffer, A J Oakley and N E Dixon: *A molecular mousetrap determines polarity of replication fork arrest by Tus-Ter sites in E. coli*

A-Y Park, S Hamdan, M J Headlam, P Prosselkov, P D Carr, D L Ollis and N E Dixon: *Deoxyribonucleotides or ribonucleotides: how does Pol III 3'→5' exonuclease discriminate?*

Pacificchem 2005, Honolulu, Hawaii, USA, 15–20 December. The following invited lectures were presented:

M A Keniry: *Insights into the association of spermine and calothrixin with DNA quadruplexes*

G Otting, K Ozawa, M Headlam, G Pintacuda, X-C Su, M John, N E Dixon, M Keniry, A-Y Park and T Huber: *Protein analysis by <sup>15</sup>N-HSQC spectra using cell-free protein synthesis and lanthanide labelling*

G Otting, G Pintacuda, X-C Su, M John, N E Dixon, M Keniry, A-Y Park and T Huber: *Protein labelling with paramagnetic lanthanides for NMR spectroscopy*

M M Sheil, J L Beck, S J Watt, R Gupta, N E Dixon, A-Y Park and P M Schaeffer: *Application of electrospray ionisation mass spectrometry to study protein-protein and protein-DNA complexes of the E. coli replisome*

### Inorganic Chemistry

7th Reactive Organometallics Symposium (ROMS-7), Australian National University, Canberra, 11 February. The following lectures were presented:

L M Caldwell, A F Hill, A C Willis: *Isoselenocyanates as selenium transfer reagents for the formation of group 6 selenoaryl complexes*



M K Smith, A F Hill: *High-valent group 4, 5 and 14 complexes of the poly(methimazolyl)borates*

I R Crossley, A F Hill, E R Humphrey, A C Willis: *Metallaboratranes: transition metal cage complexes exhibiting dative metal→boron bonding*

**9th Annual National Symposium on Computational Science and Engineering (ANSCSE9)**, Bangkok, Thailand, 3–25 March

A D Rae presented an invited lecture: *The pseudo symmetry of interfaces and their role in defining twin disorder parameters for the refinement of problem crystal structures*

**24th Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ)**, Marysville, Victoria, 29 March–1 April. The following lectures were presented:

Y Liu, R L Withers and L Norén: *The pyrochlore to 'defect fluorite' transition in the  $Y_2(Zr_yTi_{1-y})_2O_7$  system and its underlying crystal chemistry*

L Norén, R L Withers and F J Brink: *Tin ordering in  $LaSn_xSb_2$  ( $0.1 \leq x \leq \sim 0.75$ )*

A D Rae: *The pseudo-symmetry of interfaces and their role in determining twin disorder mechanisms in problem structures*

V Ting, Y Liu, R L Withers and L Norén: *A phase analysis, TEM and powder diffraction study of the  $Ca_2InNbO_6$ – $Ca_3(CaNb_2)O_9$  solid solution*

R L Withers: *Local crystal chemical flexibility and its (modulated) structural consequences*

**South African Chemical Institute Conference on Inorganic Chemistry**, Pietermaritzburg, South Africa, 10–13 April. The following lecture was presented:

N Tshabang, A F Hill, M K Smith, A C Willis: *Soft scorpionates: coordination and heterobimetallic complexes of poly(methimazolyl)borate ligands*

**4th Asian Electroceramics Conference**, Hangzhou, China, 27–30 June. The following lecture was presented:

Y Liu, R L Withers, T R Welberry, H Wang, H L Du and X Yao: *Direct observation of structural disordering of BZN-based pyrochlores*

**Connect 2005 – 12th Royal Australian Chemical Institute (RACI) Convention**, Sydney, 3–7 July. The following lectures were presented:

S B Wild presented the invited lecture: *New approach to the asymmetric syntheses of tertiary arsines and related compounds*

R J Warr, A D Rae, S B Wild, and A C Willis: *Inorganic asymmetric synthesis of two-bladed propeller octahedral metal complexes for which R J Warr was awarded one of two Don Strarks Awards for best student lecture*

The following posters were presented:

N L Kilah and S B Wild: *Deracemisation of chiral phosphine by asymmetric transformation*

H J Kitto, S B Wild, and A C Willis: *Stereospecific syntheses of parallel and double  $\alpha$ -helix conformations of tetra(tertiary phosphine) helicates*

**12th Royal Australian Chemical Institute (RACI) Convention**, Sydney, July 3–7. The following poster was presented:

R D Dewhurst, A F Hill, A C Willis, *Investigating catalytic demercuration of bis(tricarbido)  $[Hg(CCCWL)_2]$  complexes*

**8th Reactive Organometallics Symposium (ROMS-8)**, University of New South Wales, Sydney, 5 August. The following lectures were presented:

R J Abernethy, A F Hill, A C Willis: *Ruthenium-hydride bis(pyrazolyl)borate complexes: hemilability and reactions at the hydride ligand*

R D Dewhurst, A F Hill, M K Smith, A C Willis: *Constructing multimetallic complexes containing tricarbido ( $C_3$ ) ligands and a few diversions*

**20th Congress of the International of Crystallography (IUCr XX)**, Florence, Italy, 22–31 August

R L Withers presented the invited lecture: *Flexible local crystal chemistry and its (modulated) consequences*

V Ting presented an invited lecture: *Structural studies of the  $A_3CoNb_2O_9$  "1:2" ordered perovskites ( $A = Ca^{2+}, Sr^{2+}, Ba^{2+}$ )*



The following posters were presented:

A D Rae and H O Sørensen: *Validation of a twinned pseudo symmetric crystal using a hierarchical pathway*

W Somphon, K J Haller and A D Rae: *An order-disorder phase transition in [Ag(bipy)NO<sub>3</sub>]*

**9th Reactive Organometallics Symposium (ROMS-9)**, Australian National University, 25 November. The following lectures were presented:

L R Caldwell, A F Hill, A C Willis: *Chemistry of heteronuclear di-metal complexes containing  $\mu$ -alkylidyne ligands: reactions of iron molybdenum complexes with alkynyl chalcogenolates*

I R Crossley, A F Hill, A C Willis: *Unlocking the cage: metallaboratranes let loose and explained at last*

M K Smith, A F Hill: *'COT' stabilised high-valent poly(azolyl)borate complexes*

**International Conference on Neutron Scattering (ICNS 2005)**, Sydney, 27 November–2 December. The following posters were presented:

Y Liu, R L Withers, V Ting, J D Fitz Gerald and L Norén: *Stacking faults in typical Ba<sub>3</sub>M<sub>1</sub>Nb<sub>2</sub>O<sub>9</sub> (M = Mn and Co) perovskites and their impact on electrical properties*

V Ting, Y Liu and R L Withers: *Temperature-dependent neutron powder diffraction studies of the A<sub>3</sub>CoNb<sub>2</sub>O<sub>9</sub> (A = Ba<sup>2+</sup>, Sr<sup>2+</sup> and Ca<sup>2+</sup>) perovskite*

**Singapore International Chemical Conference (SICC-4)**, Singapore, 8–10 December

S B Wild gave the keynote lecture: *Inorganic asymmetric synthesis of two-bladed propeller octahedral metal complexes*

**Pacificchem 2005**, Honolulu, Hawaii, 15–20 December. The following invited lectures were presented:

A F Hill, I R Crossley, M K Smith, M R St-J Foreman, N Tshabang, A C Willis: *Metallaboratrane formation: unusual behavior of poly(methimazolyl) borates at the "Multidentate and macrocyclic ligand electronic and steric effects in coordination chemistry: control of reactivity and structure by ligand design" session*

A F Hill, R D Dewhurst, M K Smith, A C Willis: *M≡C multiple bonding in dimetallapolycarbonyls, MC<sub>x</sub>M (x = 3,4,6) at the "Atom transfer, small molecule activation, and metal-ligand multiple bonds" session*

The following posters were presented:

R J Abernethy, A F Hill, A C Willis: *Boron-based reactivity of poly(pyrazolyl)borate complexes: B-functionalisation reactions and 3c – 2e, B–H–M hemilability*

M K Smith, A F Hill: *"Soft", sulfur – donor, high valent transition metal complexes*

L M Caldwell, A F Hill, A D Rae, A C Willis: *Reactions of a  $\mu$ -alkylidyne iron-molybdenum complex with alkynyl chalcogenolates: C–C bond formation and chalcogenolate migration*

I R Crossley, A F Hill, A C Willis: *Late transition metal poly(methimazolyl)borate complexes: the chemistry of cages and chelates*

### Organic Chemistry

**One-day Festschrift in Honour of Professor M N Paddon-Row**, University of New South Wales, Sydney, 25 February

C J Easton presented the invited lecture: *Exploiting free radical chemistry to design PAM enzyme inhibitors for the regulation of hormone production*

M S Sherburn presented the invited plenary lecture: *Diels–Alders with Paddon–Row and others*

**3rd Asian Cyclodextrin Conference**, Tianjin, China, 8–12 May

C J Easton presented the plenary lecture: C J Easton, L Barr, M Cieslinski, R Dawson, P G Dumanski, H Onagi and S F Lincoln: *Applications of cyclodextrins in the construction of molecular devices*

**Sharing the Knowledge AusBiotech Symposium**, Canberra, 24–35 May

C J Easton presented the invited lecture: *Developing pharmaceuticals through chemistry*



**39th ACS National Organic Chemistry Symposium**, University of Utah, USA, 12–16 June. The following posters were presented:

K A Fairweather: *Towards the total synthesis of the marine natural product diisocyanoadociane*

M J Harvey and M G Banwell: *Studies directed towards the assembly of the binary vinca alkaloids: a strategy for the synthesis of (+)-vinblastine*

L C H Kwan and M S Sherburn: *Towards an efficient construction of steroids using a domino IMDA reaction*

N A Miller and M S Sherburn: *Synthesis and reactions of substituted dendralenes*

A T Phillis and M G Banwell: *Novel reactions of dihalocyclopropanes for the assembly of functionalised gibbanes*

P C Stanislawski and M G Banwell: *Studies directed towards the total synthesis of the erythrinan and homoerythrinan alkaloids*

**Connect 2005 – 12th Royal Australian Chemical Institute Convention**, Sydney, 3–7 July. The following invited lectures were presented:

J C Jury: *Developing chemoenzymatic routes to the anti-mitotic macrolide tricholomenyn B for which she was awarded a prize for one of the best student talks*

L C H Kwan: *Towards an efficient construction of steroids using a domino IMDA reaction*

D T J Loong: *Chemoenzymatic syntheses of cladospolides B and C*

The following posters were presented:

Z I Watts and C J Easton: *Regioselectivity of hydrogen atom abstraction from amino acids and peptides*

G P F Wood, C J Easton, M J Davies, A Rauk and L Radom: *Radical reactions implicated in Alzheimer's disease*

**Gordon Conference on Physical Organic Chemistry**, Plymouth, New Hampshire, USA, 26 June–1 July. The following posters were presented:

R Dawson, C J Easton, A J Herlt and S F Lincoln: *Stilbene and cyclodextrins as the basis of molecular shuttles*

Z I Watts and C J Easton: *Regioselective radical chlorination of amino acids and peptides*

**Gordon Conference on Free Radical Reactions**, Plymouth, New Hampshire, USA, 3–8 July

I Li presented the invited lecture and poster: I Li, B Barratt, C J Easton, J S Simpson and L Radom: *Inhibition of peptidylglycine  $\alpha$ -amidating monooxygenase*

The following poster was also presented:

Y-C Tsai, C J Easton and R D Webster: *Oxidatively-cleavable amino acid residues and peptides*

**30th International Symposium on Macrocyclic Chemistry**, Dresden, Germany, 17–21 July. The following poster was presented:

R Dawson, C J Easton, A J Herlt and S F Lincoln: *Stilbene and cyclodextrins as the basis of molecular shuttles*

**8th International Conference on Calixarenes**, Prague, Czech Republic, 25–29 July

M S Sherburn presented the invited lecture: *Superbowl container molecules*

The following poster was presented:

N Kanizaj and M S Sherburn: *On the binding of N-methylpyridinium cation by calix[4]arene receptors*

**4th Chinese National Organic Chemistry Conference**, Kunming, China, 7–11 August.

L Mander presented a plenary lecture: *Enabling strategies for the assembly of complex polycyclic natural products*

**16th Southern Highlands Conference on Heterocyclic Chemistry**, Moss Vale, NSW, 4–6 September.

N A Miller was a postgraduate scholarship awardee and presented the invited lecture: *Synthesis and reactions of substituted dendralenes*

The following posters were presented:

L Carpinelli, LA Sharp and M S Sherburn: *The intramolecular radical carboxylation reaction: scope and application to natural product synthesis*

A D Payne and M S Sherburn: *Practical synthesis and chemistry of [4]dendralene*

E L Pearson and M S Sherburn: *The intramolecular Diels-Alder reactions of benzo-tethered 1,3,9-decatrienes*

Z I Watts and C J Easton: *Regioselectivity of hydrogen atom abstraction from amino acids and peptides*

**Wood Adhesives 2005**, San Diego, USA, 2–4 November

A Philbrook presented the invited lecture: A Philbrook, C J Blake, N Dunlop, C J Easton and M A Keniry: *Demonstration of cross-linking in cellulose-urea-formaldehyde reactions using <sup>15</sup>N NMR correlation spectroscopy*

**Frontiers of Mass Spectrometry, Drug Design and Synthesis Conference**, Wollongong, NSW, 28–30 November. The following lecture was presented:

K A Fairweather: *Towards the total synthesis of the marine natural product diisocyanoadociane*

**Royal Australian Chemical Institute NSW Organic Chemistry Group 26th Annual One-day Symposium**, University of Wollongong, 30 November.

