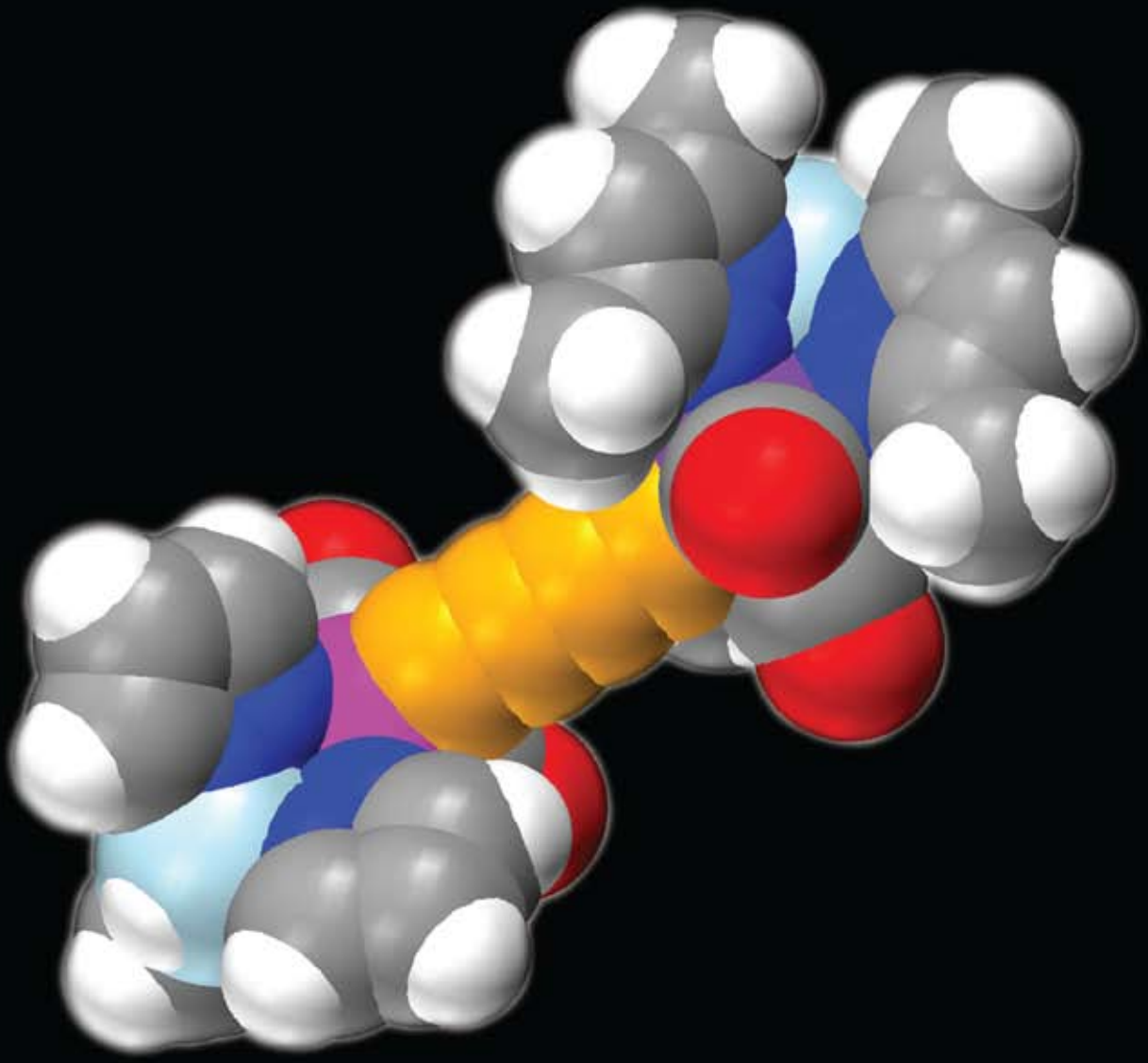
THE AUSTRALIAN NATIONAL UNIVERSITY

Research School of CHEMISTRY

2006 & 2007 ANNUAL REPORT



ANU COLLEGE OF SCIENCE

ANU College of Science

Research School of Chemistry

The Australian National University
Building 35
Science Road
Canberra ACT 0200
Australia

Telephone: +61 2 6125 3637

Fax: +61 2 6125 0755

Email: directoradm@rsc.anu.edu.au

Website: http://rsc.anu.edu.au/index.php

Editors: Professor Peter Gill
Ms Stephanie Neulinger

Coordinator: Ms Stephanie Neulinger

Front Cover:

The cover depicts a dimetallahexatriyne, a compound containing an unprecedented Mo≡C-C≡C-C≡W spine in which two metal centres are connected to a tetracarbido C_4 group via two metal-carbon triple bonds. The novel compound was prepared by Dr Rian D. Dewhurst (J. G. Crawford Prize Winner, 2005) via a [1+3] strategy involving the platinum-mediated coupling of "Mo≡C" and "W≡C—C≡C" sub-units.

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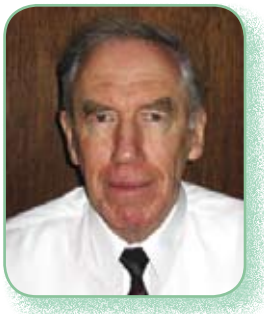
DIRECTOR'S REPORT

The present report details the circumstances of the Research School of Chemistry (RSC) during 2006 and 2007. It should also give the reader a sense of current and proposed activities within the School. In addition, we hope this document will convey a sense of the vibrancy of the organisation and the capacity it has to continue to play a vital role, both nationally and internationally, in the development of chemistry.

The preceding twenty-four months have provided exciting times for the School. Whilst a major storm and consequent flood struck us during this period, the magnificent performance of the staff allowed us to recover in a remarkably short period of time, and in some ways the Birch and Craig Buildings have never looked better. However, external appearances can be deceptive and belie the fact that some of the fabric of the now forty-year-old Birch Building is showing signs of age. As a consequence, the RSC and Department of Chemistry (DoC) will move into two new buildings and two fully refurbished ones. Whilst the move itself is still two to three years away, detailed planning is already well underway.

2007 was a very significant year for the RSC because on September 7th we celebrated its 40th birthday. Emeritus Professor David Craig, who co-founded the School with Professor Arthur Birch, was on hand to cut the birthday cake under the watchful eye of his former colleague Emeritus Professor Alan Sargeson. A more poignant moment occurred on Sunday, December 17th, 2007 with the sudden death of Emeritus Professor Rod Rickards, a remarkable individual who had made so many outstanding contributions to the School from its inception. His intellect, humour and good grace will be sorely missed by everyone.



As is always the case in any complex organisation, the last two years has been a period of transition for the RSC. In early 2006 Ms Marilyn Holloway retired after having served so admirably in the role of Academic Secretary for a number of years. Ms Lesley Harland also left in 2006 after having provided outstanding service as School Manager for nearly a decade. Ms Lorraine Scarr, a longstanding member of the School's team in the Front Office, also departed in 2006. Ms Kerryn Jackson was appointed as Business Manager of the RSC from early 2006 whilst also being involved in the implementation of the new ANU College of Science (CoS) structure. In early 2007 Mr Geoff Deeble took over the role after Ms Jackson became Executive Officer within the CoS. In the intervening twelve months, Geoff has assembled an excellent team of technical and administrative staff that is providing a fine service to both the RSC and the DoC.

There have been various changes on the academic front. Professor Nick Dixon left in 2006 to take up an appointment at the University of Wollongong, and Dr Aaron Oakley completed a five-year Research Fellowship in 2007, moving to CSIRO, Melbourne. Professor David Ollis is now Head of the DoC, while continuing to hold a substantive research appointment within the RSC. Dr Mal McLeod took up a joint appointment between the RSC and DoC in late 2007 and we wish him all the very best as he develops his research and teaching programs. Furthermore, the RSC and the DoC are currently seeking to make a joint appointment in Biological Chemistry (Protein Science). Additional appointments of this type are anticipated in the near future as we continue to expand our activities in various areas of chemistry.

Members of the RSC consistently attract significant external funding from various sources, most notably through the range of programs run by the Australian Research Council (ARC). The Canberra node of the ARC Centre of Excellence for Free Radical Chemistry and Biotechnology is now well and truly established as a vibrant entity within the RSC. It provides a major source of support and inspiration for the research activities of the groups lead by Professor Chris Easton, Associate Professor Mick Sherburn and Dr Michelle Coote.

The RSC enjoys the benefits of accommodating a large group of talented and enthusiastic undergraduate and graduate students, as well as a substantial body of post-doctoral researchers. Due to the contributions of such people, the School has a "buzz" about it as well as a strong international flavour that derives from the diverse backgrounds of this group.

On December 31st, 2007 Professor Denis Evans completed a ca. ten-year term as Dean/Director of the RSC. During this period, Denis filled the role with great zeal and, in more recent times, presided over an organisation undergoing remarkable change in many areas. I look forward, as the incoming Director, to maintaining the substantial research momentum of the RSC and to participating in its continued development as a vital organisation for promoting that wonderful subject called chemistry.

Professor Martin Banwell
Director, Research School of Chemistry

2006 & 2007 RESEARCH HIGHLIGHTS

Michelle Coote's group:
Thioketone-mediated Polymerisation

In 2006, Dr Michelle Coote and collaborators at the University of New South Wales published a new method for controlling the molecular weight and architecture of the polymer produced in free radical polymerisation. In this new process, called thioketone-mediated polymerisation, the growing polymer chains are protected from unwanted termination reactions through their reversible trapping with carefully selected thioketone compounds. As the adduct radical from this reaction is highly stabilised, this ensures that the majority of the polymer chains remain active throughout the process, and are thus the same length when a second monomer or capping group is added to the reaction mixture. The process was designed on the basis of quantum-chemical calculations from the Coote group, which were used to identify thioketones for which the corresponding adduct radicals are sufficiently stabilised to allow for control of polymerisation to be achieved. It was then confirmed experimentally in the laboratories of Professor Barner-Kowollik, and the work was featured on the cover of *Chemical Communications*. This successful example of computer-aided chemical design highlights the growing importance of computational chemistry as a partner to experiment.

Nick Dixon's group: *A molecular mousetrap in DNA replication*

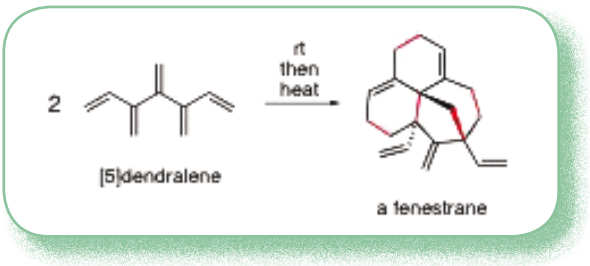
Work reported in 2006 in the premier biochemistry journal "Cell" solved a long standing puzzle regarding the last stages of copying of DNA in cells that are about to divide. DNA in chromosomes is copied by multiprotein machines called replisomes that separate the two strands of DNA and copy both of them simultaneously. On circular bacterial chromosomes, pairs of replisomes must eventually arrive from opposite directions to meet at precise positions called terminator sites. These sites, which bind tightly to a protein called Tus, stop replisomes that come from one direction, but not the other. The Dixon group showed that binding of Tus to a terminator site sets a molecular mousetrap that blocks replisomes in this directional manner. DNA strand separation by a replisome is what springs the trap; one of the separated strands moves from its normal position and binds extraordinarily tightly to a new site within the Tus protein, which now cannot be dislodged from the terminator site. In contrast, a replisome arriving from the other direction cannot spring the trap, and so passes through, knocking the Tus protein off the DNA. This mechanism was then confirmed by the structure of the trapped DNA in its complex with Tus, determined by Dr Aaron Oakley.

Chris Easton's group:
A Nanomachine at Work

As reported in *J. Am. Chem. Soc.*, 2006, *128*, 14750, Roger Coulston and Hideki Onagi developed a molecular pump as a working nanomachine. A machine is an apparatus consisting of interrelated parts with separate functions that can be used to do work. A molecular- or nano-machine is simply a machine that operates at the molecular level. Roger and Hideki designed and synthesised their molecular pump with a cyclodextrin as the cylinder and an aryl substituent as the piston, such that when 1-adamantanol is used as a fuel to drive the pump, work is done to constrain the geometry of an amide bond. The second generation of the pump incorporates a photochemically sensitive alkene as a light-driven on/off switch. This pump is a first example of the work output of a molecular machine being harnessed at the molecular level, which is an important step towards practical applications of nanotechnological devices. This research was reviewed as a "Highlight of Australian Chemistry" in the April 2007 issue of "Chemistry in Australia" and is summarised in a "Research Profile" in the text "Chemistry", A. Blackman *et al.*, eds., Wiley and Sons, Australia, 2007.

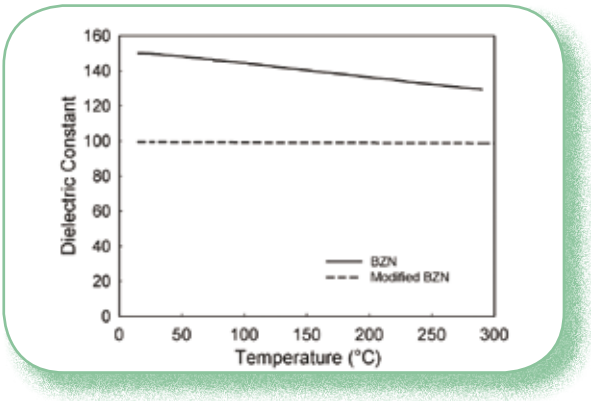
Mick Sherburn's group: *High Structural Complexity from Simple Hydrocarbons*

Dendralenes are acyclic cross-conjugated oligo-alkenes with much synthetic potential. Nevertheless, these molecules are poorly studied, due to their problematic synthesis and perceived instability. The Sherburn group were the first to prepare the dendralene family of fundamental hydrocarbons but their synthesis only allowed the preparation of very small amounts of material – too small, in fact, to study their chemical properties. In a significant breakthrough this year, they have devised a one-step synthesis of [5]dendralene, which allows the preparation of the hydrocarbon in large amounts. Their studies into its synthesis and fascinating chemical reactivity are reported in an *Angewandte Chemie* publication selected as a "Hot Paper" by the journal editors (Bojase G, Payne A D, Willis A C, Sherburn M S. *Angew. Chem. Int. Ed.* 2008, 47, 910-912). One of the highlights of their work is the dimerisation of [5]dendralene. This simple hydrocarbon undergoes an intermolecular Diels-Alder reaction followed by a 6π-electrocyclisation followed by an intramolecular Diels-Alder reaction to give a spectacularly complex fenestrane in one step without additional catalysts or reagents!



Ray Withers' group: *Bismuth-based Pyrochlores and their use for Multilayer Ceramic Capacitor Applications*

Bismuth-based, pyrochlore type, dielectric ceramics are low sintering temperature, co-fireable ceramic (LTCC) materials for multilayer ceramic capacitor (MLCC) applications. They possess good microwave dielectric properties and have potential application as multilayer microwave dielectric components. The electric field tuneability of the dielectric constants of this bismuth-based pyrochlore family of phases also makes them potentially useful as frequency agile RF/microwave components. Electron diffraction and modelling has been used to understand the local nanoscale order characteristic of these inherently disordered materials and its consequences for their dielectric properties, in particular their dielectric loss properties. Based on this fundamental research, the Materials Chemistry Group has developed a new technique to overcome a significant limitation to widespread use, their relatively poor temperature-stability characteristics. The technique enables excellent temperature stability to be achieved over a very broad temperature range (from ~ -150 °C to +200 °C) without significant deterioration of their dielectric constants and dielectric losses. This research has led to an Australian provisional patent and drawn the attention of an IP investment company.



The temperature-dependent dielectric constant of a typical $Bi_{1.5}ZnNb_{1.5}O_7$ pyrochlore ceramic before and after modification. Note that the temperature coefficient of the dielectric constant has been tuned from the original -470 ppm/°C down to only +13 ppm/°C.

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

Dean / Director

Professor Denis J Evans

Deputy Dean / Director

Professor Christopher J Easton – 2006

Professor Martin G Banwell - 2007

Associate Dean / Director (Students)

Professor Raymond L Withers

Group Leaders

Professor Martin G Banwell BSc PhD *Wellington*, FWIF, Hon FRSNZ, FRACI, FAA

Professor Michael A Collins BSc PhD *Sydney*

Dr Michelle L Coote BSc PhD *New South Wales*

Professor Nicholas E Dixon BSc PhD *Queensland*

Professor Christopher J Easton BSc *Flinders* PhD DSc *Adelaide*, FRACI, FAA

Professor Denis J Evans BSc *Sydney* PhD *ANU*, FRACI, FAA

Professor Peter M W Gill MSc (Hons) *Auckland* PhD *ANU*

Professor Anthony F Hill MSc (Hons) *Auckland* DrRerNat *Bayreuth*, FRSC

Dr Max A Keniry BSc PhD *Sydney*

Professor Elmars R Krausz BSc PhD *Sydney*, FRACI

Emeritus Professor Lewis N Mander (Adjunct) MSc *Auckland* PhD *Sydney*, FRACI, FAA, FRS

Dr Aaron J Oakley BSc *Tasmania* PhD *St Vincent's IMR Melbourne*

Professor David L Ollis BSc *New South Wales* PhD *Sydney*

Professor Gottfried Otting Dipl *Freiburg* PhD *ETH Zürich*

Associate Professor Edith M Sevick BSE *Pittsburgh* PhD *Massachusetts*

Associate Professor Michael S Sherburn BSc PhD *Nottingham*

Professor Richard T Welberry MA *Cambridge* PhD *London*

Professor John W White CMG MSc *Sydney* MA DPhil *Oxford*, FAPS, FRACI, FRSC, FAA, FRS

Professor S Bruce Wild BSc *New South Wales* PhD *Manchester*, FRACI, FRSC, FAA

Professor Raymond L Withers BSc PhD *Melbourne*

School Manager

Ms Kerryn Jackson - 2006

Mr Geoff Deeble - 2007

PROTEIN STRUCTURE AND FUNCTION

Professor Nick Dixon (Head of Section)

http://rsc.anu.edu.au/research/dixon.php

Some biological processes, such as the cellular synthesis of the nucleic acids DNA and RNA, are carried out by large protein machines that cycle through a perfectly orchestrated series of chemical processes as they function. Both strands of DNA in the cell are copied simultaneously at the rate of about 1000 nucleotides per second by a dynamic multiprotein machine called the replisome, which almost never falls off the DNA it is copying, and almost never makes mistakes. Discovering how the 30 or so proteins that collaborate in the bacterial replisome do this has been the primary research objective of the Protein Structure and Function group for the last 21 years. To succeed, we need to understand the chemistry that governs the specificity and strength of interactions of proteins with substrates, nucleic acids, and other proteins, and how effects exerted on one interaction in the replisome affect other interactions.