A T Phillis presented the invited lecture: *Exploitation of novel cyclopropane ring-cleavage reactions in the rapid assembly of tetracyclic frameworks related to the gibberellins*

E L Pearson presented the lecture: *The intramolecular Diels-Alder reaction: a combined experimental-computational investigation for which she was awarded a prize for the best student talk*

The following poster was also presented:

K A B Austin, M G Banwell, G J Harfoot and A C Willis: *A chemoenzymatic total synthesis of (–)-complicatic acid for which Ms Austin was awarded the prize for the best poster presentation by a student*

**Pacificchem 2005**, Hawaii, USA, 15–20 December. The following invited lectures were presented:

M G Banwell: *Total synthesis of pyrrole- and indole-containing alkaloids of biological interest*

M G Banwell: *Exploiting the whole-cell biotransformation of arenas as a source of enantiomerically pure building blocks for the chemical synthesis of biologically active natural products*

C J Easton, B Barratt, C J Easton, I Li, J S Simpson, L Radom and Z I Watts: *Exploiting free radical chemistry of amino acids and peptides to regulate hormone production and synthesise peptide secondary metabolites*

M S Sherburn presented the invited lecture at the "Organic Free Radicals in Biology and Synthesis" symposium: *Total synthesis through radical carboxylation*

The following posters were presented:

L Barr, C J Easton and S F Lincoln: *Cyclodextrin molecular reactors in cycloaddition chemistry*

E L Pearson and M S Sherburn: *The intramolecular Diels-Alder reactions of benzo-tethered 1,3,9-decatrienes*

A D Payne, T Bradford and M S Sherburn: *Practical synthesis and chemistry of [4]dendralene*

N A Miller and M S Sherburn: *Synthesis and reactions of substituted dendralenes*

### Physical and Theoretical Chemistry

**Congress of the World Association of Theoretical and Computational Chemists (WATOC)**, Cape Town, South Africa, 16–21 January. The following lecture was presented:

M L Coote: *The origin of retardation and inhibition effects in the RAFT polymerisation process*



**16th Biennial Congress, Australian Institute of Physics, Canberra, Australia, 30 January–4 February.** Two invited talks were presented:

E Krausz, J L Hughes, P J Smith, R J Pace and S Peterson Årsköld: *The most energetic process in biology*

E M Sevick gave the keynote address: *Experimental demonstrations of a new Second Law-like theorem*

The following talks were also presented:

A G Beasley, T R Welberry, A P Heerdegen and A C Willis: *The influence of molecular flexibility and disorder on polymorphism*

D M Carberry: *The optical tweezers capture experiment to demonstrate the fluctuation theorem and the Kawasaki identity*

D J Goossens, T R Welberry and A P Heerdegen: *Modelling dynamic disorder in 3,3'-dimethoxybenzil, C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>*

M J Henderson, A M Hawley and J W White: *Neutron reflectivity of titania and zirconia-based films self-assembled at the solid/liquid interface*

T R Welberry, D J Goossens and A P Heerdegen: *Problems encountered in the measurement of diffuse X-ray scattering*

K F Wilson, D J Goossens and M James: *Magnetic properties of Gd<sub>1-x</sub>Sr<sub>x</sub>CoO<sub>3-δ</sub> (x = 0.67, 0.90 and 0.95)*

A poster was also presented:

J L Hughes, E Krausz, P J Smith and R J Pace: *Investigating a novel spectral hole-burning mechanism in photosystem II*

**7th Annual South Australian Physical Chemistry Symposium, Adelaide, 11 February.** The following keynote lecture was presented:

P M W Gill: *Calculation of molecular vibrational frequencies by quantum chemistry*

**Australian Colloid and Interface Symposium (ACIS), Sydney, 14–17 February.** Professor J W White organised the *Scattering in colloidal systems* section and the following talks were presented:

K J Baranyai, P A Reynolds, M J Henderson, and J W White presented the poster: *Hydrocarbon solvency and reverse micelle formation in micro emulsions*

M J Henderson, A Gibaud, J-F Bardeau, A R Rennie and J W White: *An X-ray reflectivity study of evaporation induced self-assembled titania-based films*

A J Jackson: *Nanoscale structure of milk: milk protein aggregation*

A W Perriman, M J Henderson and J W White: *Unfolding free energy changes of β-lacto globulin at the air-water interface: a neutron and X-ray reflectometry study*

**Satellite Conference to ACIS, Canberra, 21–22 February.** The following talks were presented:

M J Henderson: *Protein-silicate surfaces*

A J Jackson: *Small angle scattering – milk protein concentrates*

A Perriman: *Protein denaturation at interfaces*

P A Reynolds: *High internal phase emulsion structure*

J W White: *General discussion – new horizons*

**229th American Chemical Society Meeting and Exposition, San Diego, 13–17 March**

M A Collins presented the invited lecture: *Approximate ab initio energies by systematic molecular fragmentation*

P M W Gill presented the invited lecture: *John Pople: The later years: CMU, Stockholm and beyond*

**Society of Crystallographers in Australia and New Zealand Conference Crystal 24, Victoria, March.** The following lectures were presented:

D J Goossens, T R Welberry and A P Heerdegen: *Molecular Flexibility in 3,3'-dimethoxybenzil, C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>*

T R Welberry, D J Goossens, and M J Gutmann: *Neutron diffuse scattering and Monte Carlo study of the relaxor ferroelectric PbZn<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub> (PZN)*

**19th Thermodynamics Conference, Sesimbra Portugal, 6–8 April.** The following lecture was presented:

D J Evans, E M Sevick, G M Wang, D M Carberry, J C Reid: *The Fluctuation Theorem*

**2nd Asian Pacific Conference on Theoretical and Computational Chemistry**, Bangkok, 1–8 May. The following invited lecturer were presented:

M A Collins: *Molecular energies and potential energy surfaces*

P M W Gill: *Hartree-Fock-Wigner models for computational chemistry*

**AINSE Annual Meeting**, Sydney, 26 May. The following talk was presented:

A W Perriman: *Orientation of lysozyme at the air/water interface*

**8th International Conference on Non-destructive Investigations and Microanalysis for the Diagnostics and Conservation of the Cultural and Environmental Heritage**, Lecce, Italy, May. The following paper was presented:

G Di Pietro, P J Mahon, D C Creagh, M Newnham: *The identification of photographic dyes in cultural materials using Raman spectroscopy*

**Order, Disorder and Criticality Symposium**, Centre of Science and Engineering of Materials (CSEM), ANU, Canberra, 16 June. The following invited talk was presented:

E M Sevick: *Experimental demonstrations of two new theorems in nonequilibrium thermodynamics*

**Symposium to Commemorate the 80th Birthday of Professor Noel Hush**, University of Sydney, 1–2 July. The following lecture was presented:

M L Coote and E I Izgorodina: *A computational approach to modeling radical polymerisation processes*

**6th Liquid Matter Conference**, Utrecht, The Netherlands, 2 July. The following talk was presented:

E M Sevick, D J Evans, G W Wang, D M Carberry, J C Reid: *New theorems in nonequilibrium thermodynamics, demonstrated using a colloidal bead and an optical trap*

**AINSE Winter School**, Sydney, 2–6 July. The following talks were presented:

J W White: *Suitcase science*

J W White: *Stem cell research*

**Connect 2005, 12th Royal Australian Institute, International Congress**, Sydney, 3–7 July.

M L Coote and D J Henry: *A computational approach to RAFT agent design*

D J Evans presented the plenary lecture: *The Fluctuation Theorem*

E Krausz presented the invited talk: *The engine-room of life revealed*

J W White presented the plenary lecture: *An address to the "enabling sciences" problem in Australia*

J W White presented the plenary lecture: *Small science at big facilities*

Poster presentations:

L Debono, P Smith, R Pace and E Krausz: *Secondary Electron Pathways in Photosystem II*

A Dick, M Riley, E Krausz and G Schenk: *MCD Spectroscopy of a model complex for a bimetallic enzyme*

J Kilmartin, M Riley, S Luthi and E Krausz: *Ni<sup>2+</sup> doped CsCdBr<sub>3</sub> as a Novel Molecular Switch*

**RACI Young Chemists Symposium**, Sydney University, 3 July. The following lecture was presented:

E I Izgorodina and M L Coote: *Ab initio prediction of the propagation rate coefficient in free-radical polymerisation*

**XXth Conference on the Dynamics of Molecular Collisions**, Pacific Grove, 10–15 July

M A Collins presented the invited lecture: *Molecular potential energy surfaces: a feasible strategy*

**VIIIth Workshop on Quantum Reactive Scattering**, Santa Cruz, 15–19 July

M A Collins presented the invited lecture: *Nonadiabatic dynamics on interpolated diabatic potentials*

**Dynamics Days 2005**, Technical University, Berlin, Germany, 25–28 July

D J Evans presented a lecture: *The Fluctuation Theorem*



**International Conference on Luminescence**, Beijing China 25–29 July. The following invited talk was presented:

E Krausz, J L Hughes, P J Smith and R J Pace: *Low energy absorption and luminescence of higher plant photosystem II core complexes*

**Wisenet (Women in Science Network) 28 July meeting**. The following lecture was presented:

Maria Kubik: *Paintings conservation: An interface between art and science*

**Society for Photonic and Illumination Engineering – Optics and Photonics**, San Diego, USA, 31 July–4 August. The following invited talk was presented:

D M Carberry: *Experimental demonstrations of the Fluctuation Theorem in a viscoelastic solvent using a colloidal particle held in an optical trap*

**Dynamical Processes in the Excited States of Solids Conference**, Shanghai China 1–5 August. The following invited talk was presented:

E Krausz, J L Hughes, P J Smith and R J Pace: *The amazing charge separating state of photosystem II*

**News and Expectations and Trends in Statistical Mechanics**, Kolymbari, Crete, August 13–18

D J Evans: *The fluctuation and nonequilibrium free energy theorems – theory and experiment*

**XX Congress of the International Union of Crystallography**, Florence, Italy, 23–31 August

T R Welberry presented the invited lecture: *Diffuse scattering and Monte Carlo studies of relaxor ferroelectrics*

D J Goossens, A P Heerdegen and T R Welberry: *Modelling disorder in 3,3'-dimethoxybenzil, C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>*

**ACS National Meeting**, Washington DC, 28 August–8 September. The following were presented at the Controlled Radical Polymerisation Symposium:

M L Coote and E I Izgorodina presented the invited lecture: *Quantum-chemical tools for understanding and controlling free-radical polymerisation*

A poster was also presented:

M L Coote and J L Hodgson: *Radical ring-opening polymerisation: a new route to polyphosphines*

**DFT 2005**, Geneva, Switzerland, 11–15 September. The following invited lecture was presented:

P M W Gill: *Post-DFT: Beyond the one-particle density*

**3rd International Conference on the Application of Raman Spectroscopy in Art and Archaeology**, Paris, France, September. The following posters were presented:

A S Lee, P Vandenbeeke, P J Mahon, D C Creagh: *Raman analysis of iron gall ink*

A S Lee, P J Mahon, D C Creagh: *Analysis of iron gall ink parchment degradation by vibrational spectroscopy*

**6th Australian Conference on Vibrational Spectroscopy**, Sydney, Australia, 26–30 September. The following posters were presented:

A S Lee, P J Mahon, D C Creagh: *Vibrational spectroscopy in the analysis of the degradation of iron gall inks on parchment*

M E Kubik, A S Lee: *Identifying pigments in paint: The development and application of a Raman spectral database*

**Workshop on High Dimensional Quantum Dynamics**, Leiden, 28 September–1 October

M A Collins presented the invited lecture: *Molecular potential energy surfaces*

**ICCMSE Computational Science Conference**, Loutraki, Greece, 21–26 October. The following invited lecture was presented:

P M W Gill: *Two-electron reductions of many-electron wavefunctions*

**International Workshop on Charge Separation in Photosystem II**, Loosdrecht, The Netherlands, 28–30 October

E Krausz presented the plenary lecture: *Spectroscopic identification of the native reaction centre and photophysical characterisation of the charge-separating state in active PSII*



**International Conference on Neutron Scattering (ICNS),** Sydney, 27 November–2 December. The following talks were presented:

D J Goossens, T R Welberry, A P Heerdegen and M J Gutmann: *Monte Carlo analysis of neutron diffuse scattering data*

M J Henderson, A Rennie and J W White: *Swelling of a zirconian oxide film*

M James, L Morales, K Wallwork, R L Withers and D J Goossens: *Structural distortions in the non-Fermi liquid system  $CeCu_{6-x}Au_x$*

A W Perriman and J W White: *Kinetics of adsorption of lysozyme at the air-water interface and the role of protein charge*

Poster presentations:

A J Jackson and J W White: *Small angle scattering from protein/sugar conjugates*

J Zank, P A Reynolds, A J Jackson, K J Baranyai, A W Perriman, J G Barker, M H Kim and J W White: *Aggregation in high internal phase emulsion observed by SANS and USANS*

**Australian Synchrotron Research Program User's Meeting**, Melbourne, December. The following lectures were presented:

D J Goossens, A G Beasley, A P Heerdegen, T R Welberry and P L Lee: *Diffuse X-ray scattering from Ibuprofen,  $C_{13}H_{18}O_2$*

A G Beasley, T R Welberry, D J Goossens A P Heerdegen: *The influence of disorder on polymorphism*

**Singapore International Chemical Conference IV (SICC-4)**, Singapore, 8–10 December

M L Coote and J L Hodgson presented the invited lecture: *A radical route to polyphosphines*

**BioNano**, Queensland, December

J W White, M J Henderson and A W Perriman presented the plenary lecture: *Protein-inorganic interactions and self-assembly*

**Pacificchem 2005**, Honolulu, USA, 15–20 December

M L Coote and E I Izgorodina presented the invited lecture: *Ab initio Polymerisation: methodology and applications* at the Symposium on Computational Quantum Chemistry, Methodology and Application

P M W Gill presented the invited lecture: *Benchmark correlation energies for small molecules*

## Plenary and Invited Lectures

### Professor M G Banwell

*Bugs for drugs: exploiting whole-cell biotransformations in the total synthesis of natural products and other biologically active compounds*, Institute of Chemical and Engineering Sciences, Singapore, 4 February

*Enabling methodologies for natural product synthesis*, Royal Society of Chemistry Synthetic Organic Chemistry Award Lecture, Burlington House, London, 18 March

*Enabling methodologies for natural product synthesis*, MerLion Pharmaceuticals, Singapore, 24 March

*Chemoenzymatic methods for the assembly of biologically active natural products*, Department of Chemistry, Nanyang University, Singapore, 15 August

*A little bit of strain can be good for you: gem-dihalogenocyclopropanes as building blocks for chemical synthesis*, Department of Chemistry, University of Canterbury, Christchurch, New Zealand, 12 September

Opening plenary lecture: *Enabling methodologies for natural product synthesis at the meeting "Novel Molecules, New Materials and Small Rings"* (a symposium to honour Professor Brian Halton on the occasion of his retirement), The Victoria University of Wellington, New Zealand, 29 and 30 June

He also presented the following named lectures:

2005 Merck (UK) Lectures: *Adventures in natural products synthesis down under*, Universities of Leeds, Liverpool, Manchester, and Nottingham on 6, 7, 8 and 9 June, respectively

2004 Novartis Chemistry Lectures (carried over into 2005):

- (i) *Enabling methodologies for natural product synthesis*, Novartis Institutes for Biomedical Research, Boston, 2 August
- (ii) *Chemoenzymatic methods for the assembly of biologically active natural products*, Novartis Research Facility, East Hanover, New Jersey, 4 August
- (iii) *A little bit of strain can be good for you: gem-dihalocyclopropanes as building blocks for chemical synthesis*, Novartis Institutes for Biomedical Research, Vienna, Austria, 8 August
- (iv) *Chemoenzymatic methods for the assembly of biologically active natural products; and A little bit of strain can be good for you: gem-dihalocyclopropanes as building blocks for chemical synthesis*, Novartis Tsukuba Research Institute, Tsukuba, Japan, 11 August

### Professor M A Collins

*Molecular potential energy surfaces: a feasible strategy*, Dalian Institute of Chemical Physics, Dalian, China, 11 May

### Dr M L Coote

*Free-radical polymer chemistry by computer*, Department of Chemistry, Carnegie-Mellon University, 29 August; Ames Laboratory, Iowa State University, USA, 31 August; Laboratoire de Synthèse Organique, Ecole Polytechnique, Paris, 6 September; Laboratoire de Chimie des Polymères, Université Pierre et Marie Curie, Paris, 7 September

### Professor N E Dixon

*Termination of E. coli DNA replication: the end of one story and the beginning of others*, Institute for the Biotechnology of Infectious Diseases, University of Technology, Sydney, 5 April

*The bacterial replisome (DNA replication factory) as an antibacterial target*, CSIRO Molecular Science, Clayton, Victoria, 11 April

*A molecular mousetrap determines polarity of fork arrest during replication termination in E. coli*, Laboratory of DNA Replication, Rockefeller University, New York, USA,

21 June; and also the Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, USA, 23 June

*Mechanism of replication termination in E. coli: a new protein-nucleic acid interaction*, School of Chemistry, University of Southampton, UK, 28 June

*The DNA replication factory as an antibacterial target*, Novartis Institute for Tropical Diseases, Singapore, 12 July

### Professor C J Easton

*Cyclodextrin-based catalysts, molecular reactors and microelectronic devices*, University of Notre Dame, South Bend, Indiana, USA, 24 June

*Design, synthesis and evaluation of molecular reactors*, CSIRO Molecular Health and Technologies, Melbourne, 5 April

*Manipulating free radical reactions to regulate biochemical processes*, University of Melbourne, 25 November and Monash University, 28 November

### Professor D J Evans

*The Fluctuation Theorem*, Colloquium, University of New South Wales, 26 May

### Professor P M W Gill

Five lectures on *Quantum Chemistry*, Distinguished Visitor Series, Departments of Chemistry and Mathematics, University of Auckland, NZ, 18 March–7 April

*Everything you ever wanted to know about two electrons*, Department of Chemistry, University of California, Berkeley, USA, 22 July; and Faculty of Information and Communication Technologies, Swinburne University of Technology, 26 August

### Professor A F Hill

*Metallaboranes: metal-boron dative bonding and masked metal-bases*, University of Wollongong, 10 August; and the University of New South Wales, 16 August

### Professor E Krausz

*The 'REAL' charge separating state of PSII and the nature of PSII fluorescence*, University of California, USA, 25 January

*Spectroscopy and photosynthesis*, University Bonn, Germany, 27 October

*The elusive charge separating state of PS II*, Max-Planck Institute for Bio-inorganic Chemistry, Mülheim, Germany, 27 October

### Ms M Kubik

*Painted surface project: two nondestructive analysis techniques applied to the identification of pigments*, Australian War Memorial, 10 November

### Dr P Mahon

*Chemistry at the interface: convolution voltammetry and other stories*, University of Adelaide, 4 October

### Professor G Otting

*Paramagnetism in high-resolution NMR*, NMR Discussion Group, University of New South Wales, 7 April

*Paramagnetic NMR spectroscopy: a fast route for structure AIBN*, University of Queensland, 28 July

### Associate Professor E M Sevick

*Experimental demonstrations of two new theorems in nonequilibrium thermodynamics*, Monash University, 2 June; and the University of New South Wales, 26 May

### Associate Professor M S Sherburn

*Domino reactions in total synthesis, superbows in host-guest chemistry and other short stories*, Department of Chemistry, University of Leeds, UK, 1 August

*Using free radicals to fight cancer, why pacman should be chiral, chemistry on steroids and other short stories*, University of Adelaide, 1 September, and the Flinders University of South Australia, 2 September

### Professor J W White

Invited lecture: *New materials from biomimetic processes*, International Science Advisory Committee Korean Atomic Energy Commission, Korea, March

*Chemistry at interfaces*, Craig Medal Lecture, Australian Academy of Science, Canberra, May

*Stem cell ethics*, University House, ANU, September

## Service to External Organisations

**Professor M G Banwell:** Chair, Editorial Advisory Committee, *Australian Journal of Chemistry*; Consultant, Genencor International Inc, Palo Alto; Consultant, Biota Holdings Ltd, Melbourne; Member, Scientific Advisory Board, Cryptopharma Pty Ltd, Melbourne; Member, Editorial Board, *Synlett*; Member, Board of Consulting Editors, *Tetrahedron and Tetrahedron Letters*; Member, International Advisory Board, *Chemistry – An Asian Journal*; Guest Editor, *Tetrahedron Symposium-in-Print on Natural Products Chemistry*; Asia-Pacific Representative, Advisory Committee to the International Society for Heterocyclic Chemistry; Member, Advisory Board, Special Centre for Green Chemistry, Monash University; Member of the College of Experts, Australian Research Council; Member, Scientific Advisory Committee, 21st International Congress for Heterocyclic Chemistry (ICH21) (to be held in Sydney 15–20 July, 2007)

**Dr M L Coote:** Member IUPAC Task Group on RAFT Polymerisation Kinetics; Treasurer, Royal Australian Chemical Institute, ACT Branch; Secretary, Royal Australian Chemical Institute, Physical Chemistry Division

**Professor N E Dixon:** Visiting Lecturer, School of Chemistry, University of Sydney; Assessor, NH&MRC, and MRC (UK) grant applications

**Professor C J Easton:** Chair, Organic Chemistry Division, RACI; Chair, RACI Fellowships Committee (ACT Branch); Member, External Academic Advisory Board (Chemistry), Deakin University; Member, Academic Advisory Board (Chemistry), University of Adelaide; Member, Editorial Board, *ARKIVOC*; Member, Referee Panel, Chemical Communications; Member, Editorial Advisory Board, *Current Organic Synthesis*; Member, Editorial Advisory Board, *Mini Reviews in Organic Chemistry*; Member, Editorial Advisory Board, *Letters in Organic Chemistry*; Board Member, Asian and Oceanian Cyclodextrin League; Chair, Organising Committee, Symposium on Free Radicals in Chemistry and Biology, Pacificchem 2005; Chair, Management Committee, UniChe Program; Chair, Organising Committee, 10th International Symposium on Free Radicals, 2008; Deputy Director, ARC Centre of

Excellence in Free Radical Chemistry and Biotechnology; Member, CSIRO Science Review Panel; Member, Level E Appointment Committee, University of Sydney; Member, Australian Academy of Science, International Programs Committee

**Professor D J Evans:** Member, Skills Audit Steering Committee for the Australian Academy of Science, Minister for Education, Science and Training (2005–present); Member, Organising Committee, Liblice Conferences on Statistical Mechanics of Liquids; Member, Editorial Advisory Board, *Chemical Physics*; Member, Editorial Boards, *Molecular Simulation*, *Molecular Physics*; Assessor/Reader, ARC grant applications

**Professor P M W Gill:** Member, International Panel (SPP 1145), Deutsche Forschungsgemeinschaft; Member, International Advisory Board, *Physical Chemistry Chemical Physics*

**Professor A F Hill:** Member, Referee Panel, Chemical Communications; Editor, *Advances in Organometallic Chemistry* (Academic Press); Member, Editorial Advisory Board, *Organometallics*; Member, International Editorial Advisory Board, *Dalton Transactions*; Member, EPSRC (UK) Peer College Review

**Professor E R Krausz:** Assessor on DOE, NSF and ARC grant applications; Member, Spectroscopy Committee, Academy of Sciences; Member, RACI Physical Chemistry Committee

**Professor L N Mander:** Member of Finance and Audit Committee, Australian Academy of Science; Member, Editorial Advisory Boards, *Current Organic Chemistry*, *Dictionary of Organic Compounds*, *Heterocycles*, *Natural Product Reports*, *Synthesis*, *Synlett*; Member, Board of Consulting Editors, *Tetrahedron*, *Tetrahedron Letters*; Assessor, ARC, PRF and NSF grant applications

**Dr A J Oakley:** Peer reviewer for *Bioinformatics*, *Acta Cryst. D*, and *Biochemistry*; Consultant, BetaBiotics

**Professor D L Ollis:** Assessor, ARC and NH&MRC grant applications; Member, Editorial Board, *Protein Engineering Design and Selection* (PEDS)

**Professor G Otting:** Member, Editorial Board, *Journal of Biomolecular NMR*; Assessor, ARC grant applications, Netherlands Organisation for Scientific Research, and Czech Research Council

**Associate Professor E M Sevick:** Referee, *Physical Review Letters*, *Europhysics Letters*, *Journal of Chemical Physics*, *Macromolecules*

**Associate Professor M S Sherburn:** President, ACT Branch, Royal Australian Chemical Institute; Treasurer, Organic Division, Royal Australian Chemical Institute

**Professor T R Welberry:** Co-editor, *Journal of Applied Crystallography*; Member, Journals Commission of the International Union of Crystallography; Guest Editor, *Special Issue of Zeitschrift für Kristallographie on 'Diffuse Scattering'*; Member, Nominations Committee of SCANZ (Society of Crystallographers in Australia and New Zealand); Member, Single Crystal Instrument Advisory Team, ANSTO; Alternate (for Professor J W White), Australian Synchrotron Research Program Policy and Review Board

**Professor J W White:** Member, Royal Australian Chemical Institute Steering Committee for the forthcoming review: *Future of chemistry: review of the pathway to chemists – from education to employment*; Member, RACI Policy and Nomination Committee; Chair, Advisory Committee on Replacement Research Reactor, Australian Academy of Science; Member, Emerging Science Panel, CSIRO; Program committee member, 9th International Conference on Surface X-ray and Neutron Scattering, Taiwan, July 2006; Member, Prime Minister's Science, Engineering and Innovation Council Working Group on Antarctic Science; Chair, Scholarships Committee, Oxford–Australia Scholarship Fund; President, AINSE; Member, Australian Synchrotron Research Program Policy and Review Board; Member, International Advisory Board, Centre of Excellence for Nanotechnology, University of Queensland; Member, Council, Asian Crystallographic Association; Member, Board of Governors, Consortium for Advanced Radiation Sources, CARS, University of Chicago; Member, International Science Advisory Committee,



Central Laboratory of the Research Councils, UK; Member of Council, AINSE; Member, Neutron Scattering Specialist Committee, AINSE; Member, Advisory Committee, School of Chemistry, University of Sydney; Chair, International Advisory Committee for Japanese Atomic Energy Research Institute/KEK J-PARC Project; Member, International Advisory Committee, Hanaro Reactor Project, Korean Atomic Energy Institute; Member, International Advisory Panel, Faculty of Science, National University of Singapore; Member, Editorial Boards, *Advances in Physics*, *Journal of Materials Chemistry*; Assessor/Reader, ARC grant applications; Member, Institute for the Study of Christianity in an Age of Science and Technology; Founding member, International Society for Science and Religion

**Professor S B Wild:** Consulting Editor, *Tetrahedron Asymmetry*; Guest Professor, PhD Program, University of Leipzig; Member, Royal Australian Chemical Institute Professional Assessment Committee

**Professor R L Withers:** Chair, Aperiodic Commission of the International Union of Crystallography; Member, Editorial Board, *Journal of Solid State Chemistry*; Member of Council, Society of Crystallographers in Australia and New Zealand (SCANZ); Australian Microscopy and Microanalysis Society (AMMS) Representative, Australian National Committee for Crystallography; Co-organiser, Satellite Workshop "Structural Analysis of Aperiodic Crystals" held in August in Florence preceding IUCr XX

## External Lectures and Courses

**Professor M G Banwell:** *Practical methods for organic synthesis*, Honours-level course of eight lectures presented in the Department of Chemistry, University of Canterbury, Christchurch, New Zealand, September and October

**Professor D J Evans:** *Nonequilibrium statistical mechanics – a modern perspective; computer simulation as dynamical system, chaos, Lyapunov exponents and transport coefficients*, Special Lecture Series, Macquarie University, 9–10 May

## Outreach Activities

### Conference Organisation

**Professor R L Withers**, in conjunction with Professor S van Smaalen, University of Bayreuth, Germany, organised and co-chaired a full day pre-conference workshop on the *Structural Analysis of Aperiodic Crystals* as part of the 20th Congress of the International of Crystallography (IUCr XX), Florence, Italy.

**Professor N E Dixon** and group organised the 4th East Coast Bacillus Meeting, ANU, Canberra, 14 October.

**Professor J W White** organised the Mini Satellite Pre-ICNS Conference, Canberra, November.

2005 saw three instalments of the highly successful Reactive Organometallics Symposia (ROMS) Series, two of which were hosted by the RSC. These symposia bring together research groups in organometallic chemistry from the University of Sydney (L D Field), the University of New South Wales (B A Messerle) and the RSC (A F Hill) and provide a forum for postgraduate and early career researchers to present their latest results. The diverse range of topics covered included recent advances in ligand design, ligand transformations and catalysis (nitrogen fixation, hydroamination).



Participants of the 7th Reactive Organometallics Symposium, ANU, 11 February.





### *Australian Academy of Science (AAS)*

Professor J W White participated in the Academy's National Conference on Stem Cell Research, in May, and continues to contribute to the national debate in this area.

### *Australian Institute of Nuclear Science and Engineering (AINSE)*

Professor J W White, President, continued the strategic planning process at AINSE, the benchmarking process of AINSE performance, and the development of a *tenure track* research fellowship scheme – agreed by the AINSE Council in December 2005. He has developed two submissions from AINSE for the National Competitive Research Infrastructure Scheme (NCRIS).

### *CSIRO Student Research Scheme*

Ms Anni Ajmera (St Clare's College) and Mr Kirk Foy (St Francis Xavier College) worked in Professor Wild's group between 11–13 April under the CSIRO Student Research Scheme.

### *International Conference on Neutron Scattering in the Asia Pacific Region*

750 people attended possibly the largest International Conference on Neutron Scattering in the Asia Pacific region in Sydney in November. Professor John White and Professor Trevor Hicks (Monash) were honoured for their long association with the development and use of neutron scattering methods (Professor White for over forty years and Professor Hicks for approximately thirty years).

### *National Science Summer School*

Emeritus Professor R Rickards continued to serve on the Council and Executive Council of the National Science Summer School Inc. This organisation runs the National Youth Science Forum, a two-week program held in Canberra in January for each of two groups of 144 year-12 school students from around Australia who are considering careers in science, engineering and technology. The Council early this year appointed a Director to succeed the Foundation Director, Professor R Jory, who served for 22 years, and recently they also appointed a Communications and Marketing Officer.