We use molecular genetics to engineer rich sources of the proteins and to produce mutant derivatives and segments of them. Conventional enzymology, DNA synthesis assays, protein chemistry and biophysical techniques, such as surface plasmon resonance, are used 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.

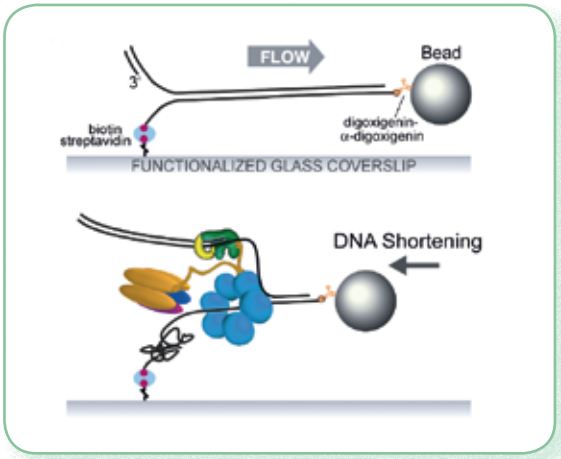
Protein Interactions During DNA Replication

One current focus of our work is on the interactions among the ten different subunits of DNA polymerase III holoenzyme (Pol III), the enzyme that actually makes new DNA. Another is on the hexameric replicative DNA helicase (DnaB), the motor protein that separates the two strands of DNA so that they can be copied. We are interested in how DnaB interacts with the DnaG primase that starts DNA chains, the DnaC helicase loader protein, and the t subunit of Pol III. In other work reported in 2006 in the journal *Cell*, we showed how the activity of DnaB determines how a complex of the Tus replication terminator protein, with DNA sites in the terminus region of the chromosome, can stop a replisome moving towards it on DNA from one direction, but not the other. This was a problem that had puzzled scientists in the field for more than 20 years. Moreover, the new protein-DNA interaction we discovered has applications in biotechnology that will be explored in future work. In a collaborative study with colleagues at the University of Wollongong, we have used a new extended-mass-range electrospray ionisation mass spectrometer, purchased with funds from the ARC LIEF program and the two universities, to obtain the first mass spectra of the DnaB hexamer and its complex with six molecules of DnaC. This is a remarkable achievement because the latter complex has a molecular weight near 500,000. *(With P D Carr, R Chan, M J Headlam, S Jergic, M John, M A Keniry, K V Loscha, M D Mulcair, A J Oakley, G Otting, K Ozawa, A-Y Park, R Qi, P M Schaeffer, X-C Su, P S C Wu, and G Schenk [U Qld]), T M Hill [U North Dakota], C Neylon [U Southampton], C Ioannou, P Soultanas [U Nottingham]*

Single-molecule Studies of DNA Replication

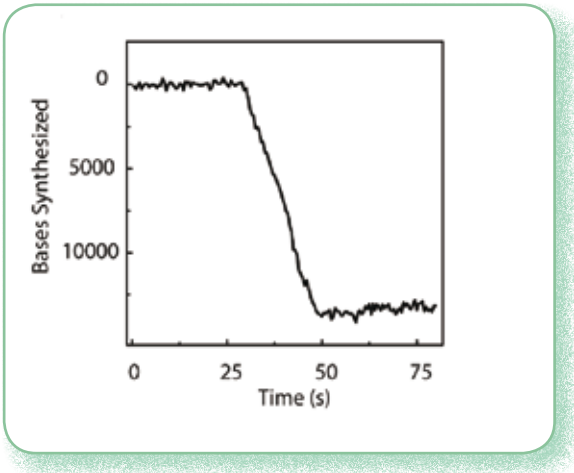
In an exciting new collaborative venture, we have initiated a project with colleagues in the Department of Biological Chemistry and Molecular Pharmacology at Harvard Medical School to produce the first real time observations of replication of individual DNA molecules by the *E. coli* replisome complex. DNA molecules are fixed at one end to a surface and at the other to a small bead, and stretched out in a gentle flow of water. Under the conditions we used for the experiment shown in the top panel of Figure 1, replication of one strand of the double-stranded DNA converts the other to the single-stranded form. Single-stranded DNA is much shorter than double stranded DNA, so the length of the DNA

shortens as one strand is copied. As shown in Figure 2, a single replisome could copy 13,000 bases of DNA on average without falling off, within about 25 seconds. *(With S Jergic, P M Schaeffer, and N A Tanner, S M Hamdan, A M van Oijen [Harvard Medical School])*



Above: Figure 1

Below: Figure 2



New Protein Technologies

Because we understand them so well, many of our DNA replication proteins are also being used for the development of a suite of new techniques in protein chemistry, including methods for *in vitro* evolution of new protein functions, cell-free 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. We are also developing methods for cell-free incorporation of unnatural amino acids into proteins, and efficient ways to identify sites of protein-protein interaction. 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. *(With M J Headlam, M D Mulcair, S Noor, G Otting, K Ozawa, A-Y Park, Y Pham, P M Schaeffer, I Ugwumba, P S C Wu, and S E Brown, Z Xu [CSIRO Entomology], P Hendry [CSIRO Molecular & Health Technologies], J L Beck, M M Sheil [U Wollongong], D Spencer, H-X Zhou [Florida State U])*

In August 2006, after 20 years as a member of the RSC, Professor Dixon moved to the University of Wollongong, and his group followed over the next eight months. He continues to have strong research collaborations with members of the Biological Chemistry section at RSC, and retains an adjunct appointment.

Nick Dixon's farewell morning tea

NUCLEAR MAGNETIC RESONANCE

Dr Max Keniry

http://rsc.anu.edu.au/research/keniry.php

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. The NMR group has solved the structures of an insulin-like growth factor and a large complex formed by two of the components from the catalytic core of DNA polymerase. We continue to investigate the structures of biologically significant DNA quadruplexes and their interactions with natural products. The association of spermine and calothrixin with DNA quadruplexes continues to present surprising results. 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 DNA Quadruplexes

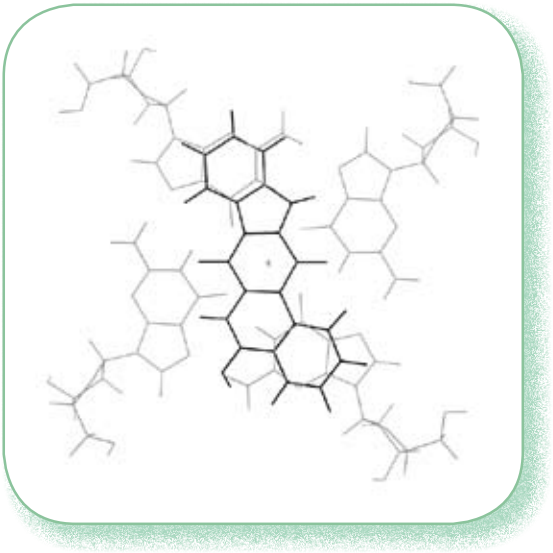
Spermine, an aliphatic polycationic molecule found in all cells, plays an essential role in cell growth and differentiation. At present, there is no thorough understanding of how polyamines exert their physiological effects. Spermine is known to interact both with DNA and with proteins, yet the details 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-quadruplex DNA using a specifically ^{13}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}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 but is still independent of the tumbling 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. A detailed description of this work has recently been published in the *European Biophysics Journal. (With E A Owen)*

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 exact mechanism of the biological activity has yet to be elucidated. With this in mind, we have investigated the association of the calothrixins and their synthetic analogues with various structural forms of DNA by NMR, circular dichroism (CD) and fluorescence. Calothrixin binds to DNA quadruplexes as shown by UV, CD and NMR spectroscopy but the low solubility of calothrixin in aqueous solution has been an obstacle to determining accurate dissociation constants. We have overcome this problem by incorporating a fluorescent analogue of adenine into the quadruplex formed within the hypersensitive site of the *c-myc* oncogene promotor. The analogue does not change the quadruplex structure but its fluorescence is very sensitive to local changes induced by the binding of other molecules. By following the changes in the fluorescence of this DNA quadruplex on binding of calothrixin, we have confirmed that calothrixin binds with micromolar dissociation constants. Further work

with several different DNA quadruplex structures has confirmed that calothrixin will bind only if there is an exposed external quartet.

One possible binding mode is shown below with calothrixin superposed on the exposed quadruplex quartet. *(With E A Owen)*



Interaction of the θ-subunit and the ε-subunit of DNA Polymerase III

The catalytic core of *Escherichia coli* DNA polymerase III contains three tightly associated subunits (α, ε, and θ). The refinement of the three-dimensional structure of the θ-subunit was completed by the NMR group. The θ-subunit has three α-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 θ- and ε-subunits. The structure of the θ-subunit bound to ε- 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 ε. We have mapped the binding surface of ε on θ to a hydrophobic patch on θ using advanced NMR techniques. The structure of the complex between ε and θ has been assembled using the same paramagnetic restraints that were used to refine the structure of ε. The structure is now complete and the work was recently published in the *Journal of Bacteriology. (With E M Bulloch, N E Dixon, S Hamdan, G Otting, A Y Park, G Pintacuda, T K Ronson, and S E Brown [Entomology, CSIRO])*

Nuclear Magnetic Resonance

We continue to explore new ways of using NMR to study chemical and biochemical problems. An ongoing theme is the use of liquid cross polarisation (CP) techniques in our research. The work with spermine has benefited from the use of doubly selective CP to isolate the interactions and dynamics of protons bound only to isotopically enriched carbon-13. We have also used CP to devise a rapid technique for characterising the reaction products in polymer chemistry.

STRUCTURAL BIOLOGY

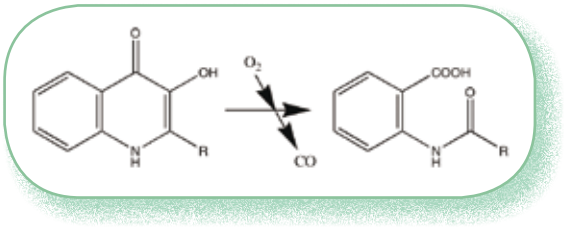
Dr Aaron Oakley

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

Broadly defined, structural biology is the study of the three dimensional structure of biological molecules such as proteins and nucleic acids. Structural biology is one of the many approaches used to understand biological systems at the molecular level, and complements other approaches such as molecular genetics, enzyme kinetics and mechanistic studies. Advances in medicine, biotechnology and industry result, in part, from an understanding of structure. Within this sphere, our group conducts fundamental and applied research.

Co-factor Free Oxygenases

We have determined the structure of a co-factorless oxygenase called QDO from *Pseudomonas putida*. The structure is remarkable for two reasons: it is a member of the α/β–hydrolase superfamily, and it is able to catalyse oxygenolysis without heme or other cofactors.



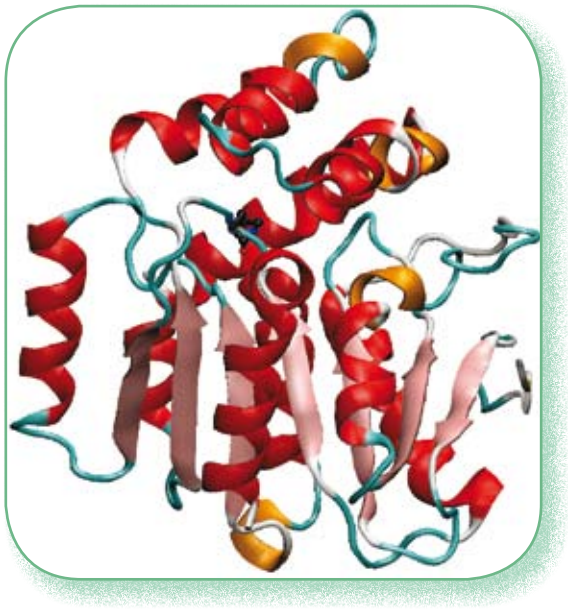
Co-factor free oxygenases

Most members of this very large group of enzymes catalyse hydrolysis reactions, ie. reactions utilising water to break chemical bonds, such as esterases and peptidases. The parsimonious approach to understanding the evolution of the enzyme superfamily suggests that QDO evolved from an ancestral protein possessing hydrolase activity. Two important questions motivate this research project: (i) how does QDO catalyse oxygenolysis without aid of cofactors, and (ii) how does an enzyme scaffold evolve so as to fundamentally change the type of reaction catalysed? Understanding the second question will help to light a new path to the creation of new enzymes in the laboratory for medicinal or industrial applications. In line with our expectation, the determination of the three-dimensional structure of QDO revealed that the enzyme adopted the classic fold indicative of the alpha/beta-hydrolase superfamily. We are now working to understand the catalytic mechanism of the enzyme. *(With R Qi, and S Fetzner [U Oldenburg])*

Termination of DNA Replication in Bacteria

The replication of double-stranded DNA is fundamental to all living things, and understanding the processes underlying DNA replication represents one of the most exciting challenges in biological chemistry. The gut bacterium *E. coli* is a model organism for understanding DNA replication, and is the subject of ongoing collaborations with the research group of Professor Nick Dixon (University of Wollongong). A multi-protein complex called the replisome is the driver of chromosomal DNA replication. *E. coli*, like other bacteria, has a carefully coordinated system for DNA replication: the process starts at a specific site (OriC), and is halted at specific sites on the chromosome called *Ter* sites. At the head of the replisome is a DNA-unwinding protein called a helicase, and the single-stranded DNA created by the action of helicase is a template for the production of new strands.

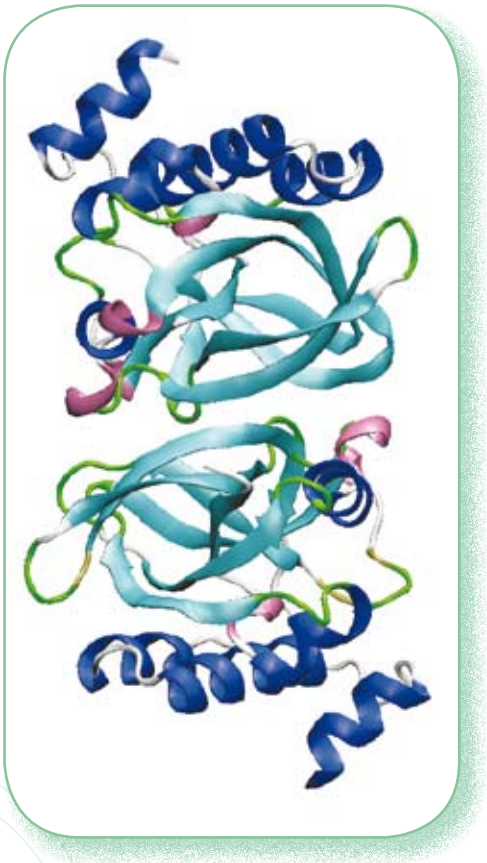
A protein called Tus recognises and binds to *Ter* sites. Professor Dixon and co-workers have shown that by breaking a specific DNA-base-pair interaction, the helicase causes Tus to bind more tightly to DNA, preventing the replisome from progressing. We have determined the three-dimensional structure of this locked form of the Tus-*Ter* complex. The structure revealed the physical process underlying the halting phenomenon and revealed a new type of protein-DNA interaction. An image of the structure was featured on the cover of the journal *Cell* in 2006. *(With N E Dixon, M D Mulcair and P M Schaeffer [UOW])*



Human Omega-class Glutathione S-transferases and Glutathione Metabolism

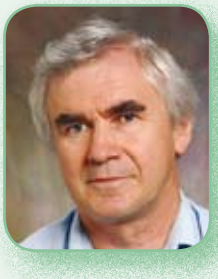
The tripeptide glutathione is central to biological detoxification in eubacteria and eukaryotes. The cytosolic enzyme γ-glutamyl cyclotransferase catalyses the formation of 5-oxoproline (pyroglutamic acid) from γ-glutamyl-dipeptides and plays a significant role in cellular glutathione homeostasis. We recently determined the three-dimensional structure of the human isozyme, which revealed a novel fold that we have dubbed the "cyclotransferase fold":

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. This enzyme, as the name suggests, utilises glutathione. Genetic polymorphisms may alter their structure and function and cause individual variations in toxicity and response to arsenic. The structure of the enzyme indicates an active site arrangement not seen in other members of this family of proteins. We are investigating how substrates interact with the enzyme. *(With P G Board [JCSMR])*



Human omega-class glutathione S-transferases and glutathione metabolism

PROTEIN CRYSTALLOGRAPHY AND ENGINEERING



Professor David Ollis

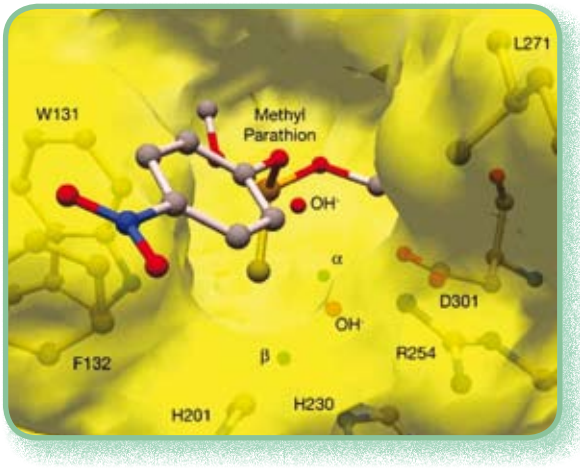
http://rsc.anu.edu.au/research/ollis.php

The group works at the interface between chemistry and biology - working out how proteins function and how they might be modified for new and useful purposes. We use directed evolution to produce mutant proteins with interesting properties that can be utilised in industrial and environmental applications. We also want to understand how mutations change the properties of a protein - as a way of better understanding how proteins fold and function. To this end we use a variety of techniques, including enzyme kinetics and X-ray crystallography, to come to grips with the detailed mechanics of protein function.