Attendees of the International Conference on Neutron Scattering in the Asia Pacific Region.



## NATIONAL AND INTERNATIONAL LINKS

### National Youth Science Forum

In January, Professor A F Hill, Mr H Neumann, and members of inorganic research groups, hosted the National Youth Science Forum. After attending a short introductory



Mr Horst Neumann demonstrates infrared spectroscopy to NYSF students, using samples they have themselves prepared.

lecture given by Professor Hill and Dr I Crossley, four groups, each of sixteen students, prepared various transition metal complexes and characterised them by infrared spectroscopy. As usual, the students appeared to enjoy the opportunity to try hands-on chemistry and gave the RSC *good to excellent* evaluations.



High school students using infrared spectroscopy to investigate coordination complexes they have prepared.

### Royal Australian Chemical Institute (RACI)

Associate Professor M S Sherburn is President of the ACT Branch of the Royal Australian Chemical Institute, that organises the joint RSC-RACI seminar series, which forms the cornerstone of the RACI's professional activities in the ACT. Other important activities include coordinating the ACT Schools Titration Competition, sponsoring student travel awards and visiting local schools to award national chemistry prizes. A number of social events were held, including a Christmas dinner, a chemistry ball and a paint-ball event. All social events were well attended and expertly organised by RSC PhD students Nathan Kilah, Lucy Carpinelli and Amy Philbrook.

### UnlChe (Universities, Industry, Chemistry)

The UnlChe project is an industry-linked chemistry outreach program funded by DEST, Orica Pty Ltd, and the Departments of Chemistry and Chemical Engineering, Universities of Queensland, Melbourne, Newcastle, and the ANU. The project was coordinated nationally by Dr P A Reynolds and chaired by Professor C J Easton. It includes an undergraduate enrichment program for the most able students, aimed at increasing high-potential chemistry graduates' awareness of career possibilities in industry; a school outreach program to raise awareness of the many interesting options in chemistry; and an industry-relevant research PhD and Honours program.

The undergraduate program continued with field trips for elite students from each of the four universities. A group of 37 students participated in the two-week UnlChe Summer School conducted in Canberra and Melbourne between 5–18 February. This group of students, selected for their high potential, learnt about business and business practice in the classroom in Canberra, followed by visits to Orica industrial sites in Melbourne to see what they had learnt being put into practice. A winter field trip to the Newcastle–Hunter Valley region was organised in July for 20 students, giving them an opportunity to discover the *ammonium nitrate trail* from synthesis by Incitec Ltd to the final end-use in open-cut mining *via* the Orica explosives facilities.

A high priority for the UniChe project is to attract more students to the enabling sciences and to increase the retention rate of students in chemistry. In order to achieve this, UniChe coordinators were appointed: Dr M J Ellison, ANU; Dr S Leitch, University of Newcastle; and Dr P Myatt, University of Queensland. Among the activities organised by the UniChe coordinators in 2005 were:

- Peer Assisted Study Sessions (PASS) in chemistry
- Career days – highlighting the wide-ranging career choices available after a Chemistry degree
- a symposium on *Research and Industry Linkage*
- an e-newsletter with information on lectures, job and scholarship opportunities distributed in Brisbane

- development of classes suitable for Years 11 and 12 to entice students to study chemistry at university level
- support of the Titration Competition

A well attended lecture titled *UniChe – a Scheme bringing Australian School and University Students into touch with Chemical Industry* was given by Professor John White at the CONNECT 2005 conference organised by RACI in July in Sydney.

Finally, UniChe organised and financed eleven honours students, ten PhD students and sixteen Summer Scholars, selected on fundamental scientific merit, but who are also of interest to five of Orica's business areas.



Professor John White with students at the UniChe Summer School in February.





## POST-GRADUATE CAREER DEVELOPMENT, EDUCATION AND TRAINING

### The David Craig Lecture Series

The Craig Lecture was entitled *Photosystem II structure-function: the EPR years*. Other lectures in the series were: *Photosystem II reaction centre photochemistry: an evolutionary view*; *The oxygen evolving enzyme*; and *Photosystem II: regulation of electron transfer*. The series was delivered by Professor Bill Rutherford, Research Director CNRS and Head of Section, Bioenergetics CEA, France.

### Graduate Program in Chemistry – Lectures

Professor M G Banwell presented an Honours course of eight lectures: *Methods for the formation of small and medium ring carbocycles*

Dr M L Coote presented an Honours course of eight lectures: *Free-radical polymerisation kinetics and mechanism*

Professor R L Withers presented a lecture in the Series on *Advanced TEM* organised by the ANU Electron Microscope Unit. He also presented a lecture on *Imaging* as part of the Dean of Science's Advanced Studies Course for PhD scholars

### Degrees Awarded and Present Employment of Graduates

#### For the Degree of Doctor of Philosophy

Dr Brendon Jeffrey William Barratt BSc Deakin

*The Development of PAM Enzyme Inhibitors and Cleavable Amino Acids for the Control of Peptide Hormone Levels*

Supervisor: Professor C J Easton

Currently: Postdoctoral Fellow, School of Medicine, University of New South Wales

Dr Elizabeth Sarah Barrett BSc Sydney

*The Synthesis of Functionalised Cavitands and their Applications in Host-guest Chemistry*

Supervisor: Associate Professor M S Sherburn

Currently: Scripps Research Institute, California

Dr Franciscus Joseph Brink BAppSc SAust MAppSc LaTrobe

*Oxygen/Fluorine Ordering, Modulated Structures and Solid Solutions in Metal Oxyfluorides*

Supervisor: Professor R L Withers

Currently: Senior Technical Officer, RSBS, ANU

Dr Satish Chand BSc USP MSc Macquarie

*Synthesis of Phenolic Natural Products of Biological Interest*

Supervisor: Professor M G Banwell

Currently: Research Officer, Institute of Molecular Bioscience, University of Queensland

Dr Alexander Hamish Duncan BSc Macquarie

*Scalable Iterative Potential Energy Surface Construction using Constraints*

Supervisor: Professor M A Collins

Currently: Senior Software Engineer, ADI Limited

Dr Gwion James Harfoot BSc MSc Waikato NZ

*Chemoenzymatic Studies in Sesquiterpene Synthesis*

Supervisor: Professor M G Banwell

Currently: Alexander von Humboldt Research Fellow, Institut für Organische Chemie der RWTH, Aachen, Germany





**Dr Oliver Earl Hutt** BSc Otago NZ Hons ANU

*Studies Directed Toward the Total Synthesis of the Diterpene Alkaloids*

Supervisor: Professor L N Mander

Currently: Postdoctoral Fellow, Kansas University

**Dr Elizabeth Helene Krenske** BSc Queensland

*Phosphine-stabilised Arsenium Salts: Applications to the Asymmetric Synthesis of Tertiary Arsines*

Supervisor: Professor S B Wild

Currently: Postdoctoral Fellow, RSC

**Dr David William Lupton** BSc Adelaide

*Studies Directed Towards the Assembly of the Binary Vinca Alkaloids: A Total Synthesis of (±)-Aspidospermidine*

Supervisor: Professor M G Banwell

Currently: Postdoctoral Fellow, Stanford University

**Dr Samuel Alexander Margerison** BSc Canterbury NZ

*Applications of Laser, Optical and Paramagnetic Spectroscopy*

Supervisor: Professor E R Krausz

Currently: National Registration Authority for Agricultural and Veterinary Chemicals, ACT

**Dr Darragh Paul O'Neill** BA Mod Comp Chem Trinity College, Dublin

*Electron Correlation by Wigner Intracules*

Supervisor: Professor P M Gill

Currently: Postdoctoral Fellow, University of Mainz, Germany

**Dr Lisa Ann Sharp** BSc Sydney

*The Intramolecular Carboxylation Reaction: Scope and Applications to Natural Product Synthesis*

Supervisor: Associate Professor M S Sherburn

Currently: Postdoctoral Fellow, DCSO, École Polytechnique, Cedex, France

**Dr Rebecca Marie Taylor** BSc MSc Waikato NZ

*Exploiting Ring-fused gem-Dibromocyclopropanes in Novel C-C Bond Forming Reactions: Applications to the Synthesis of Natural Product Frameworks*

Supervisor: Professor M G Banwell

Currently: Canberra

**For the Degree of Master of Philosophy**

**Mr Bogdan Victor Banciu** Dipl Cuza Iasi, Romania

*Analysis of Selectively <sup>15</sup>N Labelled PpiB, Proinsulin Connecting Peptide and DnaG-C by NMR*

Supervisor: Professor G Otting

Currently: Secondary school teacher, Romania

## Postdoctoral Fellows, Research Fellows and Fellows – Completions and Destinations

The School provides one of the very best environments for the education and research training of graduate students and postdoctoral fellows. Our interest in their welfare extends well beyond the time spent at the RSC, in part through a comprehensive alumni program. Although the School was founded only thirty-three years ago, many of our alumni now occupy senior positions in academia, government and industry, both in Australia and overseas.

**Dr Elizabeth Barrett** accepted a Postdoctoral Fellowship at the Scripps Research Institute, California, USA

**Dr Simon Bennett** accepted a position with the Office of Chemical Safety, Therapeutic Goods Administration, Canberra

**Dr Helen Berney** returned to Ireland

**Dr Muriel Bonnet** accepted a position at the Institute of Chemical and Engineering Sciences, Singapore

**Dr German Cavigliasso** accepted a position at the University College, London UK

**Dr Giuseppe Del Signore** accepted a Postdoctoral Fellowship at La Sapienza University, Rome

**Dr Andrew T B Gilbert** took up an appointment as Technical Officer in the Research School of Chemistry, ANU

**Dr Steffen Gross** took up an appointment as Head of Laboratory at BASF in Ludwigshafen, Germany

**Dr Gwion Harfoot** accepted an Alexander von Humboldt Research Fellowship in Bonn (Bad Godesberg)/Aachen, Germany

**Dr Andreas Kreipl** accepted a position as Head of Laboratory, Dottikon Exclusive Synthesis AG, Switzerland

**Dr Matthew McDonough** accepted a postdoctoral fellowship at the University of Sydney

**Dr Gloria Moyano** is a tutor and researcher at Massey University, New Zealand

**Dr Pavel Prosselkov** accepted a technical appointment with the Max-Planck-Institut in Germany

**Dr Jens Renner** accepted a position with BASF in Germany

**Dr Matthew Smith** accepted a position as Research Chemist, Alcan Engineering, Queensland Research and Development Centre, Brisbane

**Dr Regis Tripoli** accepted a postdoctoral fellowship at the University of Strathclyde, Glasgow UK

**Dr Craig Turner** accepted a postdoctoral fellowship at the Scripps Research Institute, California, USA

**Dr Neal K Williams** accepted a research fellowship at Monash University

**Dr Adam Wright** accepted a postdoctoral fellowship at the University of Manchester, UK

**Dr Xiang Ting Zhou** accepted a postdoctoral fellowship at the University of Sydney

## PhD Scholars

Australian Postgraduate Award = APA

Australian Postgraduate Award (Industry) = APA(I)

ANU Graduate School Scholarship = GSS

Co-funded ANU Graduate School/RSC = GSS/RSC

ANU PhD Stipend Scholarship = ANU PhD

Endeavour International Postgraduate Research Scholarship = EIPRS

University-Industry Linkages in Chemistry = UniChe

Deutscher Akademischer Austausch Dienst e.V. = DAAD

RSC Tuition Fee Scholarship = RSCT

CSIRO Postgraduate Studentship = CSIRO

CSIRO Tuition Fee Scholarship = CSIRO T

Abernethy, Robyn BSc *Massey NZ* BSc Hons *ANU* – ANU PhD

Austin, Kerrie A J BSc *Auckland NZ* – APA

Baranyai, Krisztian J BSc MSc *Monash* – ANU PhD

Beasley, Andrew G BSc Dip Ed BSciTech *WA* – APA

Beck, Daniel BSc *RMIT*

Bilski, Tomasz BSc Chem *Curtin UT* – APA(I)

Bojase-Moleta, Gomotsang BSc MSc *Botswana* – U Botswana

Bowen, Saara K BSc *New England* – ANU PhD

Brittain, David R B BSc *Adelaide* – APA

Buchan, Alexander MChem *Aberdeen* – ANU PhD/CSIRO

Caldwell, Lorraine M BSc *UQ* – GSS/RSC

Carberry, David M BSc BEng Hons *ANU* – ANU PhD

Carpinelli, Lucinda L BSc *Melbourne* – ANU PhD

Chien, Siu-Hung BSc *USciTech Hong Kong* MPhil *Chinese U Hong Kong* – ANU PhD/RSCT

Chow, Leonie BSc *Melbourne*

Cieslinski, Marta M BSc *Adelaide* – GSS/RSC

Dawson, Ryan E BSc *Adelaide* – ANU PhD

Debono, Lesley BSc *New South Wales* – ANU PhD



- Deev, Vitali BSc *Canterbury* NZ – GSS/RSC  
Dewhurst, Rian D BSc *Canterbury* NZ – ANU PhD  
Dietinger, Christine MSc *Helsinki* – ANU PhD  
Evenhuis, Christian R BSc *Tasmania* – APA  
Fairweather, Kelly A BSc *Auckland* NZ Hons *ANU* – APA  
Fearnside, Luisa BSc *Melbourne* BSc Hons *UQ* – APA(I)  
Foo, Jee L BSc *Nat U Singapore* – ANU PhD/*Orica/UnlChe*  
Friend, Martin P BSc *Murdoch* – APA(I)  
Goodwin, Shelley K BSc *Griffith* – ANU PhD  
Harvey, Michael J MSc *Waikato* NZ – ANU PhD  
Hawley, Adrian M BSc *Melbourne* Hons *ANU* – APA  
Hughes, Joseph L BSc *ANU* – GSS/RSC  
Hutt, Oliver E BSc *Otago* NZ Hons *ANU*  
Jackson, Colin J BSc *Otago* NZ – GSS/RSC  
Jergic, Slobodan AssocSc *La Guardia Coll NY* BSc *Belgrade* – ANU PhD/*EIPRS*  
Jones, Matthew T BSc *La Trobe* – APA  
Jury, Jasmine C BSc *Massey* – ANU PhD  
Kanizaj, Nicholas BSc PGDip *UQ* – ANU PhD  
Khurana, Jeevan L BScAgr *Sydney* – CSIRO  
Kilah, Nathan L BSc *UQ* – APA  
Kitching, Jacki A BMedChem *Wollongong* – GSS  
Kitto, Heather J BSc *Canterbury* NZ – GSS/RSC  
Kokas, Okanya J BBiotech *UQ* – ANU PhD  
Krenske, Elizabeth H BSc *UQ* – APA/VC  
Kubik, Maria E BA *UQ* BAppSc *Canberra* – GSS  
Kwan, Ching H L BSc/BCA *Victoria U Wellington* NZ MSc *LSE UK* – GSS  
Li, Iris H W BSc *Auckland* NZ – ANU PhD  
Lin, Ching-Yeh BS App Chem *National Chiao Tung* Taiwan – ANU PhD/*RSCT*  
Lloyd, Paul BMedSc *ANU* – ANU PhD  
Lording, William J BAppSc *RMIT* – ANU PhD  
Loscha, Karin V BSc Dipl *Göttingen* – ANU PhD/*DAAD*  
Lupton, David W BSc *Adelaide* – GSS/VC  
Maniam, Subashani BSc *Kebangsaan* Malaysia – ANU PhD  
Matveencko, Maria BSc *Victoria U Wellington* NZ – APA  
Miller, Natalie A BSc *Sydney* – ANU PhD  
Mortimer, Adam J BSc *Wollongong*  
Mulcair, Mark D BSc *Monash* – ANU PhD  
O'Neill, Darragh BA Mod Comp Chem *Trinity College* Dublin – ANU PhD/*RSCT*  
Padmakshan, Dharshana BSc MSc BEd *Kannur* – ANU PhD/*RSCT*  
Park, Ah-Young BSc *Victoria U Wellington* NZ Hons *ANU* – ANU PhD  
Pearson, Emma L BSc *WA* – ANU PhD  
Perriman, Adam W BSc *James Cook* – ANU PhD  
Philbrook, Amy A BSc *Maine* – UnlChe  
Phillis, Andrew T BSc MSc *Waikato* NZ – ANU PhD  
Reid, James C BSc LLB *Victoria U Wellington* NZ – GSS  
Sandala, Gregory M BSc *Windsor* – ANU PhD/*EIPRS*  
Smith, Michael H BSc *Melbourne* Hons *Sydney*  
Stanislawski, Pauline C BSc *Monash* – ANU PhD  
Stevenson, Bradley J BSc *Lincoln* NZ – GSS/VC  
Taylor, Rebecca M BSc MSc *Waikato* NZ  
Teese, Mark G BBiotech *UQ* – CSIRO  
Ting, Valeska P BSciTech *Victoria U Wellington* NZ – ANU PhD  
Tsai, Yi-Chin C BSc *Canterbury* NZ – ANU PhD  
Tshabang, Never BSc *Botswana* MSc *Sussex* – U Botswana  
Warr, Rebecca J BSc *Canterbury* NZ – GSS  
Watson, Morgan A BSc Biochem *Canterbury* NZ – GSS/RSC  
Watts, Zachary I BAppSc *RMIT* – ANU PhD  
Wells, Kerrina BSc *ANU* – ANU PhD  
Wu, Peter S BAppSc *QUT* BSc Hons *ANU* – APA/VC

## Visiting Scholars

As part of the recruitment program the School hosts international and Australian scholars for visits of two to six months to undertake research projects with individual staff members. In most instances the projects formed part of course requirements, and the scholars were financially supported by their home institution:

Ackermann, Thibaut MChem <i>ENS de Lyon</i>	C J Easton
Addicoat, Magdalene PhD <i>Adelaide</i>	P M W Gill
Clapet, Laurent DiplomEng <i>ENSICAEN</i>	M S Sherburn
Cross, Hannah PhD <i>Southampton</i>	N E Dixon
Hennessy, James MChem <i>Aberdeen</i>	C J Easton
Locke, Jennifer BSc <i>British Columbia</i>	L N Mander
Thomas, Lynne PhD <i>Cambridge</i>	T R Welberry
Vogt, Florian Masters <i>Tech U Munich</i>	M G Banwell
Wouterse, Alan PhD <i>Utrecht</i>	S R Williams

## Honours Scholars

The following scholars undertook Honours projects within the School:

Bissember, Alexander <i>ANU</i>	M G Banwell
Bradford, Tanya <i>UQ</i>	M S Sherburn
Coulston, Roger <i>ANU</i>	C J Easton
Hodgson, Jennifer <i>ANU</i>	M L Coote
Pinkerton, David <i>ANU</i>	M G Banwell
Statham, Georgina <i>ANU</i>	C J Easton
Weir, Michelle <i>ANU</i>	S B Wild

## Summer Scholar Program

Summer Research Scholarships, of eight to ten weeks duration, were awarded to twenty-six undergraduate students from Australia and New Zealand from November

2005 to February 2006. All were involved in research projects with individual staff members:

Anastasas, Mark <i>WA</i>	G Otting
Bradford, Tanya <i>ANU</i>	M S Sherburn
Burns, Nicolas <i>Otago NZ</i>	M Keniry
Cain, Nicole <i>Flinders</i>	A F Hill
Dao, Chau <i>UQ</i>	G Otting
Fallon, Thomas <i>Flinders</i>	M S Sherburn
Gan, Hui Peng (Pamela) <i>Monash</i>	N E Dixon
Hallam, Donna <i>LaTrobe</i>	A J Oakley
Holden, Kate <i>ANU</i>	M G Banwell
Lee, Yeng Ying <i>Deakin</i>	A F Hill
Ley, Dianna <i>ANU</i>	M Keniry
Luo, Qiong <i>ANU</i>	C J Easton
Mak, Tim <i>Monash</i>	A J Oakley
McConnell, Anna <i>Canterbury NZ</i>	S B Wild
Nielsen, Kresten <i>UQ</i>	E M Sevick
Oh, Ding (Thomas) <i>Monash</i>	N E Dixon
Reekie, Tristan <i>ANU</i>	M G Banwell
Rowley, Jessica <i>UQ</i>	M S Sherburn
Schneider, Caspar <i>Monash</i>	C J Easton
Scott, Daniel <i>Sydney</i>	N E Dixon
Sedgwick, Kathryn <i>Deakin</i>	E R Krausz
Sharp Phillip (Pat) <i>ANU</i>	M G Banwell
Sheridan, Morgan <i>ANU</i>	D L Ollis
Spindler, Xanthe <i>Newcastle</i>	M L Coote
Wanty, Christopher <i>Canterbury NZ</i>	D L Ollis
Wilson, Gregory <i>UQ</i>	R D Webster



# INTERACTIONS ACROSS THE UNIVERSITY

## Undergraduate Lecture Courses Presented in The Faculties

The following RSC staff gave lecture courses to undergraduate and Honours scholars in The Faculties:

### *Department of Chemistry, Faculty of Science*

Chem 3101 Concepts in Medicinal Chemistry – Radicals and Pericyclics in Synthesis and Nature – 10 Lectures (Sherburn)

Chem 2104 Principles of Organic Chemistry – 16 lectures, 5 tutorials (C J Easton)

Chem 3102 Applied Physical Chemistry – 12 lectures (E M Sevick)

C3105 Selected Topics in Physical Chemistry – 10 lectures (M Collins)

Third-year research projects in Organic Chemistry, two students supervised (M L Coote)

PhB add-on module: *Introduction to Quantum Chemistry* (P M W Gill)

The following research students undertook demonstrating and marking in the Department of Chemistry:

Chem A15/A17 2 semesters (D Beck)

Chem A15/A17 2 semesters (N Kilah)

Chem A15/A17 2 semesters (J Hodgson)

Chem A15/A17 2 semesters (D Brittain)

Chem 2012 Physical Chemistry 2nd semester (J Hughes)

Chem 2014 Principles of Organic Chemistry 1st semester (O Kokas)

### *Division of Biochemistry and Molecular Biology, Faculty of Science*

BIOL 2162 Molecular Biotechnology – 3 lectures (P Schaeffer)

The following research student undertook demonstrating and marking:

BIOL1007 Human Biology (P Lloyd)

In addition the following chemistry teaching work was undertaken outside of the Faculties:

ANU College (ANUTECH) Foundation Chemistry lecturing, demonstrating, exam setting/marking (D Beck)

PEMS, University College, ADFA, UNSW Chem 1A/Chem 1B demonstrating and marking (D Beck)

## University Service

**Professor M G Banwell:** IAS Representative, Admissions Committee; Chair, Working Group on Research Development, ANU

**Dr M L Coote:** Examination Panel Member, Chemistry Honours Program

**Professor N E Dixon:** Member, ANU Radiation Safety Committee; Liaison Officer, Institutional rDNA Committee; Member, Medical Sciences Board of Studies

**Professor C J Easton:** Convenor, Graduate Studies in Chemistry; Member, Institute Forum; Member, Divisional Research Committee (SHE); Member, Graduate Studies Committee (SHE)

**Professor D J Evans:** Convenor, College of Science; Member, Academic Board; Chair and IAS representative, Consultative Committee; Chair, Centre for the Science and Engineering of Materials (CSEM); Chair, Supercomputer Time Allocation Committee; Member, Research Advisory Board

**Professor P M W Gill:** Member, Divisional Information Committee (SHE)



**Professor A F Hill:** Member, National Institute of Science Steering Committee; Member, Research Committee; Member, Forum of the Institute of Advanced Studies; Coordinator, National Youth Science Forum

**Dr M A Keniry:** Head, University Nuclear Magnetic Resonance Centre; *ex officio* Member, University Nuclear Magnetic Resonance Centre Management Committee

**Professor E Krausz:** Member, CSEM Board; Member, OHS Radiation Safety Committee

**Professor D L Ollis:** Member, Board of Studies, Biochemistry and Molecular Biology Graduate Program

**Professor G Otting:** Member, Academic Promotions Committee; Member, Research Advisory Board, JCSMR

**Professor A D Rae:** Member, Radiation Safety Subcommittee, ANU Occupational Health and Safety Policy Committee

**Associate Professor E M Sevick:** Member, ANU Major Equipment Committee (MEC); Member, RSC Tenure Review Committee; Member, RSPHYSSE Tenure Review Committee; Member, Teaching and Learning Committee, Dept Chemistry, The Faculties; Member, ANU MSTAG (Microscopic Strategic Advisory Committee)

**Associate Professor M S Sherburn:** Management Representative, ANU Occupational Health and Safety Policy Committee

**Professor T R Welberry:** Member, RSES and RSAA Promotions Committee

**Professor J W White:** Member, University Staff Consultative Committee; Member, Art Acquisitions Committee

**Professor R L Withers:** Member, ANU Science, Health and Engineering Post-graduate Research Scholarships Committee (SHE); Member, ANU Science, Health and Engineering Divisional Education Committee (SHE)

# INTERNAL MANAGEMENT

## Administrative Support Structure

The management of the School is coordinated through the Business Office and the Academic Secretary's Office. The senior administrative staff in 2005 comprised:

- the Laboratory Manager (*L Harland*): who is responsible for non-academic functions in the School, including managerial, financial and budgetary, occupational health and safety, and the supervision and wellbeing of the technical support staff;
- the Business Officer (*L Scarr*): who is responsible for the supervision of the School's administrative and security/cleaning staff, and assists the Laboratory Manager with the business management of the School;
- the Academic Secretary (*M A Holloway*): who is responsible for matters pertaining to academic staff and students, particularly appointments, promotions, current rules, regulations and practices, and is the focus for outreach issues. The Academic Secretary acts as secretary to the Faculty Board and their committees, and provides advice and administrative assistance to the Dean;
- the Facilities Officer (*K Cooper*): who is responsible for the maintenance, operation and safety of the building plant and services;
- the Laboratories and Safety Coordinator (*L L Welling*): who is responsible for the maintenance and operation of laboratory facilities, and oversees the control of hazards in all of the School laboratories;
- the Purchasing Officer (*N Bayley*): who is responsible for the supervision of the purchasing/stores staff and the procurement of goods and services for the School. The Purchasing Officer is responsible for the provision of the imprest store, which services the RSC and other areas of the ANU.

## Technical Support and Research Services

The capacity of the School to undertake leading-edge research is underpinned by highly skilled technical staff, whose expertise complement those of the academic staff. The skills and dedication of staff in these areas were instrumental in bringing the School back into operation following the fire/explosion, which occurred in the Birch Building on 5th August.

Technical staff attached to individual groups support and contribute to the research work of experimental groups in the RSC and this is acknowledged by co-authorship of publications. Their broad technical expertise is enhanced by additional specialist knowledge and skills in areas of direct relevance to the research groups. Technical staff provide continuity within particular groups, however their expertise is also made available to other groups. In addition, the technical staff assist the Laboratory Manager in implementing and monitoring safety policy within the groups.

Staff of the Research Services section provided expert advice on the design, manufacture, maintenance and refurbishment of equipment to the academic and research staff of the School, the ANU and the broader community. The primary focus of this section is the support of RSC research and teaching programs.

### ANU Microanalytical Services Unit

During 2005, the Unit completed a total of 1944 analyses on samples submitted by 179 individuals, most of which (81%) were CHN analyses. This year 41% of requests originated in the RSC. External educational institutions requesting analyses (40% of total requests) included the University College UNSW ADFA, Curtin University of Technology, James Cook University, Kent State University, Newcastle University, University of New South Wales, Sydney University, Sydney Grammar School, Deakin University, University of Western Australia, University of Western Sydney and University of Wollongong.

Significant requests continue to come from Commercial and Governmental sources (14%). Commercial and Governmental clients included the Institute for Drug Technology, Children's Cancer Institute, CSIRO (Centre for Materials and Infrastructure Technology), Prana Biotechnology and Dyesol.

The fire/explosion of 5 August necessitated the closure of the Unit for some weeks whilst it was cleaned and equipment tested. Two pieces of equipment (the DX-120 ion chromatogram and Mettler UMT2 balance) have required some repair. We are very grateful for the contribution of members of RSC staff who have helped in the major endeavour of cleaning every bit of equipment in the lab to the exacting standards that we maintain, and wish to thank the Chemistry Department in particular for the space they have given us for several months to house our balances and sample preparation equipment when we have been unable to use our laboratory due to construction works in the adjacent rooms.

Reet Bergman was again able to contribute her time and expertise to the running of the Unit, returning on a casual basis. Details of instrumental techniques used and submission of samples can be found on the web site.

External earnings for 2005 were \$53,964.45. (*V L Withers, A Melnitchenko*)

<http://rsc.anu.edu.au/facilities/micro.php>

### Computer Unit

The Computer Unit provides support for the diverse range of software and hardware used in the School. The School has 45 Unix workstations (Linux, SGI and Sun). These Unix computers are used for a variety of purposes including data-reduction, desktop use and a small amount of computation. 160 Macintosh computers are used as the desktop systems for most staff and students. In addition, 85 PCs mainly running Microsoft Windows are used for controlling experimental and data collection equipment. Printing services are provided by 20 laser printers and 4 thermal wax colour printers.