In the past few years, we have developed a technique to evolve the proteins to be more soluble. This process has given some insight into structural requirements for metal binding proteins. We have also used directed evolution to evolve a protein to be antibiotic resistant – mimicking a clinically important process. We have also used a variety of techniques to better understand the detailed mechanism of an organophosphate-degrading enzyme from *Agrobacterium radiobacter* (OPDA) – the structure of the protein in the presence of a substrate has been determined.

Enzyme Engineering with an Organophosphate-degrading Enzyme

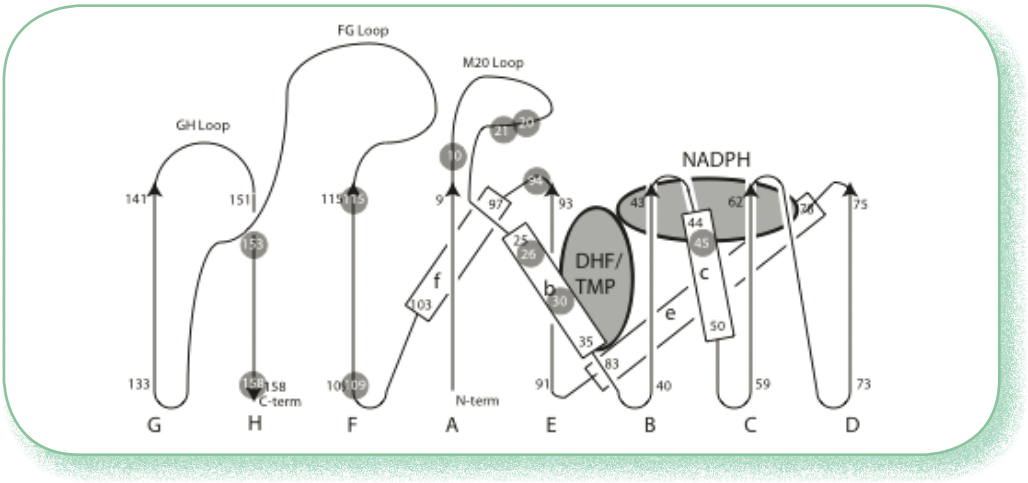
OPDA is a bacterial enzyme that shows considerable utility in bioremediation. In the last few years we have obtained the structure of OPDA using directed evolution to improve its expression in *E. coli.* We have also been involved in studies to better understand the mechanism of the protein, and to this end we have solved the structure of the protein in the presence of its reaction product along with a slow turnover substrate. These structures give clear indications as to how the substrate binds to the proteins and how the attacking water is activated within the active site. *(With C Jackson, P D Carr, J-W Liu)*



The pesticide methyl parathion is shown in the active site of OPDA. The diagram shows the active site residues that are in close proximity to the substrate.

Antibiotic Resistance at the Molecular Level – New Targets for Drug Design

The enzyme dihydrofolate reductase (DHFR) is an essential component of cellular metabolism. It is the target for a number of drugs, some of which are directed towards the bacterial form of the enzyme and function as antibiotics. Trimethoprim (TMP) is one such compound. Unfortunately, bacteria quickly evolve variants of DHFR that are both active and resistant to TMP. We have used directed evolution to mimic this evolutionary process, and have produced mutants that are both active and bind TMP with very low affinity. Analysis of these mutants reveals a great deal about DHFR as well as providing a great deal of useful information for designing new drugs. *(With M Watson and J-W Liu)*



Schematic diagram showing the secondary structure elements of DHFR – arrows representing β strands, and rectangles represent α helices. The binding sites for substrate (DHF), inhibitor (TMP) and co-factor (NADPH) are shown along with the locations of mutations (circles) that confer antibiotic resistance.

Improving Protein Solubility

Industrial applications of enzymes 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 DHFR that, as noted above, is inhibited by the antibiotic 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. This technique has been applied to an insoluble metal binding domain of aminopeptidase P from *E. coli.* The results of this study have implications for the metal binding requirements of the protein. *(With J-W Liu)*

BIOMOLECULAR NMR

Professor Gottfried Otting

http://rsc.anu.edu.au/research/otting.php

The group develops novel tools for the application of NMR spectroscopy to the study of biological macromolecules (proteins and DNA). Emphasis is placed on the study of protein-protein, protein-DNA and protein-ligand interactions, with applications for drug development in the pharmaceutical industries in mind. In particular, NMR is used to determine the three-dimensional (3D) structures of protein domains and protein-ligand complexes. This research is supported by 800 and 600 MHz NMR spectrometers equipped with a cryoprobe.

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 the NMR spectra very straightforward. We have written software to achieve such assignments fully automatically.

We have developed new approaches for site-specific attachment of lanthanide ions to proteins, involving lanthanide-binding peptides or synthetic organic molecules with high lanthanide affinities. This allows the attachment of lanthanide ions to proteins devoid of a natural ion binding site. We are currently working on techniques to attach lanthanide ions to proteins synthesised in cell-free extracts. Inexpensive cell-free protein synthesis technology is available in-house. It is particularly powerful in combination with the analysis by NMR spectroscopy. As only isotope labelled protein products are observed by NMR, the requirements for protein purity are greatly relaxed.

Labelling proteins with lanthanide tags opens 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, ie. to "zoom" in on a region of a protein and study its

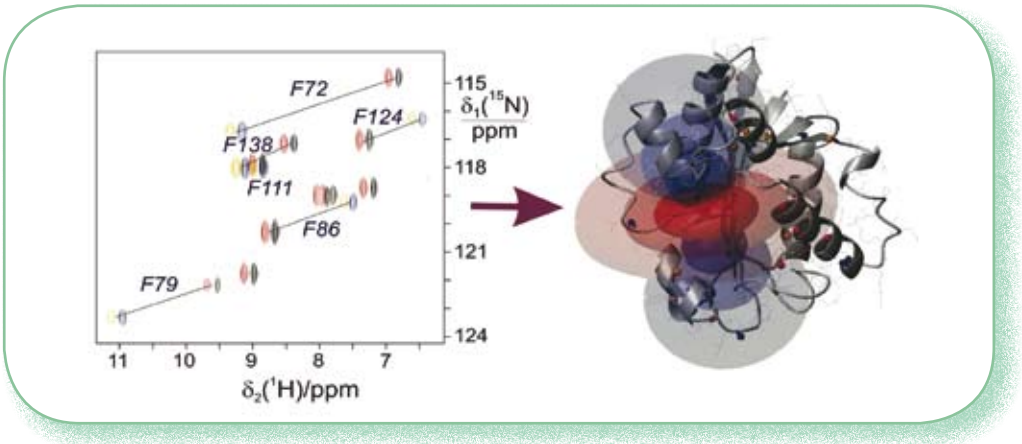


Figure 1: From NMR spectra to resonance assignment, structure determination and interaction studies of proteins. A wealth of structural information is gained by labelling with a paramagnetic ion. Isosurfaces of the anisotropic magnetic susceptibility (blue and red) are superimposed on the structure of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

structure without having to analyse the rest of the protein. It has long been known that lanthanides confer structural information. The lanthanide tagging approach available in the laboratory considerably broadens conceivable applications. 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. Finally, the luminescence properties of some of the lanthanide ions make them suitable probes for distance measurements by FRET. Furthermore, the distance between two lanthanide ions can be measured by EPR. These techniques are extremely sensitive and independent of the molecular weight of the samples.

Structure Determination of a Protein-Ligand Complex Using Paramagnetic NMR

The 3D structure of the 30 kDa complex formed between the *E. coli* proteins epsilon and theta with the small ligand thymidine was determined. One-dimensional NMR spectra recorded of the thymidine yielded sufficient structure restraints to provide an accurate structure of the complex that is closely similar to the structure determined by X-ray crystallography. *(With M John, G Pintacuda, A Y Park, N E Dixon)*

Cell-free Protein Synthesis

The cell-free expression system available in-house was enhanced by a protocol that allows the expression of proteins from linear PCR-amplified DNA. The protein yields achieved with the new protocol are as good as those achieved from conventional plasmid DNA. Site-directed mutations can readily be accommodated by the PCR protocol. The strategy allows going from cDNA to protein NMR spectrum in 24 hours. *(With P S C Wu, K Ozawa, N E Dixon)*

Lanthanide-labelling of Proteins

A generic protocol was developed that allows site-specific tagging of proteins with a lanthanide-binding peptide or organic molecule. The protocol relies on established sulfur chemistry and has been shown to procede with high yields in all proteins tested to date. *(With X C Su, T Huber, N E Dixon)*

Protein Structure Determinations

The 3D structure of the monomeric C-terminal domain of the *E. coli* primase DNA-G was determined by NMR spectroscopy.

SYNTHETIC ORGANOMETALLIC AND COORDINATION CHEMISTRY

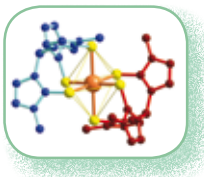
Professor Anthony Hill (Head of Section)

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

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.

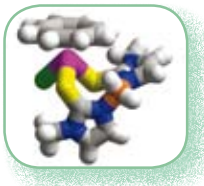
Early Transition Metal Poly(methimazolyl)borate Chemistry

Poly(methimazolyl)borates '$H_xB(mt)_{4-x}$' (x = 1, 2; mt = methimazolyl) are a class of chelating ligands that present two or three 'soft' sulfur donors to a metal centre and as such are especially suited to the later 'soft' transition metals in low oxidation states. The question arises, therefore, as to whether these ligands might also bind effectively to early 'hard' transition metals in high oxidation states. We have begun to explore this possibility and whilst our initial efforts indicated that there were considerable synthetic hurdles associated with attendant redox, hydrolysis and ligand degradation processes, these have now been circumvented. The first examples of complexes of these ligands bound to titanium, zirconium, tantalum and niobium have now been successfully prepared with metals in high formal oxidation states III – V. Selected examples include (a) the first homoleptic titanium complex $[Ti\{HB(mt)_3\}_2]^+$; (b) an alkyne complex of tantalum(III) in which the alkyne (red) binds in a chiral pocket $[TaCl_2(\eta^2\text{-}PhC{\equiv}CPh)\{HB(mt)_3\}]$ and (c) a cyclooctatetraene complex of zirconium $[ZrCl(\eta\text{-}C_8H_8)\{H_2B(mt)_2\}]$ that is devoid of B–H–Zr interactions despite the metal being coordinatively unsaturated. *(With M K Smith)*



(a)

(b)

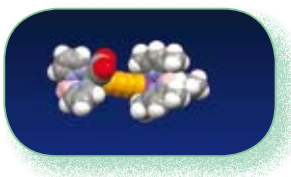


(c)

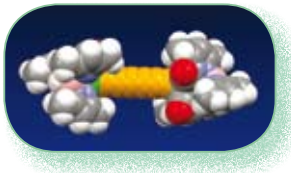
Carbon Wires with Metal-carbon Multiple Bonding

Our recent contributions to this very active field have focused on two features that differ from the vast majority of other studies (i) The construction of bimetallic species separated by odd-numbered carbon chains (L_nMCML_n, $L_nMC_3ML_n$ etc), a situation that requires that at least one of the metal-carbon linkages involves M–C multiple bonding; (ii) the construction of bimetallic species separated by even-numbered carbon chains where *both* metal–carbon linkages involve metal-carbon multiple bonding. Recent examples of the former include the synthesis of tricarbido complexes of tungsten and the metals ruthenium, rhodium, iridium, gold platinum and mercury, e.g. as shown (d) for the complex $Pt[C_3W(CO)_2\{HB(pzMe_2)_3\}]_2(PPh_3)_2$ (pz = pyrazol-1-yl). Examples of the latter are provided by (e) the first structurally characterised dimetallahexatriyne $[MoW(\mu\text{-}C_3)(CO)_2\{HB(pz)_3\}\{HB(pzMe_2)_3\}]$ and (f) the first dimetallaoctatetrayne (polycarbon linkages are shown in orange). *(With R D Dewhurst, M K Smith, A C Willis)*

(d)



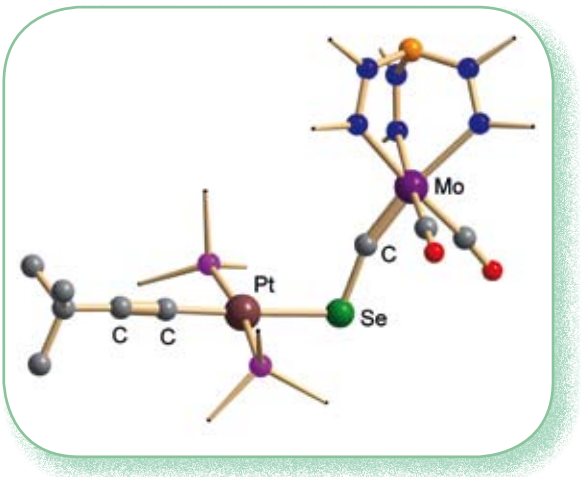
(e)



(f)

Alkynylselenolatoalkylidynes and Related Unsaturated Organoselenium Ligands

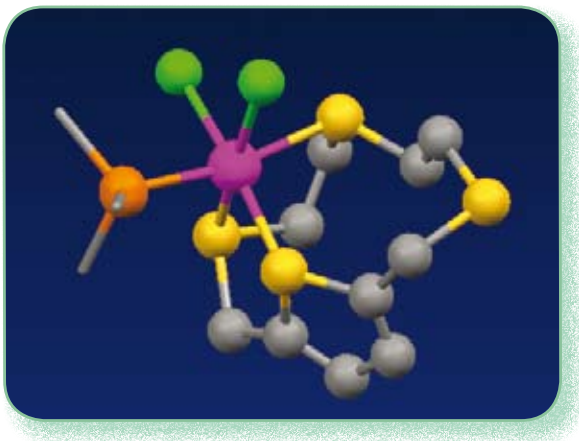
In contrast to the organometallic chemistry of carbon monoxide, that of carbon monosulfide is somewhat limited, whilst there are very few examples (all mononuclear) of complexes involving carbon monoselenide. Continuing our studies on the chemistry of alkynylselenoethers (RSe–C≡CR′) and alkynylselenolates (L_nM–Se–C≡CR′), we have now turned our attention to the study of the previously unknown alkynylselenolatoalkylidyne class of compounds, L_nM≡C–Se–C≡CR. In addition to simple cluster building reactions of these unusual unsaturated species that ultimately leave the L_nM≡C–Se–C≡CR spine intact, we have also encountered remarkably facile reactions that result in regioselective cleavage of one C–Se bond to provide the first examples of 'isoselenocarbonyls', i.e. bimetallic species in which a CSe diatomic unit bridges two distinct metals. The inner coordination geometry of one such complex, [MoPt(μ-CSe)(C≡C*t*Bu)$(CO)_2(PPh_3)_2${HB$(pzMe_2)_3$}], is shown. *(With L M Caldwell, R L Cordiner, A D Rae, A C Willis)*



Alkynylselenolatoalkylidynes and related unsaturated organoselenium ligands

Models for Thiophene Hydrodesulfurisation

The reduction in sulfur dioxide emissions from petrochemical combustion remains a key requisite for adherence to the Montreal protocol. The majority of organosulfur compounds in crude petroleum are thiophene derivatives that may be reduced to hydrocarbons (hydrodesulfurisation) over molybdenum sulfide catalysts doped with a variety of late transition metals including ruthenium. Despite much effort directed towards understanding this heterogeneous process, the vast majority of model studies in homogeneous systems do not involve metal centres in a sulfur-rich coordination environment as would be found on the surface of these sulfided catalysts. We have, therefore, begun to explore the organometallic chemistry of thiophene when bound to hydrodesulfurisation-active metals in which a range of sulfur donors complete the coordination environment. The example shown involves a polydentate macrocycle that combines both a thiophene unit and three thioether donors. Notably, with only three coordination sites available at ruthenium, the thiophene coordinates in preference to one of the thioether groups, which remains pendant. *(With R L Cordiner, A C Willis)*



Models for thiophene hydrodesulfurisation

INORGANIC STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS

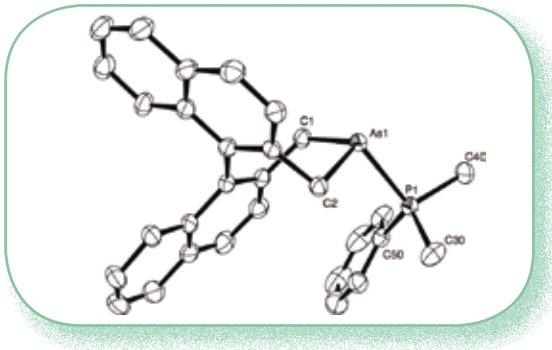
Professor Bruce Wild

http://rsc.anu.edu.au/research/wild.php

Coordination chemistry has merged with catalysis, organic and organometallic chemistry 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.

Chiral Arsenium–Phosphine Complexes

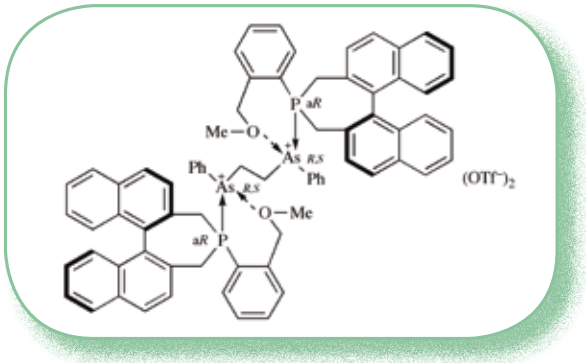
The first enantiomerically pure secondary chloro- and iodoarsines based on the 2,2′-bis(methylene)-1,1′-binaphthyl group have been prepared. The seven-membered (a*R*)-iodoarsepine has been prepared by the disproportionation of the corresponding enantiomerically pure (a*R*)-phenylarsepine with one equivalent of triiodoarsine in boiling toluene. The (a*R*)-chloroarsepine was prepared from the iodoarsepine by metathesis with silver chloride in dichloromethane. The isolation of these novel compounds facilitated an investigation of the interactions between chiral arsenium ions and symmetrical and chiral tertiary phosphines with the view to developing a new asymmetric synthesis of tertiary phosphines by deracemisation. Crystal structure determination on several phosphine-stabilised arsenium salts derived from the (a*R*)-iodoarsepine indicated orthogonal coordination of the phosphine to the trigonal plane of the AsC2 core of the six-electron arsenium ion. The 1H NMR spectra of the phosphine-stabilised salts derived from the (a*R*)-iodoarsepine indicate rapid exchange of the phosphine at 25˚C, but the rate of exchange is reduced when there is a 2-methoxylmethylphenyl substituent on the phosphine because of a moderately strong interaction of this substituent with the phosphorus and arsenic atoms in the complex. *(With N L Kilah)*



Chiral arsenium–phosphine complexes

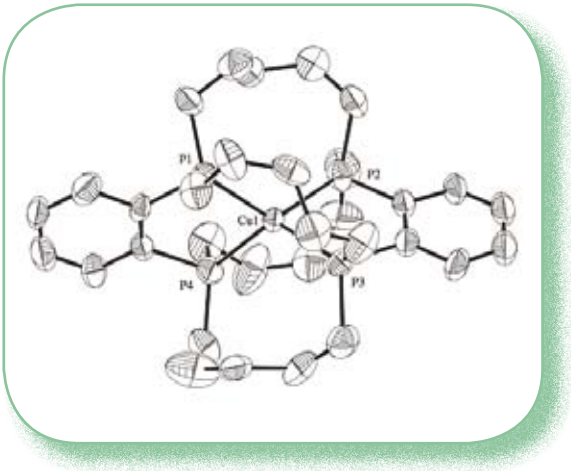
Phosphine-stabilised Arsenium Salts and the Asymmetric Synthesis of Tertiary Arsines

Our work in this area has been extended to the asymmetric synthesis of ditertiary arsines. Thus, the bis(a*R*)-phosphepine-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 Weir)*



A Tetrahedral Cage Phosphine

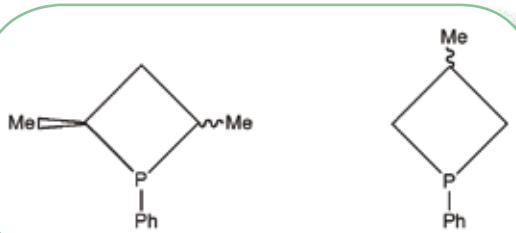
A polycyclic tetra(tertiary phosphine) cage ligand has been synthesised by the spontaneous intramolecular cyclisation of 1,2-phenylenebis[di(4-pentyl)phosphine with 1,2-phenylenebis(phosphine) on copper(I). The mixed-ligand copper complex was generated in acetonitrile by mixing together the corresponding homoleptic complexes and the progress of the redistribution of the ligands was monitored by electrospray mass spectrometry. The copper(I) complex of the cage phosphine has been characterised by $^{31}P\{1H\}$ and ^{63}Cu NMR spectroscopy and X-ray crystallography. Current work is concerned with the synthesis of related complexes with use of Grubbs' catalysts and appropriate homoleptic copper(I) complexes of 1,2-phenylenebis(dialkenylphosphines). *(With K Wells, A C Willis)*



A tetrahedral cage phosphine

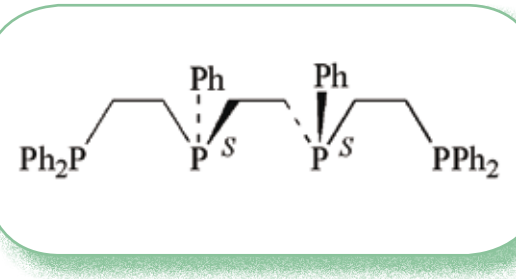
Quantum Chemical Design of Stereoregular Polyphosphines

A number of methyl-substituted phenylphosphetanes have been synthesised for an investigation of the stereoselective synthesis of polyphosphines by free radical polymerisation. Methyl substitution at the 1,3 positions of the phosphetane compared to the parent monomer, but the 2-methyl compound displays a reasonable rate of polymerisation in hot benzene and copolymerisation with oleferic monomers is being investigated. *(With M L Coote, I Maulana)*



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 helicating 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)-$[M_2\{(R,R)\text{-tetraphos}\}_2](PF6)_2$ upon reaction with univalent silver and gold salts and (M)-$[Pt_2\{(R,R)\text{-tetraphos}\}_2](OTf)_4$ 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 δ or λ twist of the ring generates a parallel or double α-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 α-helix conformer of the helicate over that of the parallel helix conformer. *(With P Gugger, A D Rae, A C Willis)*



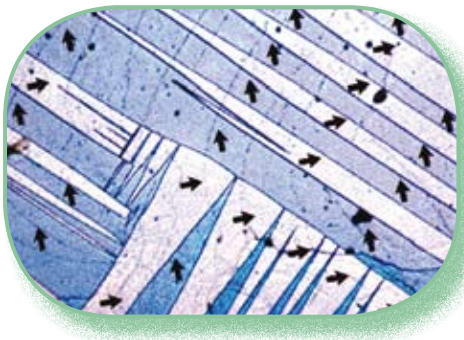
(S,S)-tetraphos

INORGANIC MATERIALS CHEMISTRY

Professor Ray Withers

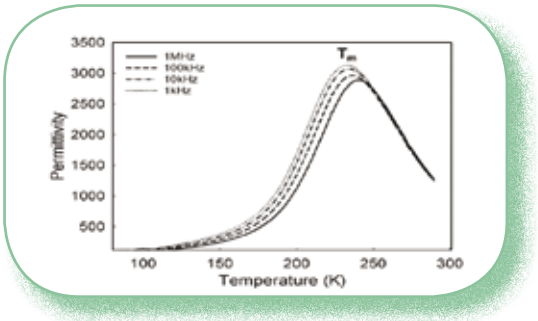
http://rsc/anu.edu.au/research/withers.php

We aim to understand and exploit the factors that determine structure and function in the crystalline solid state. As part of ongoing ARC-funded projects, we are currently particularly interested in polar (ferroic) behaviour in the solid state and the exploitable physical properties associated with it such as ferroelectricity, pyroelectricity, piezoelectricity and dielectric behaviour. We also have long term interests in structured diffuse scattering, crystal chemistry and local order in a wide range of compositionally and/or displacively flexible crystalline phases. Systems investigated include flexible framework structures, ferroic materials, dielectric materials, modulated structures, piezoceramics, microporous molecular sieve materials, non-stoichiometric solid solutions, solid ionic conductors and functional electroceramics. The principal experimental research tools used include a wide range of synthesis techniques (conventional solid state, sol-gel, the use of metallorganic precursors etc), transmission and scanning electron microscopy in combination with powder and single crystal diffraction, as well as physical properties measurements including resistivity, dielectric, pyroelectric, piezoelectric and ferroelectric properties using a recently commissioned aix-ACCT ferroic properties measurement apparatus.



Structurally Frustrated Polar Nano-regions in $BaTiO_3$-based Relaxor Ferroelectric Systems

$BaTiO_3$-doped relaxor ferroelectrics (RF's) exhibit a broad frequency dispersive dielectric constant maxima at a "diffuse phase transition" temperature T_m and a slim P-E ferroelectric hysteresis loop. They have widespread applications as lead-free, electrostrictive and/or piezoelectric sensors and actuators as well as for the electrical field-tuneability of their dielectric properties. RF behaviour has long been attributed to the existence of polar nano regions (PNRs). The nature of these PNR's and their relationship to compositional heterogeneity, however, is still far from well understood. We have recently found direct experimental evidence for inherently polar, displacively disordered 1-d PNR's in four different types of doped $BaTiO_3$ RF compounds in the form of {001}* sheets of diffuse intensity. The role of the dopant ions in these RF systems appears to be to set up random local strain fields suppressing transverse correlations of these <001> chain dipoles and frustrating the development of long range ferroelectric order. Below the freezing temperature of the dipole dynamics, the application of a sufficiently large applied electric field aligns the 1-d PNRs and gives rise to macroscopic spontaneous polarisation. *(With Y Liu, B Nguyen, K Elliott)*



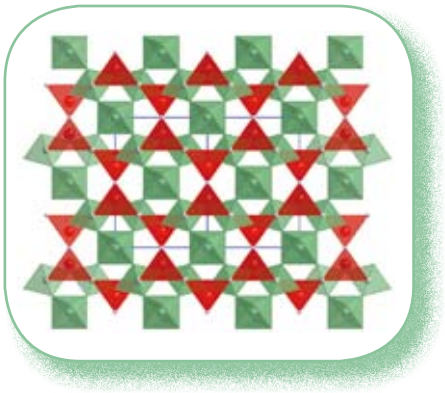
Structurally frustrated polar nano-regions in $BaTiO_3$-based relaxor ferroelectric systems

Precise Diffraction Studies of Temperature-dependent as well as Composition Induced Structural Phase Transitions

As part of an ARC-funded project involving precise diffraction studies of compositionally and/or temperature induced structural phase changes, coupled electron, X-ray and neutron diffraction studies of composition as well as temperature induced structural phase changes in the $NiGe_{1-x}P_x$, $Ni_{3\pm x}In_{1-y}Te_{2+y}$ and $Ba_{4-x}Sr_xNaSb_3O_{12}$ systems have been carried out. Wide range non-stoichiometric solid solutions of average B8 structural type have been identified in the $NiGe_{1-x}P_x$, and $Ni_{3\pm x}In_{1-y}Te_{2+y}$ systems and their (3+1)-d incommensurately modulated structures determined at several distinct compositions. The mechanism allowing compositional flexibility has thereby been identified in both cases. In the 1:3 ordered perovskite $Ba_{4-x}Sr_xNaSb_3O_{12}$ system, diffraction studies have revealed a complex series of temperature and composition dependent phase transitions associated with ordering of the Na and Sb cations on the perovskite *B* site as well as with octahedral tilting. *(With A-K Larsson and L Norén, and C J Howard [ANSTO], B J Kennedy [U Sydney], H Rundlöf [U Uppsala, Sweden], FJ Garcia-Garcia [U Augsburg, Germany])*

The Crystal Chemistry of Misplaced-Displacive Bi-based Pyrochlores

Bi-based, cubic pyrochlore phases have been of considerable interest over recent years as a result of their relatively high dielectric constants and low dielectric losses over a considerable frequency range around room temperature, coupled with their relatively low sintering temperatures, enabling the possibility of co-firing with e.g. Ag electrodes. This combination of properties makes such materials attractive candidates for multilayer capacitor and integrated device applications. The disordered structures and low temperature dielectric relaxation properties of two such misplaced-displacive cubic pyrochlores found in the Bi_2O_3-$M^{II}O$-Nb_2O_5 (M = Mg, Ni) systems, $Bi_{1.667}Mg_{0.70}Nb_{1.52}O_7$ (BMN) and $Bi_{1.667}Ni_{0.75}Nb_{1.5}O_7$ (BNN), have been determined. As for other recently reported Bi-pyrochlores, metal ion vacancies are found to be confined to the pyrochlore *A* site. The B_2O_6 octahedral sub-structure is found to be fully occupied and well-ordered. Considerable displacive disorder, however, is found associated with the $O'A_2$ tetrahedral sub-structure in both cases. *(With Y Liu, H B Nguyen, L Norén, and M M Elcombe [ANSTO], X Wei [Xian Jiaotong U, China])*



A Method for Tuning the Temperature Coefficient of Capacitance of Bi-based Pyrochlore Dielectric Ceramics

Bismuth-based pyrochlore dielectric ceramics possess good microwave dielectric properties and have potential application as multilayer microwave dielectric components. The electric field tunability of the dielectric constants of this Bismuth-based pyrochlore family also make them potentially useful as frequency agile RF/microwave components. To date, however, the relatively poor temperature stability characteristics of the dielectric properties of these Bismuth-based pyrochlore ceramics is a significant limitation to their widespread use. As part of an ongoing ARC-funded project, we have developed a method to tune the temperature coefficient of capacitance of these promising bismuth-based pyrochlore ceramics to a close to zero value without significant deterioration of their original dielectric properties. A provisional patent based on this method has been filed.

SYNTHESIS AND MECHANISM

Professor Martin Banwell (Head of Section)

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

The group's activities continue to be 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), quinine (the famous anti-malarial alkaloid), various Amaryllidaceae alkaloids (e.g. lycorine, galanthamine and nobistiline A) and the potent new antibiotic platencin represent key targets and have inspired a considerable number of methodological studies. Australian industry has funded a significant portion of our work, while a new collaboration has just started with the German-based company BASF and is focused on developing novel agrochemicals based on marine natural products found in the cooler parts of the southern hemisphere oceans.

Other research highlights include:

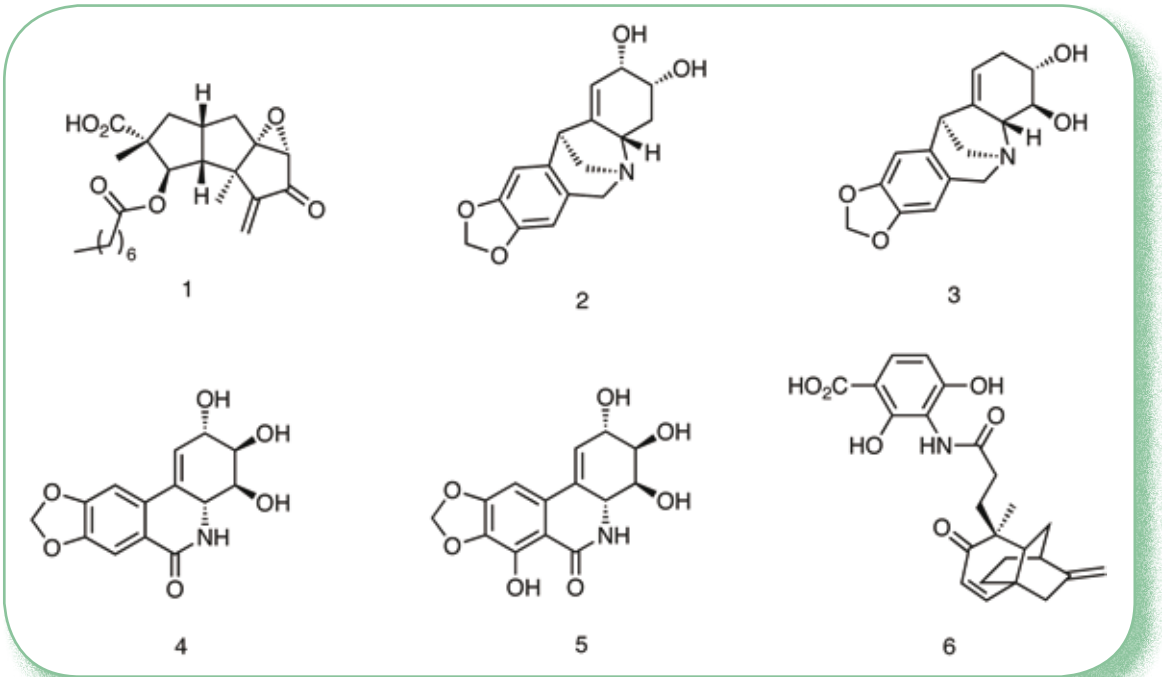
(i) the completion of a chemoenzymatic total synthesis of the triquinane-type natural product phellodonic acid (**1**), a fungal metabolite possessing powerful anti-bacterial properties;

(ii) the completion of a total synthesis of the non-natural enantiomeric forms of the montanine alkaloids brunsvigine (**2**) and nangustine (**3**);

(iii) the completion of total syntheses of the non-natural enantiomeric forms of the alkaloids lycoricidine (**4**) and narciclasine (**5**);

(iv) the completion of total syntheses of most members of the tamjamine family alkaloids, some of which are expected to possess potent immunosuppressive properties;

(v) the identification of a new method for constructing annulated pyrroles;



(vi) the rapid assembly of the tricyclic framework associated with the potent antibiotic platencin (**6**);

(vii) the exploitation of the palladium[0]-catalysed Ullmann cross-coupling reaction in the generation of oxindoles.

During the course of the last two years, a number of group members reached significant milestones and/or received important recognition for their research efforts. For example, Drs Michael Harvey, Dan Beck, Pauline Stanislawski, Jasmine Jury and Martin Friend each received PhD degrees while Mr Okanya Kokas has submitted his thesis and the examination process has been completed. Pauline has been awarded a Johnson&Johnson Postdoctoral Fellowship that is enabling her to work at the company's laboratories in Belgium. Martin has joined the pharmaceuticals manufacturing company IDT based in Melbourne while Dan is now with IP Australia having spent a period as a researcher with Novartis in Basel, Switzerland. Shortly, Okanya will move to Imperial College, London to take up a Postdoctoral appointment with Professor Tony Barrett FRS. Jasmine will move to a Postdoctoral position at the University of Wollongong where she will work with Professor Steve Pyne. Another member of the group, Andrew Phillis, has joined GSK's manufacturing facility in Singapore, whilst two former Postdoctoral members of the group, Drs Muriel Bonnet and Christian Bluechel, have also secured positions in the same country. Two former members of the group have recently taken up academic appointments - Dr Scott Stewart is now working at The University of Western Australia and Dr David Lupton at Monash University. Dr Rajeev Menon has been awarded an ARC Postdoctoral Fellowship (APD) that will allow him to continue his work.