The School's main servers run Debian or Red Hat Linux. These servers provide external services including the School's e-mail and web services and internal services such as authentication and file serving, plus the ability to run small- to medium-sized computational tasks. A separate server provides mirroring of all the Unix disks and most of the machines running OSX. Archives and backups of the School's computers are now done to hard disk. The backup server is currently located in the Department of Chemistry and will soon be moved off-site.

The major hardware acquisitions this year have been two raid arrays to support the offsite-backup and local-backup servers. We also purchased some Macintosh Dual G5s, iMac G5s, eMacs, iBook G4s, G4 Laptops as well as a small number of PCs running Microsoft Windows.

In July, Rado Faletic moved to FEAST (Forum for European-Australian Science and Technology). The School's web page at <http://rsc.anu.edu.au> is administered by Chris Blake. (*P R Cohen, C D Delfs, R Faletic, G A Lindsell*)

<http://rsc.anu.edu.au/~rscu/index.html>

### Single Crystal X-ray Diffraction Unit

The unit performs crystal structure analyses on samples provided by various groups within the RSC. X-ray diffraction data sets are collected on a Nonius Kappa-CCD area-detector diffractometer equipped with IFG capillary X-ray-focusing collimators and an Oxford Cryosystems crystal cooling device. Several members of the RSC collect and refine their own structures. Some structures needed to be refined in non-standard ways to allow for twinning, stacking faults and composite space groups, and these were done in collaboration with Professor David Rae.

Source of Crystal	Data Sets Collected	Reports Completed
RSC (performed by unit)	137	97
RSC (performed by others)	57	48
Others (performed by unit)	13	6
TOTAL	207	151

In total, 207 data sets were collected and 151 final reports produced for the year. External work was performed for University College UNSW ADFA, the South Australian Museum and RMIT University. (*A C Willis*)



### Mass Spectrometry Service

From August to November all five main mass spectrometers were refurbished. Both electrospray machines received new data stations, and the VG Autospec and VG Zab were given a full refurbishment plus cleaning inside and new parts fitted.

5875 measurements were made throughout the year on the five different mass spectrometers in the Unit. The majority of samples were run for RSC and 500 for the Chemistry Department, ANU. Total samples run through each mass spectrometer were as follows:

VG Autospec (1909), VG Quattro 2 (1089), Micromass ZMD (1992), HP Agilent GC/MS (358), Bruker FTICR (527).  
*(J M Allen [Head], G G Lockhart, A Jeyasingham)*

<http://rsc.anu.edu.au/facilities/mass.php>

### University NMR Centre

The past year has marked the first full year of operation of the 800 MHz spectrometer, the highest field NMR instrument in Australia. This spectrometer is a joint facility of a consortium of universities from the ACT and NSW. A cryoprobe, capable of measuring very low concentrations of material was recently installed on this instrument. At the other end of the scale, the XL200, the oldest NMR instrument in the Centre and the first NMR spectrometer acquired by the Centre was recently decommissioned. The five remaining instruments at magnetic fields ranging from 7–14 Tesla have continued to operate with consistent reliability enabling a high productivity for the NMR Centre throughout 2005.

During the year the University NMR Centre catered for 120 users from RSC, RSPHYSSE, RSBS, JCSMR, The Faculties, Charles Sturt University, University College UNSW ADFA, University of Sydney, University of NSW and the University of Wollongong. Applications include *in vivo* NMR, nucleotide and protein structure determination,

analysis of natural products and synthetic intermediates, NMR of organometallic compounds and variable temperature NMR. *(M A Keniry, C J Blake, P T Culhane, P M Simmonds)*

<http://bloch.anu.edu.au/>

### Carpentry and Paint Workshops

These workshops are well equipped with carpentry and joinery machinery and spray painting facilities, and provide outstanding custom furniture and fittings for the School's laboratories and offices, in addition to specialised scientific apparatus and specialised surface finishes to engineering materials for all workshop sections. A major project in 2005 was the refurbishment of a laboratory to house a large piece of new scientific equipment (laser tweezers) funded through an ARC LIEF grant. *(I J Clarke, R J O'Brien)*

### Cryogenics Unit

This unit provides cryogens, liquid nitrogen and helium to the School and the wider ANU community (Department of Chemistry, The Faculties, and RSES). *(P Devitt, R J O'Brien)*

### Electrical Unit

This unit provides services in electrical wiring and modifications, new equipment verification and installation, maintenance of electrical research and plant equipment. The School's mandatory electrical appliance safety checks are coordinated by this unit. *(F Vera, R J O'Brien)*

### Electronics Unit

This unit is equipped with design, development, and construction facilities, including specialised services for computer-aided design and printed circuit board (PCB) manufacture. In addition, electronic repair services are provided for the research groups within the School and the instrumentation service units, *i.e.* the Mass Spectrometry Unit, in preference to using external service engineers. *(T Davenport [from 14/4/05], R T Koehne)*

### Glassblowing Unit

Staff in this unit provide expertise and resources for the design, construction and repair of glass apparatus, together with advice on any aspect of construction, materials, and safety. Throughout 2005 the unit continued to provide an impeccable service to research programs within the RSC and the wider ANU community, as well as undertaking work for external clients. (*P Siu, C J Tomkins*)

### Mechanical Workshop

This main workshop is equipped with precision engineering capabilities for instrument development (e.g. precision milling, turning, and welding), mechanical maintenance and repair, and the design and manufacture of prototype apparatus in metal or plastic. In support of all laboratory research programs, extensive maintenance, repair and fabrication services were provided by the workshop. Installation of services (gas, water, vacuum, equipment racks) associated with fume-cupboard and laboratory upgrades continued, together with support of the environmental program to convert instrument cooling systems, reliant on mains water, to recirculating chilled water systems. The workshop also continued to provide support to the wider ANU community, such as the Facilities and Services Division Zone-3 maintenance section.

The mechanical prototype workshop provides mechanical engineering services, prototypes of advanced scientific instrumentation, high vacuum, cryostat, and helium leak-detection services to the School. (*P Devitt, R Filardo, M J Hill, K L Jackman, R J O'Brien*)

### Environment Policy

A summary of management practices that benefit the environment follows:

#### Energy and Resource Conservation

- diaphragm pumps are being used in all laboratories to replace the water aspirators normally attached to rotary evaporators

- large items of equipment that require water cooling are on closed-loop recirculating systems
- double-sided printing and photocopying is encouraged
- single strand toilet tissue is used throughout the School
- the Annual Report is published mainly in electronic form

#### Re-use of Materials

- the workshop reuses off-cuts of metal/glass/wood/plastics
- the original teak laboratory benches are redressed and reused
- precious metals (in particular platinum group metals) are recovered

#### Recycling

- the workshop systematically segregates and recycles, where practicable, metals, glass, oils, and wood
- used printer cartridges are sent for charging
- liquid helium boil-off is recovered, compressed, and returned to the supplier for reliquification
- unused laboratory glassware not required, is donated to ANU School of Art, Glass Department, and local high schools
- offices have "Intershred" boxes for paper recycling

#### Use of Recycled Materials

- where possible, laminated or veneered particle board or MDF (medium density fibreboard) is used in place of exotic woods
- remanufactured laser printer cartridges are used
- 50/50 recycled environmentally friendly laser printing and copy paper is used
- 100% recycled tissues/paper towels are used in laboratories

# SCHOOL COMMITTEES, REPRESENTATIVES AND OFFICE BEARERS

## Faculty Board

Professor D J Evans, Dean (*Chair*) (*ex officio*)  
Professor C J Easton, Deputy Dean *IF rep*, *DEC(SHE)*  
*Research Committee rep* (*ex officio*)  
Professor RA Withers, Associate Dean (Students), *DEC(SHE)*  
*Education Committee rep* (*ex officio*)  
Professor M G Banwell  
Professor M A Collins  
Professor N E Dixon (*MS Board of Studies rep*)  
Professor P M W Gill  
Professor A F Hill (*Academic rep IF*)  
Professor E R Krausz  
Professor L N Mander  
Professor D L Ollis  
Professor G Otting  
Professor A D Rae  
Professor T R Welberry  
Professor J W White  
Professor S B Wild  
Associate Professor E M Sevick  
Associate Professor M S Sherburn  
Dr M L Coote  
Dr M J Henderson (*Faculty of Science rep*)  
Dr M A Keniry  
Dr A J Oakley  
Dr G Salem (*Dept Chemistry rep*)  
Dr D J Sinclair (*Faculty and IF rep*)  
Mr K Cooper  
Ms L Harland  
*Secretary: Ms M A Holloway*

## Academics-in-Charge

Mass Spectrometry: Professor C J Easton  
Microanalytical Unit: Professor C J Easton  
Crystallography Unit: Professor C J Easton  
UNMRC: Dr M A Keniry  
EPR Facilities: Dr R D Webster

## Advisory Committee on Safety

Professor T R Welberry (*Chair*)  
Professor M G Banwell  
Mr K Cooper  
Mr P A Gugger  
Mr H McGlinchey  
Ms L Harland  
Dr J-W Liu  
Dr A J Oakley  
Mr C J Tomkins  
Mr L L Welling  
Professor S B Wild  
Mrs V Withers

## Licensee for Radiochemicals, AQIS and Institutional rDNA Committee Liaison Officer

Professor N E Dixon

## Board of Studies of the Graduate Program in Chemistry

Professor C J Easton (*Chair/Convenor*)  
Professor M G Banwell  
Professor N E Dixon  
Professor A F Hill  
Professor R L Withers  
Professor Mark Humphrey (*Dept Chemistry, Faculty of Science rep*)

## Chemistry Library Advisory Committee (CHEMLAC)

Professor M G Banwell (*Chair*)  
Professor M A Collins  
Dr C Delfs  
Professor N E Dixon  
Professor A F Hill

Ms S Jackson  
 Mr P McNamara  
 Mrs J Smith  
 Dr M Humphrey (*Dept Chemistry, Faculty of Science rep*)  
 Dr R Barrow (*Dept Chemistry, Faculty of Science rep*)

### Dean's Prize and Crawford Prize Selection Committee

Professor T R Welberry (*Convenor*)  
 Professor C J Easton  
 Professor S B Wild

### Distinguished Visitors Selection Committee

Professor M G Banwell (*Chair*)  
 Professor P M W Gill  
 Professor T R Welberry  
 Professor S B Wild

### IT Committee

Professor M G Banwell (*Chair*)  
 Professor T R Welberry  
 Mr C J Blake  
 Ms P Cohen  
 Professor E R Krausz

### Local Area Consultative Committee (LACC)

Mr K Cooper (*Chair*)  
 Dr P Carr  
 Ms P Cohen  
 Dr J Renner (*Postdoctoral Fellows Rep*)  
 Mr P Siu, Mr M J Hill (*Technical Officer reps*)  
 Mr C Evenhuis, Ms H Kitto (*Grad Students reps*)  
 Associate Professor M S Sherburn (*Academic rep*)  
 Dr R Webster (*RO Rep*)

#### Ex-officio Members:

Professor D J Evans, *Dean*  
 Ms L Harland, *Laboratory Manager*  
 Ms M A Holloway, *Academic Secretary*

### National Science Teachers Summer School RSC Coordinators

Associate Professor E M Sevick  
 Professor R W Rickards

### Occupational Safety and Liaison Officers

Mrs R E Enge  
 Dr G A Lindsell  
 Mrs L M Monaghan  
 Mrs E O'Toole  
 Mrs S Riches

### Ombudspersons

Professor C J Easton  
 Ms M A Holloway  
 Associate Professor E M Sevick  
 Professor R L Withers

### Promotions Committee (Local Area)

Professor Chris Easton (*Organic Chemistry*) (*Chair*)  
 Professor Peter Gill (*Theoretical Chemistry*)  
 Professor Gottfried Otting (*Biological Chemistry*)  
 Professor Richard Welberry (*Physical Chemistry*)  
 Professor S Bruce Wild (*Inorganic Chemistry*)

#### External Members:

Dr Geoff Salem, (*Dept Chemistry, The Faculties*)  
 Adjunct Professor V James OAM, (*U Sydney, retired*)  
 Secretary: Ms M A Holloway

### Visitors Grants Committee

Professor T R Welberry (*Chair*)  
 Professor C J Easton  
 Professor N E Dixon  
 Professor S B Wild

### WWW Site Committee

Professor E R Krausz (*Chair*)  
 Mr C J Blake (*Webmaster*)  
 Ms P Cohen  
 Ms M A Holloway



# FINANCE

## Financial Summary

The School continued its success in obtaining funding through the Australian Research Council's competitive grants schemes, thus the financial strategy in 2005 was again to be focused on consolidation and upgrading of resources required to support both new and ongoing research. However, whilst expenditure on small to medium items of research and IT equipment to replace old and obsolete items continued, purchases of new items of larger equipment were deferred due to the fire/explosion which occurred in the Birch Building on 5th August.

In addition to recurrent income, the research contracts with biotechnology company Progen Industries Ltd and ORICA (Australia) Ltd continued throughout the year, as did the UniChe Project, part of the DEST Higher Education Innovation Program. Funding was also received through the Australian Research Council's Discovery and Linkage Schemes, plus from a variety of other external sources, the details of which are given below. In addition the School continued to make patent applications for work carried out by several of the research groups, and work was undertaken for external clients by the Microanalytical Unit, the Mass Spectrometry Unit, and the Glass and Mechanical Workshops. The annual recurrent grant for the School (\$10,707,000) was supplemented by external income of \$5,908,174.