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. 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 abovementioned alkaloids as well as the antibiotic platencin. *(With K A B Austin, K Ban, C Bluchel, D Bon, J S Foot, M P Friend, A Gebert, J Jury, O Kokas, X Ma, T Reekie, R White, and J Lambert [Biota Pty Ltd, Melbourne], G Whited [Genencor International Inc, Palo Alto])*

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. Certain work in this area has focused on attempts to mimic the key bond-forming events associated with the proposed biogenesis of the marine alkaloids known as the lamellarins. *(With A Augustine, L Axford, T Bilski, A Bissember, M Eyles, M J Harvey, K Hasse, K Holden, M Jones, J Kitching, A Lehmann, R Menon, D Offermann, D Pinkerton, P Sharp, P Stanislawski, J Zhou, and M Garson [U Qld], C Parish [JCSMR, ANU], J Renner [BASF], A Stewart [Cryptopharma Pty Ltd])*

BIOCHEMICAL REACTIONS AND MOLECULAR RECOGNITION

Professor Chris Easton

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

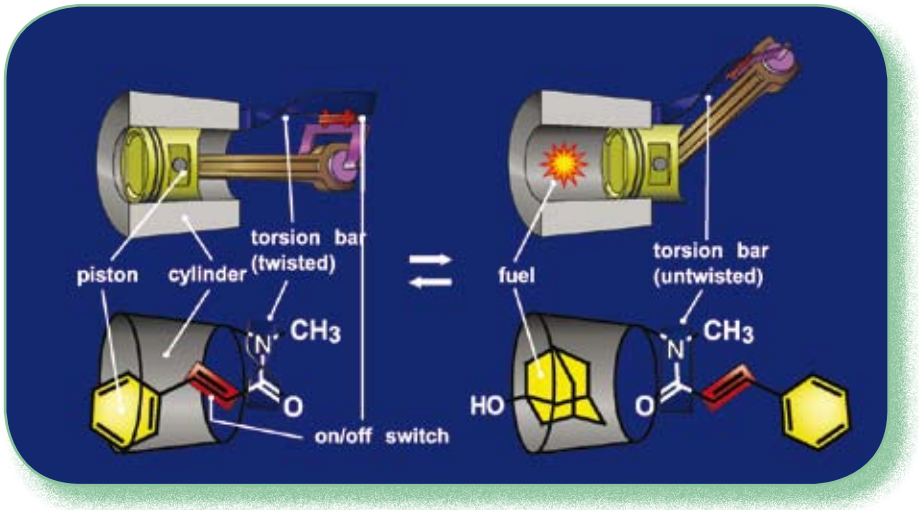
We study biochemical reactions in order to better understand the origin of a variety of disease states, with a view to producing methods for their prevention and treatment. This involves, for example, the development of enzyme inhibitors to down-regulate, and pro-hormones to up-regulate, the biosynthesis of peptide hormones in higher organisms. Our work in this area is also concerned with comprehending the evolution of biochemical systems in addition to the development of enzymes as catalysts with novel functions and mechanisms of action. Other studies involve supramolecular chemistry and molecular recognition, and include the design, synthesis and evaluation of molecular hosts, as the basis of catalysts, molecular reactors and devices, and photochemical and thermal switches. Further research concerns the development of improved resins and manufacturing processes for reconstituted wood products.

This research continues to be supported through the ARC Centre of Excellence in Free Radical Chemistry and Biotechnology, and the CSIRO Emerging Science Initiative in Synthetic Enzymes for Synthetic Chemistries.

Highlights of the research during 2006-2007 included the following.

i) The design and synthesis of a molecular piston as a working nanomachine having a photochemical on/off switch. The energy of molecular recognition is harnessed to drive the machine in what is a first example of a molecular device performing work at the molecular level. This research was reviewed as a "Highlight of Australian Chemistry" in the April 2007 issue of *Chemistry in Australia* and is summarised in a "Research Profile" in the text "Chemistry", A. Blackman *et al.*, eds., Wiley and Sons, Australia, 2007.

ii) The identification of a novel fatty acid that reduces inflammation. This is based on earlier work in the group on the synthesis of β-oxa- and β-thia-fatty acids as selective inhibitors of particular fatty acid metabolic pathways. The commercial potential of these compounds is being explored through the biotechnology company, New World Bio Ltd., with the assistance of AusIndustry.



Schematic comparison of mechanical and molecular pistons

iii) The development of a photo-responsive molecular muscle and related molecular shuttles and sensors, as well as the controlled formation of molecular wires in aqueous solution, as well as in the solid state. New methods and techniques have been developed for the synthesis and study of these species, using 2D NMR spectroscopy and X-ray crystallography, and the focus is now on producing systems that are capable of performing work or are suitable for incorporation in microelectronic devices.

iv) The preparation of new fluorescent tags to study the distribution of resins in reconstituted wood products. As a complement to earlier research on the development of improved resins, this work aims to improve the use of those resins.

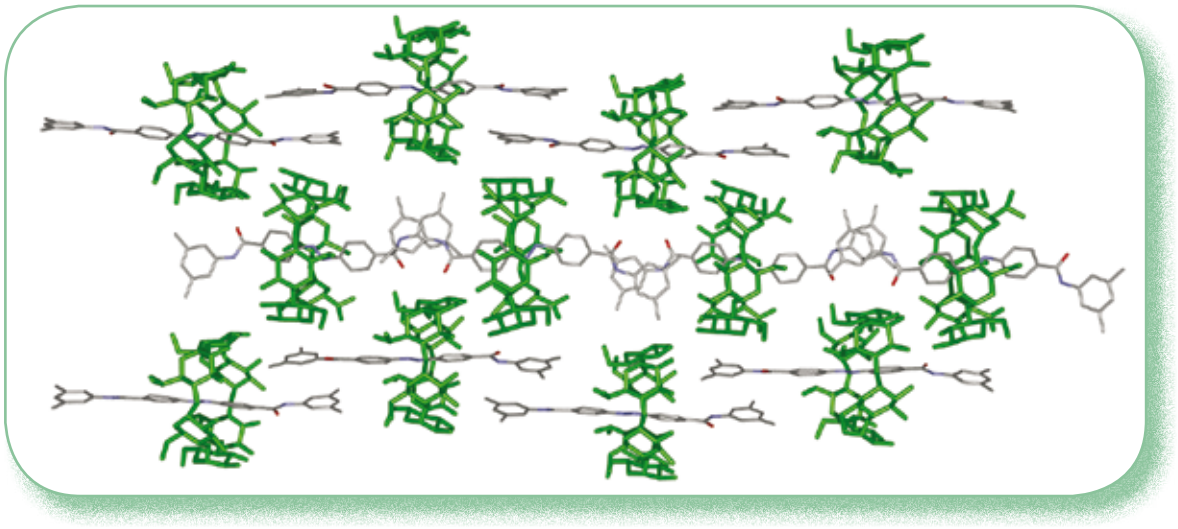
v) The discovery of the peculiar resistance of amino acids and peptides towards certain types of radical degradation. This is likely to have contributed to the evolution of peptides as biopolymers, as well as account for the preponderance of particular types of amino acids in peptides that function in oxidatively stressful environments.

vi) The production of new molecular reactions vessels as catalysts for nitrile oxide cycloadditions.

vii) The preparation of novel amino acid derivatives that function to provide photochemical, oxidative or hydrolytic release of peptide hormones.

viii) The biomimetic synthesis of oxazoles and related natural products through electrolysis of amino acid derivatives.

ix) The development of new approaches for studying radical reactions combining gas and solution phase studies and theroretical calculations.

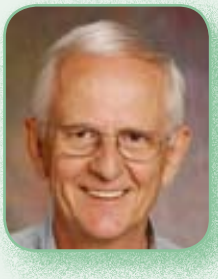


Aligned and insulated molecular wires formed by a cyclodextrin rotaxane in the solid state

ORGANIC SYNTHESIS

Emeritus Professor Lew Mander

http://rsc.anu.edu.au/research/mander.php



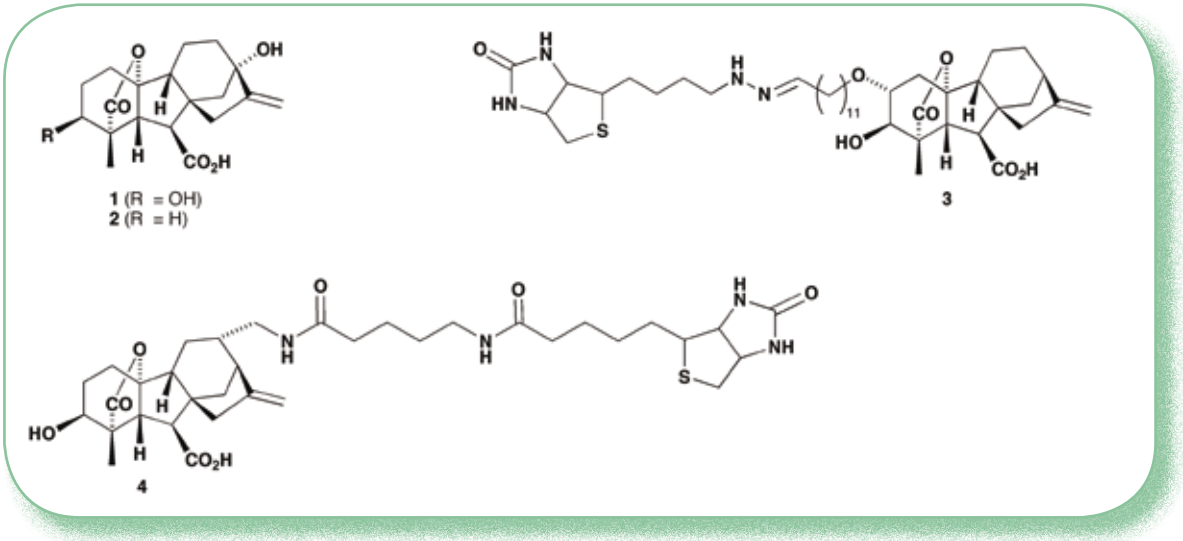
Our research interests are concerned primarily with methods and strategies for the synthesis of complex natural products that have interesting biological properties. Within this context, members of the group have successfully completed syntheses of numerous complex natural products and developed a number 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). Gibberellins 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.

The Search for Gibberellin Receptors

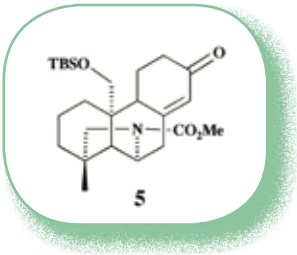
In order to understand more fully the molecular basis of gibberellin bioactivity, we are presently attempting to identify receptors in barley. In October 2005, a paper in the journal *Nature* reported the isolation and expression of a protein from rice with evidence that it was a gibberellin receptor. With the sequence information from this report we have been able to clone and express an analogous protein (GSE 1) from barley. The availability of this protein has allowed us to undertake *in vitro* binding studies with gibberellins. We have demonstrated binding between the GSE 1 protein and 14C-labelled GA1 **(1)**, whereas no binding was observed with the bio-inactive GA20 **(2)**, as would be expected. We have also prepared a series of gibberellins linked to biotin, namely **(3)** and **(4)**, but they proved to be biologically inactive *(With K A Fairweather, S M McAteer, L C Axford, B Twitchin)*

Total Synthesis of Natural Products

Following the formal retirement of the group leader in November 2002, the Synthesis group has been slowly wound up. The last of the Postdoctoral Fellows and students departed in February 2007, with the termination of the natural product synthetic program. The last "instalments" have been the preparation of



the advanced intermediate **(5)** for the synthesis of the alkaloid nominine **(6)**, and the formal total synthesis of diisocyanoadociane **(7)**, a potent antimalarial isolated from a Barrier Reef sponge. *(With O E Hutt, K A Fairweather)*



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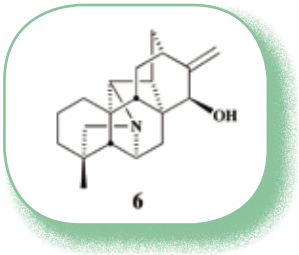

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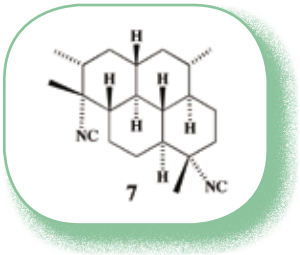

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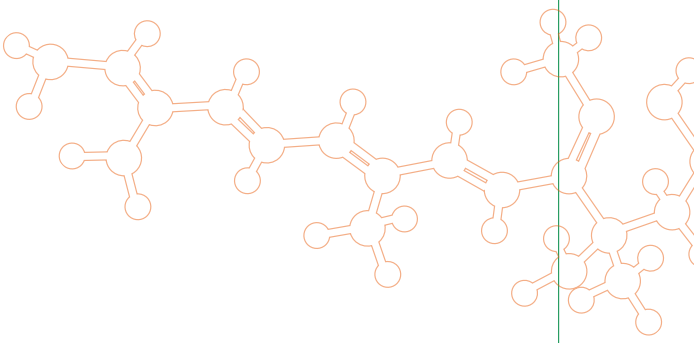
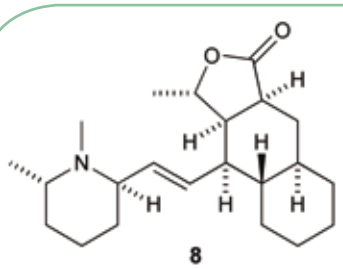
Biosynthesis of the Galbulimima Alkaloids

Several decades after the isolation and structural elucidation of the Galbulimima alkaloids there has been renewed interest in their synthesis and biosynthesis. Of particular interest is the biosynthetic relationship between the various structural types, namely **(8)**, **(9)**, **(10)** and **(11)**. We have therefore commenced a search for minor alkaloids that may prove to be "missing links" between the various skeletons. Thus far we have isolated two new alkaloids that appear to be derivatives of **(9)**. *(With A J Herlt)*





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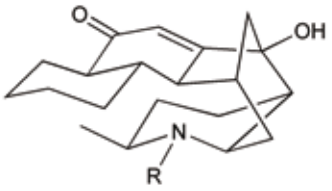

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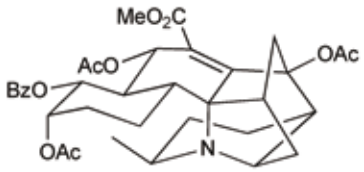


11

ORGANIC SYNTHESIS, METHODOLOGY AND HOST-GUEST CHEMISTRY

Associate Professor Mick Sherburn

http://rsc.anu.edu.au/research/sherburn.php

Domino reactions are spectacular events in which many bonds are made and broken in a single step. The reactions hold much promise for achieving more efficient syntheses - a pressing need in times of increasing production costs and 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. The 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.

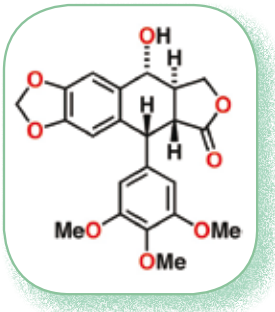
Efficient Total Synthesis of Medicinally-important Natural Products

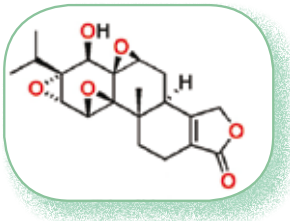
Lignans, like podophyllotoxin, have cancer-fighting properties and are used in chemotherapy. An efficient and highly modular approach for the synthesis of lignan natural products has been developed, culminating in several total syntheses, including that of podophyllotoxin. The approach involves a late stage domino radical reaction. Our 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 structures from simple, unsaturated, acyclic precursors using sequences of Diels–Alder reactions. Applications of these processes in total synthesis are being investigated. In 2007 we completed the shortest total synthesis of the natural product triptolide, which shows great potential in medicine due to its myriad biological activities.

Significant progress has also been made towards the natural product viridin, a particularly challenging structure that we have been targeting since 2003. *(With G Bojase, T A Bradford, L Carpinelli, C Gray, L C H Kwan, I Louis, N A Miller, A D Payne, E L Pearson, D Robinson, E Wiadrowski)*

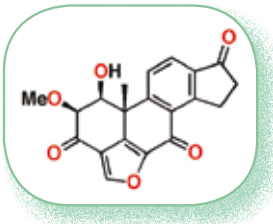
Podophyllotoxin





Tripolide

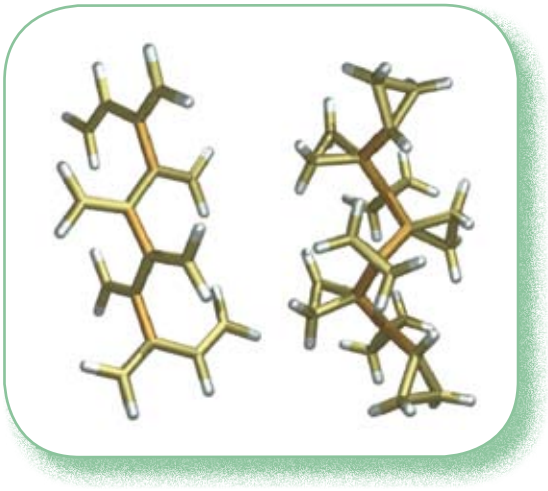
Viridin



Fascinating New Hydrocarbon Structures

Chemists are often inspired by nature's chemical structures to develop syntheses. Sometimes, structures not produced naturally initiate the development of exciting new methods, concepts and principles. Our interest in this area is focused on the dendralenes, one of the four fundamental classes of conjugated hydrocarbon structures. In earlier studies, we reported the first chemical synthesis of this hydrocarbon family, previously believed to be too unstable to prepare. One of our major advances in this reporting period includes the first practical synthesis of [5]dendralene and a demonstration of its use in the rapid formation of different polycyclic frameworks. Upon publication, the

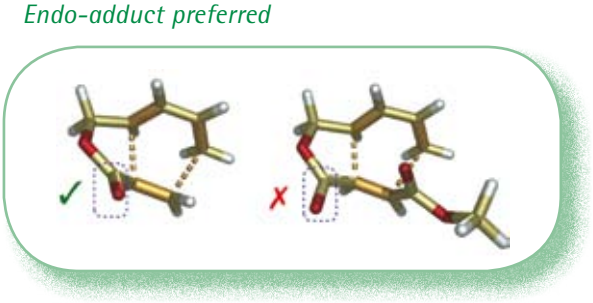
work was selected as a "Hot paper" by the editors of *Angewandte Chemie*. Another important development involves the preparation of the first saturated hydrocarbon with a helical structure. We have also uncovered new and unexpected reactivity patterns of these fundamental compounds. The results have led to a better understanding of the stability and reactivity of unsaturated organic compounds in a more general sense. *(With A Alborzi, G Bojase, T A Bradford, T Fallon, N A Miller, E L Pearson, A D Payne)*



Fascinating hydrocarbons

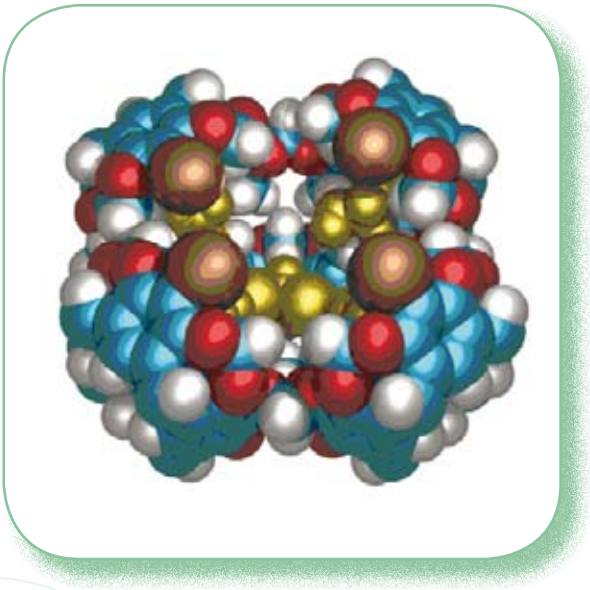
A Deeper Understanding of the Most Important Organic Reaction

The Diels–Alder reaction is one of the most powerful and 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, A Longshaw, W Lording, E L Pearson, R J-P Tripoli, and M N Paddon-Row [UNSW])*



Host-Guest Chemistry

Research in this area is concerned with the design and synthesis of our "superbowl" host molecules for molecular recognition, complexation and catalysis. Superbowls are a new class of synthetic hosts with non-collapsible interiors. Major advances in 2006-07 include the synthesis of new types of superbowl container molecules with different internal dimensions. We have also demonstrated, for the first time, that superbowl molecules selectively encapsulate certain medicinal agents. *(With M W Carland, C Gray, N Kanizaj, T V Nguyen, D J Sinclair)*



A superbowl molecule

THEORETICAL CHEMICAL PHYSICS

Professor Michael Collins

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

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 electronic energy of a molecule for any geometry. The way that atoms move during a chemical reaction is determined by how the electronic energy changes as the shape of the molecule changes. To understand the mechanism of a chemical reaction (how the atoms move) we need to know the electronic energy for all the possible molecular shapes (which is a potential energy surface or PES). The PES is constructed as an interpolation of the *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.

(i) We are developing methods to study chemical reactions that take place in multiple electronic states, such processes are dominant factors in photochemistry. 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.

(ii) 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 principle 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 Professor Dong Hui Zhang at the Chinese Academy of Science in Dalian, Professor David Yarkony at Johns Hopkins University (Nonadiabatic Dynamics), Professor Geert-Jan Kroes at the University of Leiden (Reaction at Surfaces), Professor Mark Gordon at Iowa State University, and Assistant Professor Ryan Bettens at the National University of Singapore.

Hydrogen Abstraction in X• + CH_4

The abstraction reactions, X• + RH ´ XH + R•, where X = H, F or Cl, are important in many contexts, including combustion. In collaboration with Professor Zhang, PES and quantum scattering calculations of the reaction cross sections and their dependence on the initial state of the reactants are being evaluated. 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. *(With D H Zhang [Chinese Academy of Science])*

Nonadiabatic Chemical Reactions

Many reactions, particularly in photochemistry, combustion, atmospheric and interstellar 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.

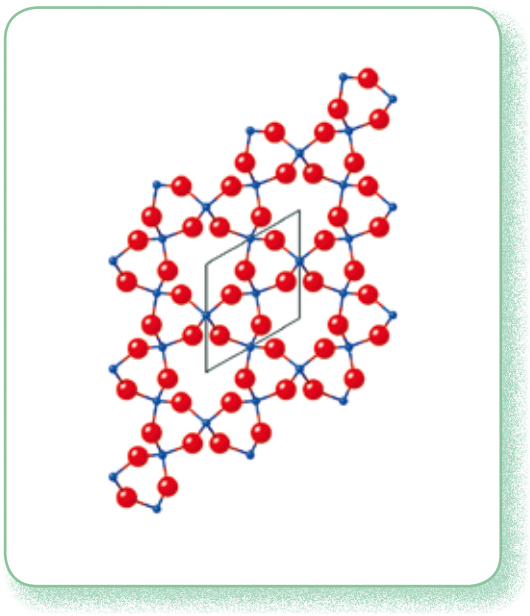
The code development for the general multi-state case is mostly completed, and is currently being tested for reactions involving H + H_2 , H_2 + H_2+, and OH(2Â) + H_2. *(With C Evenhuis, O Godsi, and D H Zhang [Chinese Academy of Science], D Yarkony [Johns Hopkins U, USA])*

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, we can calculate thermochemical properties and, in principle, the complete PES that 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. A general computer code has been developed to implement this approach to evaluate molecular energies and energy gradients (and higher derivatives in some cases) and perform geometry optimisation. This approach has recently been applied to the construction of complete PES for polyatomic reactions (for example, $H + CH_3(CH_2)_3CH_3$), opening the possibility for detailed dynamics studies of reactions of large molecules. Further development of the methodology has concentrated on the approximation of the relatively weak long-range interactions between well-separated segments of molecules, in collaboration with Professor Mark Gordon *(Iowa State U)* and Professor Peter Gill. *(With V Deev)*

Ab Initio Quantum Chemistry of Crystals

The method we have developed to approximate molecular energies has been applied to estimating the energies (and free energies) of crystals. A new approach has been developed that fragments a crystal structure into relatively small components under periodic boundary conditions. The method has been demonstarted by application to several crystal structures of SiO_2. *(With H Netzloff, and M Gordon [Iowa State U], M Jordan [U Sydney])*



A representation of the crystal structure of α-quartz. The energy of the infinite crystal is estimated from the energies of small fragments of this structure.

COMPUTATIONAL QUANTUM CHEMISTRY, POLYMER CHEMISTRY

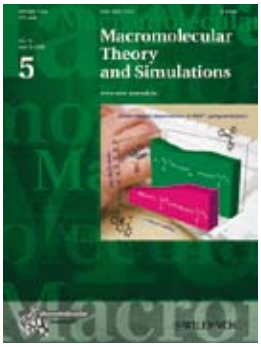
Dr Michelle Coote

http://rsc.anu.edu.au/research/coote.php

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 particular interest is in the area of radical chemistry, especially radical polymerisation. We are interested in identifying and developing cost-effective theoretical procedures for studying these difficult reactions, and then using them in mechanistic studies so as to design new and improved chemical reagents. We work very closely with experimental research groups who put our computational designs into practice. In recent years, our computational studies have led directly to the development of two new classes of reagent for controlling free radical polymerisation and a new route to polyphosphines, which highlights the growing potential of computational chemistry as a practical tool for the polymer field.

Accurate Computational Methods

Applying quantum-chemical methods to the reactions of larger molecules, such as in free radical polymerisation, 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. To address this problem, we have designed a reliable low-cost methodology for studying radical reactions that involves the use of an *ab initio* version of the ONIOM method, the design of small model reactions capable of mimicking the kinetic behaviour of their larger counterparts, and additional cost-saving measures such as our new efficient algorithm (called Energy-Directed Tree Search) for exploring the conformational space of larger molecules. We have demonstrated that our computational methodology delivers chemical accuracy for radical polymerisation kinetics, radical thermochemistry in general, and the prediction of one- and two-electron redox potentials of a range of biologically active species. We have also combined *ab initio* calculations with kinetic modelling techniques, so as to produce the first *ab initio* simulation of an entire polymerisation process from first principles. In a proof-of-principle study, we modelled initialisation in RAFT polymerisation, demonstrating excellent agreement between theory and experiment.



Macromolecular Theory and Simulations

Free Radical Chemistry

Free radicals contain an unpaired electron and as such are often highly reactive species that are utilised in many chemical and enzymatic reactions, and can also participate in a wide range of unwanted processes such as the degradation of materials and oxidative

damage to peptides. Our group is part of the ARC Centre of Excellence for Free Radical Chemistry and Biotechnology, and we have been working with other Centre members to study both fundamental aspects of radical reactivity and applications in chemical synthesis and biological processes. One of our current interests are nitroxide radicals, which are stable free radicals capable of acting as antioxidants in biological systems and materials, and as control agents in free radical polymerisation. We have recently studied the effects of substituents on their electrochemistry and radical trapping abilities, and are working with Professor Bottle (Queensland University of Technology) to use this information to identify structural improvements. We are also working with synthetic chemists to find new and improved tin-free chain carriers for organic synthesis. With Professor Zard (Ecole Polytechnique) we have been studying the kinetics and thermodynamics of reactions mediated by xanthic anhydrides, while with Associate Professor Sherburn we have been investigating tris(trim ethylsilylmethane) and derivatives of ethyl piperidinium hypophosphate. We have also been working with a team led by Professors Radom and Easton to study hydrogen atom transfer in peptide radicals, and also in coenzyme B-12 mediated reactions.

Controlled Radical Polymerisation

In recent years, the polymer field has been revolutionised by the development of techniques for controlling the molecular weight and architecture of the polymer produced in free radical polymerisation. We have been using quantum chemistry to study the mechanism and kinetics of these techniques with a view to designing improved control agents for 'difficult' monomers, such as ethylene. Our early studies focused on the Australian-invented RAFT process and this work culminated in the development and patenting of the first multipurpose RAFT agent, capable of controlling monomers with disparate reactivities. Our studies of the intermediate radical in the process also led to the discovery (in collaboration with Professor Barner-Kowollik, UNSW) of a new method for controlling free radical polymerisation using thioketone spin traps. We are now working with the inventor of Atom Transfer Radical Polymerisation (ATRP), Professor Matyjaszewski (Carnegie Mellon), to study the mechanism of ATRP with a view to improved catalyst selection and design. Recently, we highlighted the important role of penultimate unit effects on the initiation step of this process and demonstrated that, for the alkyl halides relevant to ATRP, outer-sphere electron transfer occurs preferentially via dissociative electron transfer.

Chemical Communications

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. Recently, 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. Experimental studies in the group of Professor Wild indicated that polymerisation was possible but the monomers were very reactive and thus difficult to handle. To address this problem, we have been investigating the effects of various ring substituents on the polymerisation rates, and have now designed a number of less reactive monomers that are currently undergoing experimental testing.

LIQUID STATE CHEMICAL PHYSICS

Professor Denis Evans

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

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.

In 1990 we derived the first exact, practical link between chaotic measures (namely Lyapunov exponents), and thermophysical properties. The 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 spontaneous entropy production is a negative rather than a positive value, as 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.

In 2006 we proved a new mathematical theorem: the Dissipation Theorem. The theorem shows that time-dependent fluctuations in the central argument of the Fluctuation Theorem, can be used to calculate exact expressions for the nonlinear response in nonequilibrium systems.

Experimental Demonstration of Fluctuation Theorems in Viscoelastic Media

This experimental work was carried out in collaboration with Associate Professor Sevick's group. There have now been a large number of experimental confirmations of the Evans-Searles FT. In every case, however, the system studied could be accurately modelled by the Langevin Equation with white noise. This work gave the first experimental confirmation of the FT for a system that cannot be modelled by such an equation. *(With D M Carberry, M A B Baker, E M Sevick)*

Deterministic Fluctuation Theorem (FT) Applied to Glassy Systems

We applied the FT to glassy 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 computer 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, are 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.

Statistical Mechanics of Non-dissipative Non-equilibrium States

Following on from our work on the application of the FT to glassy systems, we have developed a quantitative statistical mechanical theory that can be applied to nonergodic, time-independent, non-dissipative, non-equilibrium systems. The theory requires that the ergodic subdomains, into which these systems decompose themselves, should be *robust* with respect to small but finite changes of macroscopic state variables and fields. We show that the ergodic consistency condition required by the Evans-Searles FT provides an independent check on the robustness condition.

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* both the Evans-Searles and the Crooks Fluctuation Theorems. This derivation proves that the ensemble average of 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 tested the Second Law Inequality using molecular dynamics simulations of oscillatory shear in the linear regime. The Second Law Inequality is valid for time averaged entropy production. We observe that the ensemble average of the instantaneous entropy production is negative for various time intervals.

Time Reversibility is a Necessary Condition for the Fluctuation Theorem

It has long been known that ergodic consistency and time reversibility are sufficient conditions for the Evans-Searles FT to hold. In this work, we demonstrated numerically that these conditions are in fact necessary conditions for the FT to hold in deterministic systems.

The Dissipation Theorem

Late in 2006 we derived a new and very widely applicable theorem for nonequilibrium statistical mechanics. This theorem shows that the argument of the Evans-Searles FT is also central to nonlinear response theory. The ensemble-averaged response of an arbitrary phase function is related to the time integral of the transient time correlation function formed by ensemble averaging the product of the dissipation function evaluated at time zero (the initial state) and the phase function being studied, as a function of time. This expression for the time dependent response is exact arbitrarily far from equilibrium. It applies to all types of nonequilibrium systems including those for which there is an explicit external field driving the system away from equilibrium, and it is also the case where the nonequilibrium state is generated by an initial distribution that is not preserved by the dynamics. The theorem shows that the dissipation function is the central function for nonequilibrium statistical mechanics. The close to equilibrium dissipation theorem reduces to the well-known expressions of linear response theory.

THEORETICAL QUANTUM CHEMISTRY

Professor Peter Gill

http://rsc.anu.edu.au/research/gill.php

Quantum chemistry is the discipline in which the laws of quantum mechanics are applied to understand and predict molecular behaviour. 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.

Intracules, Conjectures and the Correlation Problem

One of the most urgent and important issues in quantum chemistry is the electron correlation problem. We have been working for several years to develop a paradigm in which the correlated motion of electrons can be understood through their two-electron probability densities, or intracules. During 2006 and 2007, we published five papers on this topic, 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 ω. Through systematic computational studies, we have shown that the correlation energies of atoms can be predicted very accurately but that molecules with small HOMO-LUMO gaps are more difficult to treat. We are determining the reasons for this so that we can then improve our models appropriately. *(With D L Crittenden, E E Dumont, D P O'Neill, and N A Besley [U Nottingham, UK])*

Q-Chem 3.0 Software Package

New quantum chemical methodology is of little use until it has been implemented into a software package that research workers can use. With this in mind, we have recently released Version 3 of the *Q-Chem* package, which is used by many groups around the world, and which is the computational engine inside the popular *Spartan* software package. As well as benefiting the scientific community, it also provides an excellent mechanism by which the work of students and postdocs can be made available, quickly and efficiently, to an international audience. *(With A T B Gilbert, D P O'Neill, C Y Lin, S H Chien, and N A Besley [U Nottingham, UK], A I Krylov [U Southern California, USA], H F Schaefer III [U Georgia, USA], M Head-Gordon [U Berkeley, USA])*

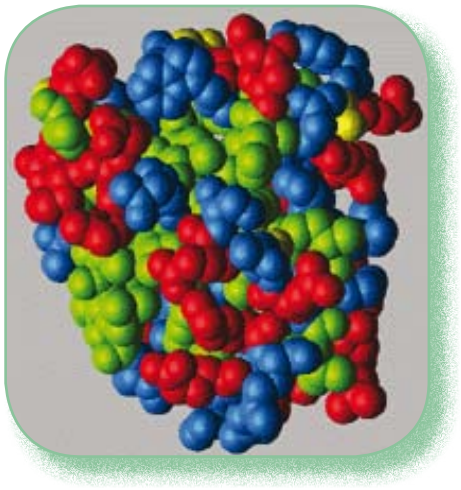
Q-CHEM

We have also developed an interface between the *Q-Chem* and CHARMM packages, allowing researchers to study very large chemical systems using a mixture of quantum mechanics and molecular mechanics. This has allowed us, for example, to investigate the mechanism of the chorismate mutase catalysed Claisen rearrangement. *(With A T G Gilbert, and H L Woodcock III [National Institutes of Health, USA], H F Schaefer III [U Georgia, USA])*

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, but none are entirely satisfactory. We have recently extended our method, which finds charges that

reproduce as many of the low-order multipole moments of the system as possible. Our algorithm is capable of dealing with very large molecules and is particularly beneficial for biochemical systems. *(With A T B Gilbert)*



Multipole–derived atomic charges

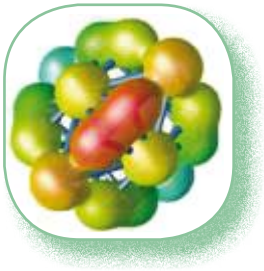
Linear-scaling Statistical Permutation Tests

In 1935, the statistician Sir Ronald Fisher introduced a class of statistical significance tests that are theoretically excellent but computationally very demanding. Until now, this has limited their practical usefulness, but we have discovered a radical new approach that allows the Fisher test to be performed at a cost that scales only linearly with the number of statistical data, thus rendering it practically feasible even for very large datasets. We hope to use a similar strategy to reduce the cost of electron correlation methods, such as Full CI.