## Outside Grants and Contracts

The recipients and sources of external grants are as follows:

\*\* denotes a new grant in 2005

### *Protein Structure and Function*

Professor N E Dixon and Dr G Schenk \*\*

*An integrated approach towards development of highly specific chemotherapeutics*

Australian Research Council, Discovery Project, January 2005–December 2007

Professor N E Dixon and Dr G Coia

*New methods for directed molecular evolution of novel protein functions*

Australian Research Council and Evogenix Pty Ltd, Linkage Project, March 2004–December 2005

Dr K Ozawa

*Subunit contacts in the replicative DNA polymerase: A new paradigm for protein-protein interactions*

Australian Research Council, Linkage–Postdoctoral Fellowship (CSIRO), October 2003–October 2006

Professor N E Dixon and Professor G Otting

*Enabling technologies for structural genomes*

Australian Research Council, Discovery Project, January 2003–December 2005

### *Protein Crystallography and Engineering*

Dr P D Carr \*\*

*Cytokine receptor complex (cytokine, alpha and beta) structure determination*

ANSTO, Australian Synchrotron Research Program, August 2005

Professor D L Ollis

*Directed evolution used to probe protein structure and function: new enzymes for bio-remediation and industry*

Australian Research Council, Discovery Project, January 2003–December 2005

### *Biomolecular NMR*

Professor G Otting

*New methods for structural biology in solution*

Australian Research Council, Federation Fellowship, January 2002–December 2006

Professor G Otting

*New methods for structural biology in solution*

Australian Research Council, Discovery Project, January 2003–December 2007

Professor G Otting and Professor N E Dixon

*Enabling technologies for structural genomes*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Coordination Chemistry and Spectro-electrochemistry**

Dr G A Heath

*The first development of multi-dimensional spectro-electrochemistry and its application to crucial transformations in inorganic systems*

Australian Research Council, Discovery Project, January 2004–December 2006

### **Disordered Materials**

Dr D J Goossens \*\*

*Diffuse neutron scattering from deuterated p-terphenyl, (C<sub>18</sub>D<sub>14</sub>)*

ANSTO, Access to Major Research Facilities Program, November 2005

Dr D J Goossens \*\*

*Finding the ferromagnetic direction in BaPrO<sub>3</sub> using high magnetic field neutron powder diffraction*

AINSE, Access to Facilities Program, July 2005

Dr D J Goossens \*\*

*Neutron diffuse scattering in p-terphenyl*

AINSE, Access to Facilities Program, June 2005

Professor T R Welberry \*\*

*Diffuse scattering from statically and dynamically disordered crystals*

ANSTO, Australian Synchrotron Research Program, July 2005

Professor T R Welberry

*Development of methods and strategies for the measurement, interpretation and analysis of diffuse X-ray scattering from disordered materials*

Australian Research Council, Discovery Project, January 2003–December 2005

Professor T R Welberry, Professor R L Withers, Professor A Pring and Dr N Ishizama

*The effects of local strain on the crystal structure of solid solutions*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Inorganic Stereochemistry and Asymmetric Synthesis**

Professor S B Wild and Dr M L Coote \*\*

*Quantum chemical design of stereoregular polyphosphine for nanowires*

Australian Research Council, Discovery Project, January 2005–December 2007

Professor S B Wild

*Asymmetric synthesis of chiral phosphines, arsines and stilbines*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Synthesis and Mechanism**

Professor M G Banwell and Mr T Bilski \*\*

*The development of new, non-steroidal anti-asthma drugs with novel modes of action*

Australian Research Council and Cryptopharma Pty Ltd, Linkage Project, December 2005–December 2007

Professor M G Banwell \*\*

*Development of 3NTA-DTDA*

Lipotek Pty Ltd, May–August 2005

Professor M G Banwell \*\*

*Generation of novel fermentation products and their exploitation in the synthesis of biologically-active organic compounds with therapeutic potential*

Australian Research Council, Discovery Project, January 2005–December 2008

Professor M G Banwell and Ms L Fearnside

*Chemoenzymatic routes to novel dendritic architectures suitable for pharmaceutical applications*

Australian Research Council and Starpharma Ltd, Linkage Project, March 2004–December 2006



**Professor M G Banwell and Associate Professor M J Garson**  
*Synthetic, molecular and biological studies on novel marine metabolites isolated from Great Barrier Reef sponges*

Australian Research Council, Discovery Project, January 2004–December 2006

**Professor M G Banwell and Mr M P Friend**

*Development of chemoenzymatic methods for the selective elaboration of polyfunctional therapeutic agents to oligomers with improved efficacy*

Australian Research Council and Biota Holdings Ltd, Linkage Project December 2003–December 2006

**Professor M G Banwell**

*Progen phase III synthesis and identification of novel, heparinoid mimetics and development of the heparanase enzyme as a diagnostic and therapeutic target*

Progen Industries Ltd, October 2002–September 2005

### **Biochemical Reactions and Molecular Recognition**

**Professor C J Easton \*\***

*Development of optimised processes for manufacturing melamine–urea–formaldehyde resins, and improved resins and reconstituted woods products derived from resins*

Australian Research Council and ORICA Australia Pty Ltd, Linkage Project, December 2005–December 2008

**Professor C J Easton and Professor S F Lincoln**

*Supramolecular assemblies as nanoscale devices to control chemical and physical processes*

Australian Research Council, Discovery Project, January 2004–December 2008

**Professor C J Easton**

*Amino acid and peptide radicals in biochemistry and synthesis*

Australian Research Council, Discovery Project, January 2003–December 2005

**Professor C J Easton and Dr M Casarotto**

*Synthetic compounds to specifically activate or inhibit ryanodine receptor calcium ion channels*

Australian Research Council and Biotron Ltd, Linkage Project, January 2003–December 2005

### **Organic Synthesis**

**Professor L N Mander**

*Preparation of photo–affinity molecular probes for the identification of gibberellin receptors*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Organic Synthesis, Methodology and Host–guest Chemistry**

**Associate Professor M S Sherburn \*\***

*Domino approaches to polycyclic natural products*

Australian Research Council, Discovery Project, January 2005–December 2007

**Associate Professor M S Sherburn and Professor M Paddon–Row**

*New horizons in Diels–Alder chemistry*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Synthetic Organometallic and Coordination Chemistry**

**Professor A F Hill and Professor M I Bruce \*\***

*Towards nano–circuits: 2– and 3–dimensional carbon–wired nano–architectures*

Australian Research Council, Discovery Project, January 2005–December 2007

**Professor A F Hill**

*Metallaboratrans: Soft scorpionates and masked metal bases*

Australian Research Council, Discovery Project, January 2003–December 2005

### **Solid State Inorganic Chemistry**

**Professor R L Withers, Dr B Kennedy and Dr C Howard \*\***

*Understanding phase transitions through precise structural studies*

Australian Research Council, Discovery Project, January 2005–December 2007

**Professor R L Withers \*\***

*Temperature-dependent structural studies of the  $A_3\text{CoNb}_2\text{O}_9$  ( $A=\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ) 1:2 b-site substituted complex perovskites*

AINSE, Access to Facilities Program, January–December 2005

**Professor R L Withers \*\***

*Structural Studies of  $\text{Sr}_{3-x}\text{Ba}_x\text{CoNb}_2\text{O}_9$  triple perovskites*

ANSTO, Australian Synchrotron Research Program, January–February 2005

**Professor R L Withers, Professor T R Welberry, Professor A Pring and Dr N Ishizama\*\***

*The effects of local strain on the crystal structure of solid solutions*

Australian Research Council, Discovery Project, January 2003–December 2005

**Theoretical Chemical Physics****Professor M A Collins and Associate Professor M Zhang**

*The energetics and dynamics of chemical reactions of polyatomic molecules involving multiple electronic states*

Australian Research Council, Discovery Project, January 2004–December 2006

**Computational Quantum Chemistry, Polymer Chemistry****Dr M L Coote \*\***

*Computer-aided design of agents for controlling free-radical polymerisation*

Australian Research Council, Discovery Project, January 2005–December 2007

**Dr M L Coote and Professor S B Wild\*\***

*Quantum chemical design of stereoregular polyphosphine for nanowires*

Australian Research Council, Discovery Project, January 2005–December 2007

**Dr M L Coote**

*Hydrogen abstraction in chemical, biochemical and polymerisation processes*

Australian Research Council, Postdoctoral Research Fellowship, June 2002–June 2005

**Liquid State Chemical Physics****Professor D J Evans, Associate Professor E M Sevick, Dr T J Senden and Dr D R M Williams \*\***

*A pico-Newton scale force measurement apparatus for polymer physics and nonequilibrium statistical mechanics*

Australian Research Council, Linkage Infrastructure Equipment Facilities, January 2005–December 2005

**Professor D J Evans and Dr D J Bernhardt**

*Fluid properties and chaotic dynamics in equilibrium and nonequilibrium states*

Australian Research Council, Discovery Project, January 2004–December 2008

**Professor D J Evans and Associate Professor E M Sevick**

*Experimental demonstrations of violations of the Second Law of Thermodynamics*

Australian Research Council, Discovery Project, January 2003–December 2005

**Polymers and Soft Condensed Matter****Associate Professor E M Sevick, Professor D J Evans, Dr T J Senden and Dr D R M Williams \*\***

*A pico-Newton scale force measurement apparatus for polymer physics and nonequilibrium statistical mechanics*

Australian Research Council, Linkage Infrastructure, Equipment and Facilities, January 2005–December 2005

**Associate Professor E M Sevick and Professor J S Williams and Professor B W Ninham**

*Salt, sugar and sequence: The effect of molecular forces on polymer conformation*

Australian Research Council, Discovery Project, January 2004–December 2006

**Associate Professor E M Sevick and Professor D J Evans**

*Experimental demonstrations of violations of the Second Law of Thermodynamics*

Australian Research Council, Discovery Project, January 2003–December 2005



### Molecular Electrochemistry

Dr R D Webster

*In situ electrochemical NMR spectroscopy*

Australian Research Council, Queen Elizabeth II Fellowship,  
June 2001–June 2006

### Solid State Molecular Science

Dr A Jackson \*\*

*Surfactant distribution in aggregates within high internal phase emulsions*

ANSTO, Access to Major Research Facilities Program,  
November 2005

Dr A Jackson \*\*

*Microphase structure in block copolymers*

AINSE, Access to Facilities Program, November–December  
2005

Professor J W White \*\*

*Structure of pristine oil/water interface: surfactant-free emulsions*

ANSTO, Access to Major Research Facilities Program,  
August 2005

Professor J W White \*\*

*Drying of dairy proteins – denaturation of proteins at interfaces at the nanometer scale*

Dairy Ingredients Group of Australia, July 2005–December  
2006

Dr P A Reynolds \*\*

*Interfacial structure of block copolymers at the oil/water interface / Cosurfactant stabilisation of high phase emulsions / Differential effects in mixed diblock copolymer amphiphiles at the air/aqueous interface*

ANSTO, Access to Major Research Facilities Program, May  
2005

Dr J Zank \*\*

*Lamellar structures formed from diblock copolymers / Aggregation of sugar/protein complexes*

ANSTO, Access to Major Research Facilities Program,  
April 2005

Dr A Jackson \*\*

*Polymeric surfactant aggregation in high internal phase emulsions / Polymeric surfactant micelle formation in high internal phase emulsions*

ANSTO, Access to Major Research Facilities Program,  
March 2005

Professor J W White

*Designer surfactants for creation of emulsion properties*

Australian Research Council and ORICA (Australia) Ltd,  
Linkage–Project, 2004–2008

Professor J W White

*High internal phase emulsions – structure and rheology control*

ORICA (Australia) Ltd, April 2004–March 2005

Professor J W White

*Making film-stars: Nano-composite films for solar energy capture*

DEST, Innovation Access Program, March 2004–May 2006

Professor J W White

*Drying of dairy proteins – strategies for preserving functional properties during dehydration*

Food Science Australia, January 2004–December 2006

Professor J W White

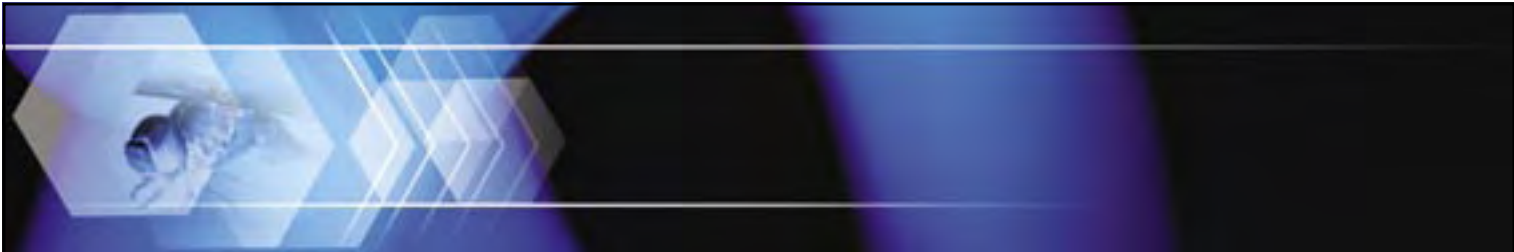
*The UnIChe project*

DEST, Higher Education Innovation Program, January  
2004–December 2005

Mr A Perriman

*Protein behaviour at interfaces*

Australian Institute of Nuclear Science and Engineering  
Student Award, July 2003–February 2006



## EQUAL OPPORTUNITY

An informal program to meet gender equity objectives is continuously in progress in the Research School. Professor Elmars Krausz, formerly a representative with the ANU Equity and Diversity Consultative Group, continues to advise the Dean on such matters as required. Dr Coote was promoted and granted tenure late in 2005, and became the second tenured female on the academic staff.

### Scholar and Academic Staff Recruitment Profiles

In the PhD annual recruitment program the percentage of successful females has steadily risen from 24% in 1994 to 44% in 2005. In the Summer Scholar program the percentage of successful female applicants was 52%.

The following table shows, in a gender specific way, the data for applications and appointments to academic positions over a ten-year period; and the percentage of females in the PhD student population from 1996.