Sir Ronald Fisher

DFT on Transition-metal Clusters

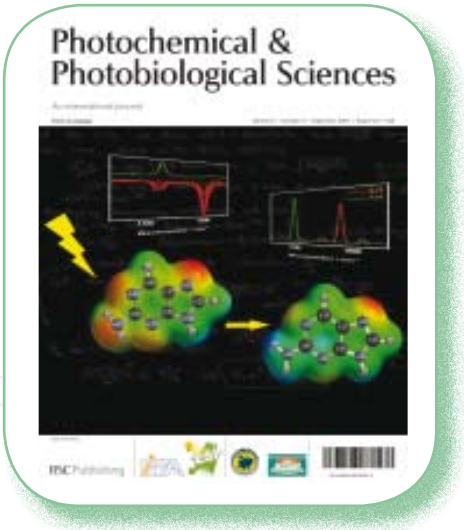
Density Functional Theory (DFT) has become extremely popular in computational chemistry, but it is far from perfect and, in particular, its accuracy depends on the exchange-correlation functional that is employed. We have constructed a new functional, BFW, which is explicitly designed for transition-metal clusters, such as the notoriously difficult "metcars". Tests on a variety of clusters showed that BFW is more accurate than the widely used B3LYP functional. *(With A T B Gilbert, and M A Addicoat [U Adelaide])*



Transition–metal cluster

Models for DNA Damage

2-aminopurine (2AP) is a DNA base analogue with a structure similar to that of adenine and guanine, and has been used as an internal fluorescent probe for the study of DNA solvation and structural dynamics. We have performed DFT calculations to aid in the assignment of intermediates observed in picosecond time-resolved infrared spectroscopy following the two-photon ionisation of 2AP in neutral and acidic aqueous solutions. Our results shed light on the nature of the species formed when DNA is damaged by radiation. *(With C Y Lin, and M W George [U Nottingham, UK])*

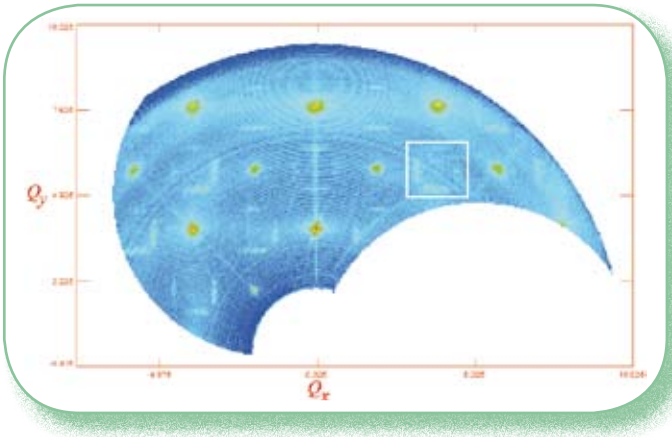


STRUCTURE AND MAGNETISM OF MATERIALS

Dr Darren Goossens, AINSE Research Fellow

http://rsc.anu.edu.au/~goossens

A material's properties must ultimately arise out of its structure. A key aspect of materials physics and chemistry lies in exploring this relationship. We use a combination of experimental techniques including neutron, X-ray and electron diffraction, and computational modelling to explore the structures of materials and relate the structures to the physical and magnetic properties. Through links with The Australian Institute of Nuclear Science and Engineering (AINSE), we particularly make use of neutron diffraction at the Bragg Institute at the OPAL reactor (ANSTO, Sydney) and the ISIS spallation neutron source (UK), as well as synchrotron X-ray sources. Many materials undergo structural phase transitions in which the crystal structure changes as a function of, for example, temperature or pressure.



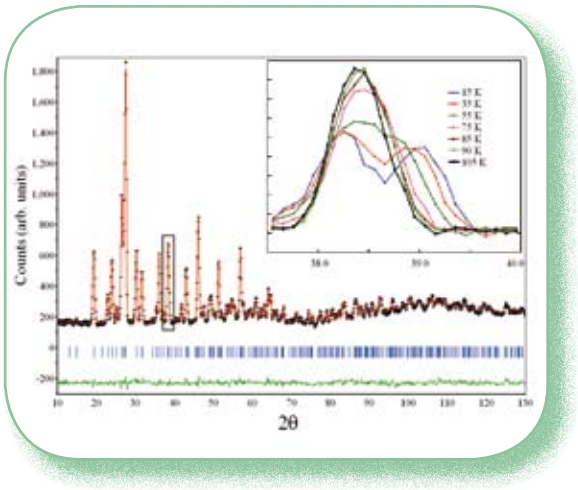
Preliminary neutron diffuse scattering from $Cu_{1.8}Se$, measured using the WOMBAT diffractometer at the Bragg Institute, ANTSO. An example of diffuse scattering is boxed.

A cubic cell may stretch along one axis, becoming tetragonal. The question arises: what drives the phase transition? This can be important when relating the structure to the properties because, first, a change in unit cell will often result in a change in physical properties and, further, while the structural modification forms a different type of long-range order in the crystal at the phase transition, at temperatures above the transition the interactions driving the transition may still contribute to governing the material's behaviour. The transition itself offers a means of studying these interactions. The magnetic phase transition is also of interest, both for fundamental and technological reasons. A powerful tool for the study of magnetic properties of materials is neutron diffraction, as neutrons can scatter off an array of magnetic moments just as X-rays scatter from electrons when performing crystallographic studies. As a result, we can follow the evolution of the magnetic structure as a function of temperature, applied magnetic field and composition. We have an interest in rare-earth magnetism and in the properties of layered magnetic systems, in which unusual magnetic phenomena can be observed.

We work to better elucidate the nature and role of short-range order in materials by studying diffuse scattering, the diffracted intensity that does *not* lie on the Bragg positions. The local ordering that diffuse scattering can study is reflective of the local crystal chemistry and physics – an individual atom does not care what 'average' it is supposed to obey, just how it interacts with its neighbours. The average may be completely non-physical. If we wish to understand how the structures and properties arise, we need to 'get inside' the long-range average using diffuse scattering. In view of the strong relationship with AINSE and ANSTO, we have driven the development of neutron diffuse scattering. The neutron is sensitive to light atoms, such as hydrogen and its isotopes, and so neutron diffuse scattering is a way to explore the behaviour of light atoms in the presence of heavier ones, such as oxygen in functional oxides like high-temperature superconductors and in ferroelectric materials such as hydrogen in organic molecular systems.

Structural Phase Transitions

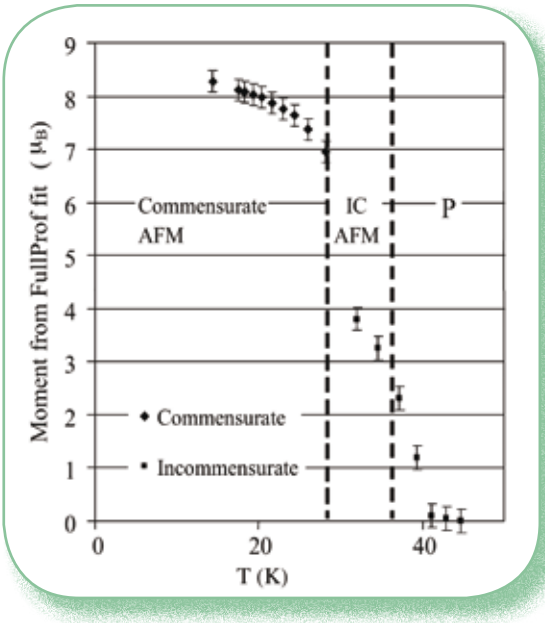
We have studied the structural phase transitions in deuterated paraterphenyl ($C_{18}D_{14}$) and deuterated benzil, $C_{14}D_{10}O_2$. The former study made use of neutron diffuse scattering, the latter used neutron powder diffraction and 3-axis neutron spectroscopy, and showed that the phase transition is a first order ferroelectric transition that occurs at 88.1K. It had previously been suggested that the transition was triggered by a phonon softening at the Brillouin zone centre, but we find that the structural phase transition in benzil is driven by a conventional phonon softening at the Brillouin zone boundary. In other words, a lattice vibration slows down until it locks into a new static ordering. *(With M E Hagen [Oak Ridge National Laboratory, USA], X Wu [Monash], M Prior [ANSTO])*



Neutron powder diffraction from deuterated benzil as a functionof temperature. Below 90K the highlighted peak splits, indicating the onset of the structural phrase

Incommensurate Magnetic Order in Rare-Earth Compounds

Magnetic phase transitions in rare-earth magnets have been studied using specific heat measurements, magnetometry and neutron powder diffraction. Experiments were per-formed on $TbNiAl_4$ and $ErNiAl_4$ to establish the magnetic phase diagram as a function of temperature and applied magnetic field. $TbNiAl_4$ was found to be particularly interesting. At the lowest temperatures, the material orders antiferromagnetically with the magnetic moment (anti)parallel with the *a* lattice vector. On heating above 28K, there is a first-order transition to an incommensurate magnetic phase, in which the moments show a canted component that does not repeat in an integer number of crystallographic unit cells. This then undergoes a second-order phase transition to paramagnetism at 34K. *(With W D Hutchison [UNSW@ADFA], K Nishimura, K Mori, Y Isikawa [Toyama University, Japan], A J Studer [ANSTO])*



Ordered magnetic moment of Tb in $TbNiAl_4$ as a function of temperature

Short-Range Order (SRO) in Crystalline Materials

Key achievements have been the first refinements of a SRO model against X-ray and neutron diffuse scattering data simultaneously, and the development of a flexible suite of computer programs to enable complex systems to be modelled routinely. The program suite has been applied to a range of materials including pharmaceuticals, polymorphic molecular systems, inorganic materials, materials with non-linear optic properties, and molecular ferroelectric materials. The time taken to establish a working simulation of the systems has been reduced from a matter of days to just hours. *(With A Beasley, A P Heerdegen, T R Welberry, R L Withers, L Norén, and P A Altin [Department of Physics], M J Gutmann [ISIS, Oxon, UK])*

LASER AND OPTICAL SPECTROSCOPY

Professor Elmars Krausz

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

Our existence on Earth is entirely dependent on photosynthesis, the process that nature uses to convert solar radiation into molecular energy. Energy stored as 'solid sunlight' is regained when biomass reacts with atmospheric oxygen to form CO_2. The combustion powers a myriad of processes, from the biochemical processes that keep us alive, to generating the vast amounts of heat, mechanical and electrical energy that has allowed modern societies to flourish. The price of our success has been a rapidly increasing human population and a dramatically increasing atmospheric concentration of CO_2, leading to global warming.

For the last decade, our research has concentrated on the photosynthetic process, which splits water into hydrogen and oxygen. An effective understanding of charge separation, electron transfer and catalytic water-splitting remains unknown, leading to considerable controversy. Harnessing these processes is a way in which our reliance on coal and oil can be addressed, leading to an alternative and renewable molecular energy source. Our efforts are being made in collaboration with a number of ANU, Australian and overseas groups and have lead to a number of remarkable discoveries and, in particular, to new ideas on Photosystem II, the enzyme responsible for splitting water.

Spectroscopy is our strength and passion. When light impinges on a sample, it can be absorbed, induce fluorescence and scattered. Each process carries a wealth of information. Lasers, having phenomenal intensity, purity and coherence, are capable of driving far less familiar processes. We combine conventional and laser techniques to provide a wide range of spectroscopic techniques. An armory of techniques is particularly valuable in studying complex systems. We construct specialised apparatus to target fundamentally important questions. A persistent theme is that molecules can behave quite differently in solution to when they are 'trapped' or enclosed in a protein or crystal. Such influences are probed *via* laser-selective spectroscopy.

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.

Professor Krausz was invited to present some of our new discoveries, particularly in regard to the 'red tail' in Photosystem II, to the 2006 Gordon Conference on Photosynthesis. This was followed by an invitation to attend a meeting at the Royal Society in 2007, which dealt with many issues bedeviling Photosystem II. Ronald Steffen and Joseph Hughes attended the Photosynthesis Congress in Glasgow in 2007, and Joseph Hughes and Professor Krausz the Physical Chemistry meeting in Adelaide. Professor Krausz was invited to a special symposium on Artificial Photosynthesis as part of the Australian Society for Biophysics meeting in Newcastle in December 2007.

An ongoing collaboration with Professor Bill Rutherford and his group at Saclay was funded by a FASTS grant. Joseph Hughes made two extended visits to the Saclay labs in 2007. Felix Ho and Stenbjorn Styring from Uppsala visited in November 2006 with Professor Rutherford, who also returned in November 2007. A joint Research School of Biologial Science (ANU)/RSC ARC Discovery grant, targeting the redox states of the metal centres in the oxygen-evolving cluster of Photosystem II cluster was won for 2007-2010.

The potential offered by artificial photosynthesis, as one arm of a range of 'Emerging Energy Sources', was communicated to Federal Parliament by Professor Krausz and Dr Ron Pace. This was part of an ANU team that presented a full suite of such activities to Parliament in the second half of 2007. Professor Krausz also appeared on a special edition of the ABC program 'New Inventors' highlighting future technologies.

The Primary Acceptor and Secondary Donors in Photosystem II

When Photosystem II spontaneously charge-separates, the critical pheophytin pigment is transiently reduced before metastable reduction of a plastoquinnone. A number of secondary donors can be formed before oxidation of the catalytic manganese cluster occurs. We have identified and quantified many processes involved, taking advantage of our new CCD spectrograph. The pheophytin can also be *chemically* reduced. This process can be followed by circular dichroism and other spectroscopies. Photosystem II, isolated from a range of organisms, shows variations that identify spectral positions and couplings to nearby pigments. *(With R Steffen, J Hughes, N Cox, and R Pace, P Smith [Department of Chemistry, ANU], A W Rutherford, A Boussac [Saclay, France]), S Styring, K Sigfridsson, F Ho [Uppsala U, Sweden]), M Sigiura [Osaka U, Japan]*

Near-IR Absorption in Photosystem II

Utilising the phenomenal capacity of our new CCD spectrograph, we have been able to study weak transient absorptions in the 700-900nm region that have been attributed to the manganese cluster of the oxygen evolving centre in Photosystem II. *(With R Steffen, and R Pace, P Smith [Department of Chemistry, ANU], W Hillier, T Wydrzynski [RSBS, ANU], A W Rutherford [Saclay, France])*

Water-soluble Chlorophyll-binding Proteins (WSCP)

WSCP proteins, which bind a small number of pigments, form a wonderful system in which to study protein-pigment and pigment-pigment interactions. WSCP can be expressed from *E. Coli* and be modified at will. CD and hole-burning studies are providing insights into electronic relaxation between pigments. *(With J Hughes, A Oakley, and T Wydrzynski, B Conlan [RSBS, ANU])*

Our High Performance CCD-based Spectrograph

We have developed a potent spectrometer system, able to accumulate extremely accurate spectra, over a wide spectral range, in less than 100msec whilst using a minimum amount of measurement light. A high-sensitivity, cooled CCD camera forms the heart of the system. Our software developments allow the system to be synchronised with a pulse laser, with changes in spectra associated with photochemical and photophysical transformations to be monitored in real time. *(With R Steffen, K Jackman)*

Our high performance CCD-based spectrograph

POLYMERS AND SOFT CONDENSED MATTER

Associate Professor Edith Sevick

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

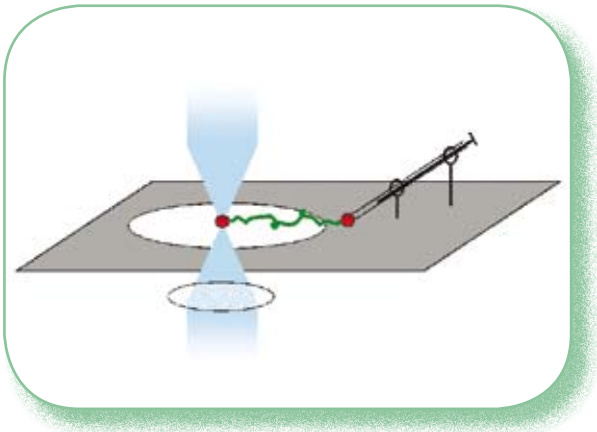
Atomic Force Microscopy (AFM) and Optical Tweezers (OT) have revolutionised molecular science by measuring picoNewton forces over lengthscales from 1 to 100 Å. Our research focuses on experiments using the technique of OT, but we are also involved in theory and simulation of polymers and soft condensed matter: materials well suited for 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 generated by the OT serves to both localise a colloidal particle and to measure the small, sub-picoNewton scale forces acting on the particle. The measurements are central to probe and develop new understandings of the energetics and dynamics of small systems, including polymers and colloids.