Academic	1996	1997	1998*	1999	2000	2001	2002	2003*	2004	2005
Positions advertised	8	17	17	7	13	10	3	16	5	5
Total applications	167	153	126	77	109	49	73	151	28	34
Appointments w/out advertisement							2	4	15	16
Total of women applicants as a %	37	18	26	22	16.5	26.5	17.8	29.67	33.3	24
Total appointments	6	12	12	6	15	12	8	25	19	21
Total of women appointed as a %	17	17	42	16	46.6	33.3	50	12	31.5	23
Female PhD scholars recruited as a %	28	26.8	30.35	25	21.4	27.2	32.7	36.5	38.5	44

\* = Rita Cornforth Fellow recruitment years (this fellowship is for early-career female researchers only)

# STAFF

## Academic Staff

\* Departed during 2005

### Professors

Banwell, Martin G BSc PhD *Wellington* FWIF, Hon FRSNZ, FRACI, FAA

Collins, Michael A BSc PhD *Sydney*

Dixon, Nicholas E BSc PhD *Queensland*

Easton, Christopher J BSc *Flinders* PhD DSc *Adelaide* FRSC, FRACI, FAA

Evans, Denis J BSc *Sydney* PhD *ANU* FRACI, FAA

Gill, Peter M W MSc *Auckland* PhD *ANU*

Hill, Anthony F MSc (Hons) *Auckland* DrRerNat *Bayreuth* FRSC

Krausz, Elmars R BSc PhD *Sydney* FRACI

Mander, Lewis N (Emeritus) (Adjunct) MSc *Auckland* PhD *Sydney* FRACI, FAA, FRS

Ollis, David L BSc *NSW* PhD *Sydney*

Rae, A David MSc PhD *Auckland* FRACI

Welberry, T Richard MA *Cambridge* PhD *London*

White, John W <sup>CMG</sup> MSc *Sydney* MA DPhil *Oxford* FRSC, FRACI, FAPS, FAA, FRS

Wild, S Bruce BSc *NSW* PhD *Manchester* FRACI, FRSC, FAA

Withers, Raymond L BSc PhD *Melbourne*

### Australian Research Council Federation Fellow

Otting, Gottfried Dipl *Freiburg* PhD *ETH Zürich*

### Associate Professors

Sevick, Edith M BSE *Pittsburgh* PhD *Massachusetts*

Sherburn, Michael S BSc PhD *Nottingham*

### Senior Fellows

Heath, Graham A BSc PhD *Melbourne*

Keniry, Max A BSc PhD *Sydney* (RSC/UNMRC)

### Fellow

Oakley, Aaron J BSc *Tasmania* PhD *St Vincent's IMR Melbourne*

### Rita Cornforth Fellow

Coote, Michelle L BSc PhD *NSW*

### Research Fellows

(\*denotes ARC grant funded)

Berney, Helen BSc *Dublin* PhD *Cork* \* (# 15/7/05)

Goossens, Darren J BAppSci *Ballarat* PhD *Monash*

Henderson, Mark J BSc PhD *WA* \*

Liu, Yun BSc MSc PhD *Xi'an Jiaotong*, China \*

Mahon, Peter J BSc PhD *Deakin*

Moyano, Gloria BSc PhD *Nat U Colombia*

Prosselkov, Pavel MSc PhD *Woronezh*, Russia \*

Robinson, J Kenneth BA PhD *Oxford* \*

Schaeffer, Patrick M DEA *Chem Louis Pasteur*, Strasbourg PhD *Basel* \*

Sinclair, David J BSc PhD *NSW* \* (RSC/Dept Chem)

Smith, Matthew K BSc PhD *James Cook* \*

Williams, Neil K BSc PhD *Sydney* \*

Zank, Johann DiplChem DrRerNat *Tech Munich* \*

### Postdoctoral Fellows

Axford, Lorraine MChem *Wales* PhD *Bristol* \*

Backes, Michael DiplChem DrRerNat *RWTH Aachen* \*

Barr, Lorna BSc *Strathclyde* PhD *ANU* \*

Barrett, Elizabeth S BSc *Sydney* PhD *ANU* (# 8/4/05)

Bennett, Simon A BSc PhD *ANU* \* (# 29/4/05)

Cavigliasso, German BSc *Córdoba*, Argentina MSc *British Columbia* PhD *Cambridge* UK \* (# 22/9/05)

Crittenden, Deborah BSc PhD *Sydney*

Crossley, Ian R MChem PhD *UMIST*\*

Dauge, Delphine M DEA *Orsay* PhD *École Polytechnique*, Palaiseau \*

Del Signore, Giuseppe Laurea *La Sapienza Rome* DrRerNat *RWTH Aachen* \* (# 24/3/05)

Foot, Jonathan S MSc *Edinburgh* PhD *York* \*

Gilbert, Andrew T B BSc *Massey* PhD *Cambridge* (# 28/11/05)

Godsi, Oded BA MA *Tel-Aviv* PhD *Technion Israel* \*

Harfoot, Gwion J MSc *Waikato* PhD *ANU* \* (# 26/4/05)

Headlam, Madeleine J BSc PhD *WA* \*

Izgorodina, Ekaterina I BSc MSc *Ivanova State U Chem/Tech*, Russia DrRerNat *Münster*

Jackson, Andrew J MChem DPhil *Oxford* \*

John, Michael DiplChem *Philipps Marburg* DrRerNat *Tech Munich* \* (# 5/8/05)

Kim, Hye-Kyung BSc MSc *Yeungnam Korea* PhD *Chalmers* \*

Knoke, Mario Diplom PhD *Göttingen* \*

Krenske, Elizabeth H BSc *Queensland* PhD *ANU* \*

McAteer, Stephen M MChem *Southampton* PhD *Leeds* \*

McDonough, Matthew J BSc PhD *WA* \*

Martin, Stephen A BSc PhD *RMIT*\*

Mulcair, Mark D BSc *Monash* PhD *ANU* \*

Offermann, Daniel A BSc PhD *Monash* \*

Onagi, Hideki BAppSc *Western Sydney* BScHons PhD *ANU* \*

Payne, Alan D BSc PhD *WA* \*

Philbrook, Amy BS *Maine* PhD *ANU* \*

Ranganathan, Prabhakar MS *Indian IT*, Madras PhD *Monash* \*

Robinson, Diane E J E MChem *Oxford* PhD *Bath* \*

Scott, Andrew J BSc *Sydney* PhD *ANU* \*

Simonsen, Shane M BSc PhD *Queensland* \*

Steffen, Ronald Dipl PhD *Tech U Berlin* \*

Steinbach, Joerg Dipl DrRerNat *Kaiserslautern* \*

Su, Xun-Cheng MSc PhD *Nankai China* \*

Tripoli, Regis J-P DEA Chem *Bordeaux* PhD *Strathclyde* \* (# 14/1/05)

Turner, Craig BSc *Massey* PhD *Sydney* (# 9/4/05)

Viswanathan, Bala BSc MSc *McGill* PhD *Dalhousie* \*

Williams, Stephen R B AppSci PhD *RMIT*\*

Wright, Adam BMedChem *Wollongong* PhD *Sydney* \* (# 28/6/05)

Zhou, Xiangting BSc *Hebei China* MSc *Zhengzhou/Hebei* PhD *NSW* \*

## Research Staff Externally Funded

### ARC Queen Elizabeth II Fellow

Webster, Richard D BSc *Auckland* Hons PhD *La Trobe*

### ARC Linkage Australian Postdoctoral Fellow (CSIRO)

Ozawa, Kiyoshi BEng *Yokohama*, MSc PhD *Tokyo*

### ARC Postdoctoral Fellows

Coote, Michelle L BSc PhD *NSW* (#20/06/05)

### Progen Industries Fellows

Bonnet, Muriel Dipl *Bordeaux* PhD *ETH Zurich*

Kreipl, Andreas T DiplChem *Hamburg* DrRerNat *Munich* (#14/4/05)

### Feodor Lynen Fellows (Alexander von Humboldt Stiftung Foundation)

Gross, Steffen Dipl PhD *Freie Berlin* (#30/6/05)

John, Michael DiplChem *Philipps Marburg* DrRerNat *Tech Munich* (from 16/8/05)

Renner, Jens Dipl DrRerNat *Kaiserslautern* (#28/1/05)

### UnIChe Project

Reynolds, Philip A BA DPhil *Oxford* FRACI

### National Science Foundation, America

Netzloff, Heather M BA *Minot* PhD *Iowa*



**Endeavour Australia Cheung Kong Award**

Somphon, Weenawan BSc *Ramkhumheang*, Bangkok PhD  
*Suranaree U Tech* Thailand

**Honourary Academic Staff****Adjunct Professors**

Amos, Roger D BSc *Glasgow* PhD *York*

James, Veronica J OAM BA BSc *Queensland* BSc PhD *NSW*

Radom, Leo MSc PhD *Sydney* DSc *ANU* FRACI, FAA

**Visiting Fellows (Post-retirement)**

Beckwith, Emeritus Professor Athelstan L J BSc *WA* DPhil  
*Oxford* FAA FRACI, FRS

Bennett, Emeritus Professor Martin A BSc PhD DIC DSc  
*London* ARCS, FRACI, FAA, FRS

Bramley, Dr Richard MSc *Sydney* PhD *London* MRACI

Brown, Dr Desmond J BSc MSc *Sydney* PhD DSc *London*

Craig, Emeritus Professor David P MSc *Sydney* PhD DSc  
*London* FRIC FRACI, FAA, FRS

MacLeod, Dr John K BSc PhD *Queensland* FRACI

Rickards, Emeritus Professor Rodney W BSc *Sydney* FRACI,  
FAA

Sargeson, Emeritus Professor Alan M BSc PhD Dip Ed  
*Sydney* FRACI, FAA, FRS

Williams, Emeritus Professor John F MSc PhD *NSW* MA  
*Oxford* DSc *ANU*, FRACI, FAIFT

**Administrative and Technical Staff**

≈ = part-time; # = left during 2005

**Business Office**

Harland, Lesley BSc MSc *E Anglia* Laboratory Manager

Scarr, Lorraine Business Officer

Bayley, Neil BInTech *ANU* Purchasing Officer

Monaghan, Lorna M Administrative Assistant

O'Brien, Brendan J Administrative Assistant

O'Toole, Elouise E

Administrative Assistant

Russell, Kurt

Requisitioning Clerk

Scarr, Barry

Administrative Assistant

Davies, Christine ≈

Receptionist

Rawlings, Kim C ≈

Receptionist

**Academic Secretary's Office**

Holloway, Marilyn A

Academic Secretary

Slocum, Maureen

Academic Staff Administrator

Murray, Valerie J ≈

Student Administrative Officer

Riches, Susan ≈

Administrative Assistant

**Departmental Administrative Assistants**

Enge, Rosemary E ≈ #

Inorganic Chemistry

Williams, Suzanne R #

Physical Chemistry

Riches, Susan ≈

Organic Chemistry

Britton, Lena BSc (Bus Admin)

Physical Chemistry (UnlChe)

*Goteborg* ≈

**Dean's Executive Assistant** Baker, Michelle

**Facilities Officer** Cooper, Kevin DipBus *AIM ACT*

**Laboratories and Safety Coordinator** Welling, Lee L  
BSc(App) *Canberra CAE*

**Engineer** King, David J BE BSc *NSW*

**Facility Coordinator, ANU NMR Centre** Keniry, Max A BSc  
PhD *Sydney*

**Technical and Research Services Staff**

Allen, John M BSc *Canterbury* NZ

Carland, Michael W BSc(Hons) PhD *Melbourne*

Carr, Paul D BSc PhD *Keele*

Cayzer, Tory N BSc(Hons) *Sydney*, PhD *ANU* #

Clarke, Ian J

Culnane, Pui T DipAppChem *Melbourne*

Davenport, Troy BEngTech *USQ*

Devitt, Peter J

Filardo, Raffaele J

Gilbert, Andrew T B BSc(Hons) *Massey PhD Cambridge*  
 Gugger, Paul A BSc(App) *Canberra CAE*  
 Heerdegan, Aidan P BSc *Massey PhD ANU*  
 Herlt, Anthony J BSc *ANU*  
 Hill, Michael J  
 Jackman, Keith L  
 Jeyasingham, Anithahini BSc *Jaffa Sri Lanka MSc Waikato*<sup>~</sup>  
 Koehne, Russell T AssocDipEng *CIT*  
 Lee, Stephen B  
 Lilley, Penny E BSc(App) *Canberra CAE*<sup>~#</sup>  
 Liu, Jian-Wei BSc *Jinan, China BSc PhD Newcastle NSW*  
 Lockhart, Gordon G  
 Ma, Xinghua H BSc *Hanzhong ME Dalian China PhD ANU*  
 Melnitchenko, Alexandre MS *Kiev*  
 Mittag, Emil J BSc(Hons) MSc *UTEP PhD ANU*  
 Neumann, Horst  
 Norén, Lasse H BSc PhD *Uppsala*  
 O'Brien, Robert J  
 Owen, Elisabeth A BAppSc GradDipChem Grad DipAdmin *WAIT*  
 Qi, Ruhua BSc *Lanzhou China PhD ANU*  
 Sharrad, Christine BSc *Melbourne Hons Monash Cert III BusComp CPTI*  
 Simmonds, Peta BSc *Monash*  
 Siu, Paul  
 Tomkins, Christopher J  
 Twitchin, Bruce  
 Vera, Fernando  
 Wang, Genmiao BSc MSc *USTC Hefei China PhD NSW*  
 Willis, Anthony C BSc PhD *WA*  
 Withers, Viki L BSc *ANU*<sup>~</sup>

### Laboratory Attendants

Hogan, Carol <sup>~#</sup>

### Programmers

Blake, Christopher J BSc(Appl) *Canberra CAE GradDip (Comp) Canberra*

Cohen, Pam BA *ANU GradDip(CompSci) Canberra CAE*<sup>~</sup>

Delfs, Christopher D BSc PhD *WA*

Faletic, Rado <sup>~#</sup>

Lindsell, Graeme A BSc *NSW PhD ANU*

### Chemistry Librarian (ANU Staff)

Smith, Joan E

### Stores Staff

Easton, Norman <sup>#</sup>

Galarza, Marcelo

### Security Officers

McGlinchey, Hugh

Jamieson, Stephen

Ross, Ian T <sup>#</sup>

Smith, Don M

Stuart, Ian

### Cleaning Staff

Antunovic, Marica <sup>~</sup>

Lauc, Draga <sup>~</sup>

Lockhart, Rosemary <sup>~</sup>

Stavreska, Luba <sup>~</sup>

### Tea Assistant

Van Kampen, Lena

## STATISTICS

<b>Total academic staff at 31 March 2005</b>			<b>82.5</b>	<b>(17)</b>
Standard appointments	17.5	(1)		
Fixed term appointments (excluding PDFs)	17	(3)		
<i>School funded</i>		4.5	(1.5)	
<i>ARC grant funded</i>		9.5	(1.5)	
<i>UnlChe grant funded</i>		1	(0)	
<i>ARC Federation Fellow</i>		1	(0)	
<i>ARC QEII Fellow</i>		1	(0)	
<b>Total Postdoctoral Fellows</b>	<b>48</b>	<b>(13)</b>		
<i>ARC PDFs</i>		.5	(.5)	
<i>School funded PDFs</i>		4.5	(3)	
<i>ARC grant funded PDFs</i>		37.5	(7.5)	
<i>Progen funded PDFs</i>		1.5	(1)	
<i>ARC/CSIRO Linkage funded PDF</i>	1	(0)		
<i>National Science Foundation Fellowship</i>	1	(1)		
<i>Feodor Lynen funded PDFs</i>	2	(0)		
<b>Visiting Fellows during 2005 (including Post-retired)</b>			<b>33</b>	<b>(3)</b>
<b>Postgraduate students at 31 March 2005 (excluding 5 students on program extension)</b>			<b>55</b>	<b>(31)</b>
<b>PhD degrees awarded</b>			<b>13</b>	<b>(4)</b>
<b>MPhil degrees awarded</b>			<b>1</b>	<b>(0)</b>
<b>General staff at 31 March 2005 (FTE)</b>			<b>69.11</b>	<b>(24.11)</b>
<b>Technical/Research</b>	<b>37.58</b>	<b>(7.08)</b>		
<b>Administrative/Computing</b>	<b>20.68</b>	<b>(13.18)</b>		
<b>Other</b>	<b>10.85</b>	<b>(3.85)</b>		

Note: Bracketed figures at right, in italics, represent female staff/students