Stretching Biopolymers Using Optical Tweezers

Research at the forefront of chemistry and biology aims to understand the energetics and dynamics of complex single molecules such as DNA, RNA, and proteins. Our approach is to use OT to "grab" the colloidal beads that are attached to the ends of a single DNA molecule, and to stretch the spaghetti-like molecule while measuring the energy required to effect tension-induced transitions. Our aim is to apply the OT technique to biophysical systems (i) to quantify the energy of specific protein/DNA interactions that are important to chromosomal replications, and (ii) to quantify the energy of local denaturation, or "melting" of *ds*DNA, an important first step in the biochemistry of DNA and RNA. The single molecule experiments are analogous to conventional calorimetry measurements that detail the energetics of an ensemble or collection of molecules. *(With G M Wang, and N E Dixon [U Wollongong])*

Hydrodynamic Interactions in Simulations of Flexible Polymers

A long, flexible polymer molecule consists of hundreds of thousands of monomeric units. Detailed atomistic simulation of such a molecule and surrounding solvent molecules is not practical if one is interested in detailing the molecule's dynamics. We could model the chain as a continuous curve of a certain atomic thickness, where the forces mediated through the surrounding solvent molecules are incorporated as hydrodynamic interactions. However, computer simulation of such



Schematic of the operating principles of OT and biopolymer stretching. Colloidal beads are tethered to the ends of the l-DNA, of contour length ~20 mm. A bead is suctioned into a micropipette fixed to a translatable stage, while the other bead is optically trapped at the fixed focal point. Translation of the stage separates the ends, or stretches the chain, while the small displacement of the optically trapped bead is measured and recorded as the stretching force or tension in the stretched chain.

a model demands a level of discritisation, which usually involves postulation of bead-spring (or pearl-necklace) models where hydrodynamic interactions are prescribed between spherical beads of fixed radii. This leads to an additional modelling parameter and is unable to accurately model dynamics of highly stretched chains without fine- (as opposed to coarse-) graining. In 2006-07 we developed a scheme for coarse–graining hydrodynamic interactions where the chain is represented by a series of orientable and stretchable Gaussian blobs, with no additional tuning parameters. We constructed Brownian dynamics simulations of the relaxation of strongly stretched chains, modelled with the new scheme, and demonstrated that the transient radius of gyration and first normal stress difference are less sensitive to the degree of coarse-graining than the conventional bead-spring model with RPY hydrodynamic interactions. *(With R Prabhakar, and D R M Williams [RSPhysSE, ANU])*

Fluctuation Theorems (FTs)

Conventional 19th century thermodynamics have limited our understanding of statistical physics to systems in the thermodynamic limit, at or near equilibrium. In the last decade two new theorems, referred to as the Fluctuation Theorems (FTs), were introduced to quantify the energy distributions of small systems that are driven out of equilibrium, possibly far from equilibrium, by an external field. The FTs represent a much-needed extension of non-equilibrium thermodynamics that can potentially address systems of interest, including nano/micro-machines and single biomolecular function. The first and original FT of Evans *et al* is a generalisation of the second law of thermodynamics to small systems over short timescales, whilst the FT of Crooks, or the Jarzynski equality, describes the evolution of systems between equilibrium states. In 2002 we demonstrated experimentally, for the first time, the FTs by analysing the trajectories of an isolated colloidal particle in a translating optical trap. However, the motion of a single colloidal particle in a purely viscous solvent is accurately described by the stochastic, inertia-less Langevin equation, and as the FTs can also be derived using this same equation of motion with uncorrelated Gaussian noise, one might argue that we merely tested the applicability of the stochastic equation of motion. In 2006 we confirmed the FT using an optically trapped bead in a viscoelastic solvent, for which the stochastic equations of motion require a dissipative term with memory and from which the FTs cannot be derived. This experimental demonstration is a confirmation of the FTs rather than a confirmation of the dynamics that satisfy the FTs. The paper describing the work was singled out and advertised by Institute of Physics editors for its "novelty, signficance and potential impact on future research". In 2006-07, we wrote a review of the FTs for *Annual Reviews of Physical Chemistry* using a new notation that emphasises the general applicability of the FTs to small dynamical systems, which are perturbed by a field that acts dissipatively and/or conservatively. *(With M A B Baker, D M Carberry, D J Evans, G M Wang, R Prabhakar, S R Williams, and D J Searles [Griffith U])*

Optical Tweezers Investigation of Liquid-Liquid Interfaces: Ultra Low Surface Tension and Micro-rheology

Mixtures of liquids that phase separate or partially de-mix are ubiquitous. Examples include mixtures that completely de-mix, such as oil and water, as well as partially de-mixed systems, in particular mixtures of colloids and polymers that form liquid-liquid interfaces of ultra-low surface tension. The boundary or interface that separates the de-mixed phases plays an important role in determining droplet size, emulsions stabilisation and flow-driven deformation of the droplets. We are working to develop OT as a technique to measure ultra-low surface tensions that cannot be measured easily by other conventional methods. We are also using OT to measure the micro-rheology at and near liquid interfaces. *(With S Martin, G M Wang)*

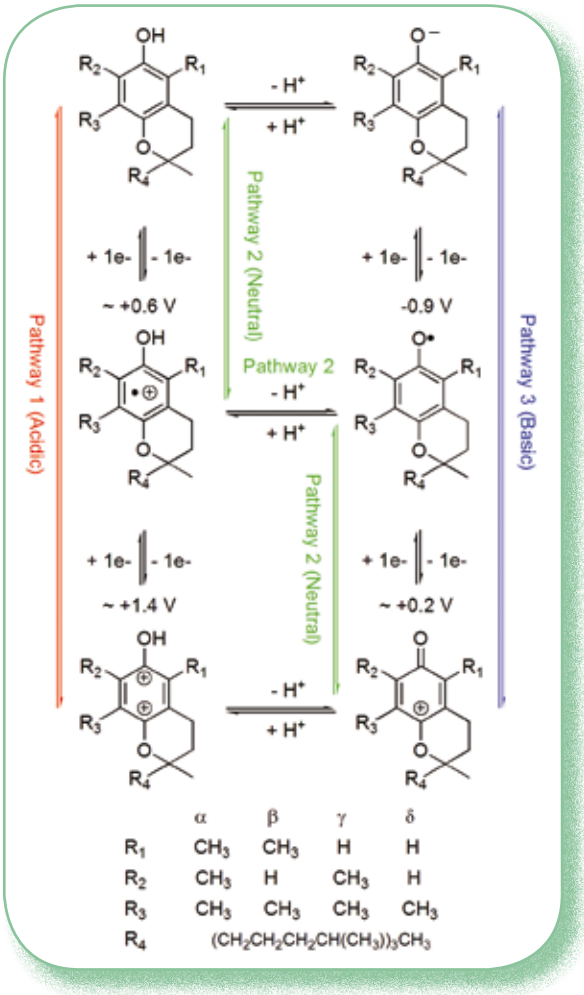
MOLECULAR ELECTROCHEMISTRY

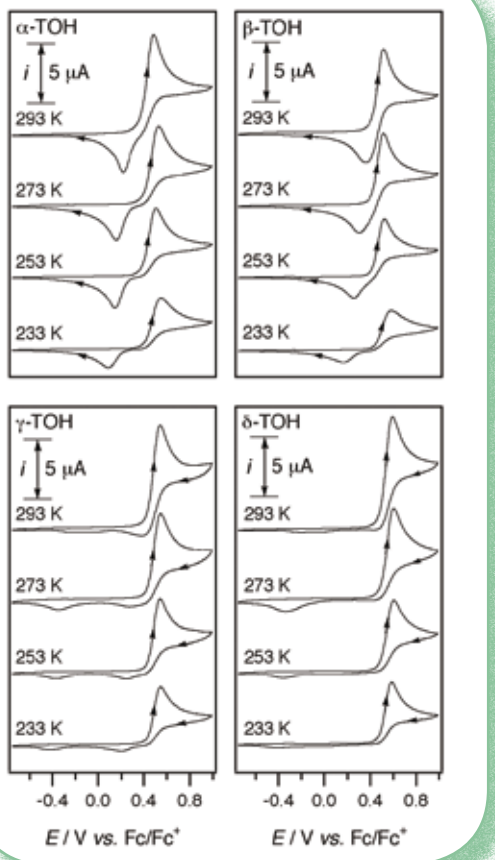
Dr Richard Webster

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 the research is to develop and utilise spectroscopic techniques, including EPR, UV-VIS, FTIR and NMR, to study processes involving electron transfer in organic and inorganic systems.

The Electrochemical Behavior of the Naturally Occurring Tocopherols

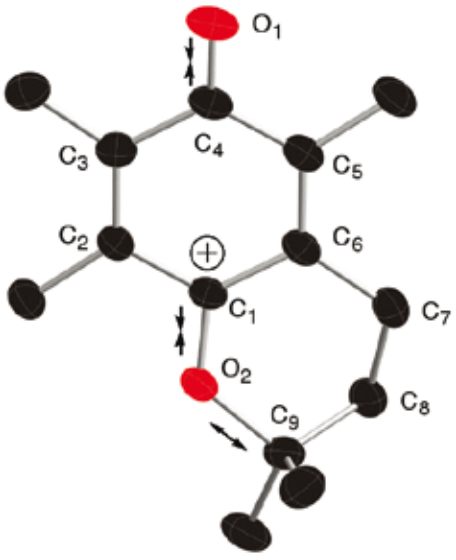
A combination of electrochemical and spectroscopic experiments have proven that the α, β, γ and δ-forms (vitamers) of the tocopherols (TOH) (vitamin E) undergo a series of chemically reversible proton and electron transfer steps in dry organic solvents, such as acetonitrile or dichloromethane, to form cationic compounds: the cation radical, the dication and the phenoxonium cation. The cationic compounds are extremely unusual in their high persistence compared to what is presently known about the oxidative stability of other phenols, particularly the phenoxonium cation of α-tocopherol, which is stable for at least several hours in non-aqueous solvents and is formed quantitatively by oxidation of the starting material at an applied potential of ~ +0.5 V *vs.* ferrocene$^{0/+}$ or with 2 mol equiv of NO^+. *(With G J Wilson, C Y Lin)*





The X-ray Crystal Structure of the Phenoxonium Cation of α-Tocopherol

The crystal structure was obtained of the phenoxonium cation (α-TO$^+$) of the α-tocopherol model compound, stabilised with the non-nucleophilic $B(C_6F_5)_4^-$ and $CB_{11}H_6Br_6^-$ anions. Due to the scarcity of long-lived phenoxonium cations, it is a remarkable observation that one obtained from a natural compound is long-lived (especially in light of the number of new non-antioxidant functions recently discovered that have been assigned specifically to the α-TOH vitamer), and raises questions as to whether the cation has any biological importance. The C_4–O_1, C_2–C_3 and C_5–C_6 bond lengths in α-TO$^+$ are typical of compounds with a quinone structure and the C_1–O_2 bond length in α-TO$^+$ is between what is expected for a single and double bond. The C_9–O_2 bond length in the phenoxonium cation (1.520 Å) is longer than expected for a C–O single bond (1.44 Å), thus the high stability of the phenoxonium cation can be rationalised by the chromanol ring maintaining structural integrity around C_9 despite the long and therefore, weak C_9–O_2 bond. *(With S B Lee, A C Willis)*



DISORDERED MATERIALS

Professor Richard Welberry

http://rsc.anu.edu.au/research/welberry.php

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.

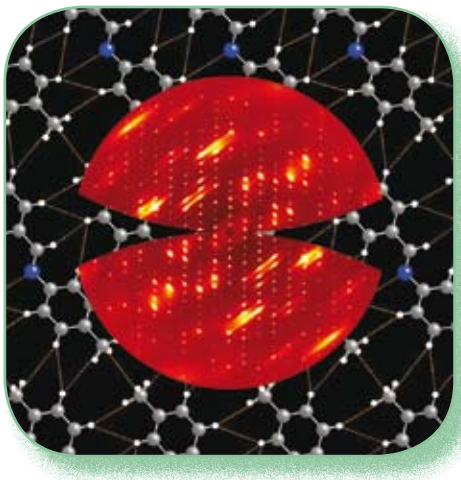
The group uses dedicated diffuse-scattering diffractometer systems. These are based on a Mar 345 image plate detector system (commissioned in July 2006) and two Stoe linear curved position-sensitive wire detectors. These allow high quality diffuse scattering data to be efficiently recorded over large 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 have been 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 investigation of the role of disorder in the occurrence of polymorphism, particularly in pharmaceuticals (supported by an ARC Discovery grant), and with the investigation of the relationship of polar nano-domain structure of relaxor ferroelectrics, such as $PbZn_{1/3}Nb_{2/3}O_3$ (PZN), with their chemical constituency.

The Influence of Disorder on Polymorphism in Pharmaceuticals

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 have studied the model compound p-(N-methylbenzylidene)-p-methylaniline (MeMe), which crystallises in three polymorphic forms.



The structure and diffuse scattering of polymorph II of MeMe

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. All three, however, show strong and highly structured diffuse scattering. A complete study of the diffuse scattering of the pharmaceutical ibuprofen has been published during 2007, and diffuse scattering data have been collected on two polymorphs of benzocaine, two polymorphs of barbital, several polymorphs of substituted sulfonamides and one polymorph of aspirin. Analyses of these systems are underway. *(With D J Goossens, A Beasley, E J Chan, A P Heerdegen, and P Chupas [APS, Argonne, USA])*

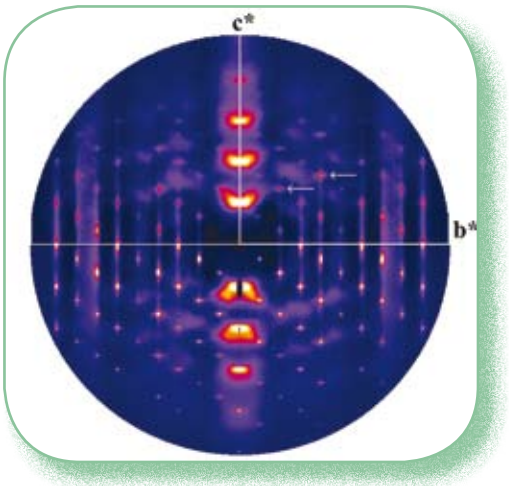
Chemical Origin of Nanoscale Polar Domains in $PbZn_{1/3}Nb_{2/3}O_3$

We have developed an atom-based Monte Carlo simulation model that gives rise to a nanoscale polar domain structure as envisaged to occur in $PbZn_{1/3}Nb_{2/3}O_3$ (PZN) and similar relaxor ferroelectric materials. Individual domains are essentially thin plate-like domains normal to each of the six <100> directions. Calculated diffuse scattering patterns from the model are in good agreement with observed neutron scattering data. Nanoscale domain formation is driven by the need for the Pb atoms to satisfy their valence requirements; within a planar domain, the Pb atoms are displaced in a concerted fashion away from the centre of their 12-fold coordination polyhedra with an in-plane displacement along <100> towards one of the coordinating O atoms. The B-site cations Zn and Nb display a strong tendency to alternate in the <100> directions but complete order is frustrated by the 2:1 stoichiometry. No diffraction evidence has been found that this B-site ordering is directly linked to the nanoscale polar domain ordering. Such a linkage cannot be completely ruled out but, if it does exist, its effect on the diffraction pattern must be quite subtle. The effect of applying an external electric field has been modelled, and the results are found to be consistent with experiment. *(With D J Goossens, A Beasley, A P Heerdegen, and M J Gutmann [ISIS, UK])*

Functional Organic Molecular Materials

Pentachloronitrobenzene, $C_6Cl_5NO_2$, (PCNB) is one of a series of chloronitrobenzene derivatives that are currently being studied because their disordered nature and propensity to undergo phase transitions are thought to be responsible for their anomalous dielectric properties. Disorder often strongly affects the electronic environment in such materials and it is considered that this may be fundamental to physical properties such as, for example, second harmonic generation. Our goal is to quantify the disorder and short-range order as fully as possible with a view to being able to control or harness such disorder and aid the design of new functional molecular materials.

Monte Carlo computer simulation has been used to interpret and model observed single-crystal diffuse X-ray scattering data for PCNB. Each site in the crystal contains a molecule in one of six different basic orientations with equal probability. However, no short-range order amongst these different orientations has been detected. The strong, detailed and very distinctive diffraction patterns can be accounted for almost entirely on the assumption of random occupancy of each molecular site, but with very large local relaxation displacements that tend to increase the neighbouring distances for contacts involving NO_2—NO_2 and NO_2—Cl with a corresponding reduction for those involving Cl—Cl. The results show that the mean NO_2—NO_2 distance is increased by ~0.6Å, compared with that given by the average structure determination. *(With D J Goossens, A P Heerdegen, and L Thomas, C C Wilson [U Glasgow], J M Cole [U Cambridge], M J Gutmann [ISIS, UK], P L Lee [APS, USA], S J Teat [Daresbury Laboratory, UK])*



Comparison of the observed (lower half) and calculated (upper half) Okl diffraction pattern of PCNB

SOLID STATE MOLECULAR SCIENCE

Professor John White (Head of Section)

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

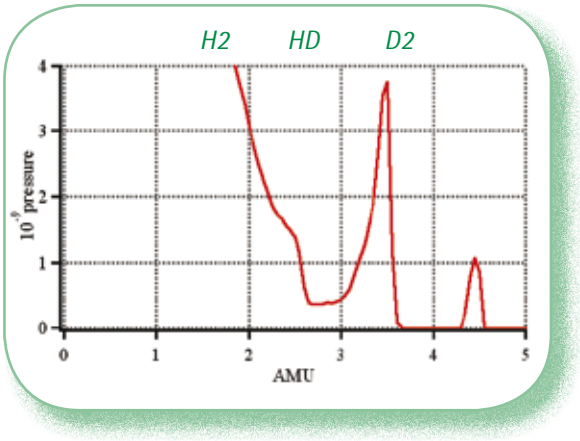
Neutron and X-ray scattering methods, developed by this research group, are used to study the structure and dynamics on nanometre and picosecond space/time scales. Adsorption, self-assembly at interfaces, polymers, the imitation of biomineralisation phenomena using "template" molecules and, most recently, 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. Recent highlights include the production of robust titanium oxide films for water splitting and bio-degradation, and observation of isotope effects in hydrogen formation. The modelling of protein orientation at the air-water interface and interfacial protein denaturation thermodynamics, as well as the first experiments showing the interfacial interaction of different milk proteins, have succeeded. For emulsions, highlights are the design of co-surfactants that greatly change high internal phase emulsion properties, the first *in situ* experiments showing the effects of shear and the first synchrotron anomalous scattering experiments on surfactant-less emulsions.

Our collaboration with Orica Australia 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

Our work to prepare thin mesoporous TiO2 films (800 – 3000 Å), doped to provide a shift in the optical response and capture sunlight, has progressed.

The films, prepared by a surfactant template route using evaporative induced self-assembly (EISA) have produced films which withstand hundreds of hours UV visible irradiation in saturated water vapour. During 2006, the collaboration identified the conditions required to form well-structured films reproducibly. Chemical control of the preparation has been consolidated and film structure characterisation using X-rays and neutron reflectometry is essential. Using 99.75% (deuterium) heavy water, a strong hydrogen isotope effect has been observed as shown in the figure below. *(With M J Henderson, and A Gibaud [Laboratoire de Physique de l'Etat Condense, France], A R Rennie [Uppsala U, Sweden])*



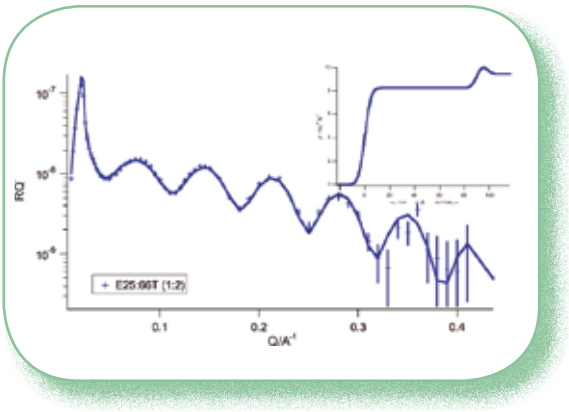
Titanium oxide films for solar energy capture

Nanometre Structure at the Oil/Water Interface

A simple method has been developed to produce a stable, thin (~90 Å) oil film on the surface of pure water, suitable for direct measurements of the oil-water interface using ellipsometry, X-ray or neutron reflectometry, or other experimental methods. The layer is simply formed from the co-spreading of an aliphatic non-volatile hydrocarbon oil (chain lengths between 8-30 methylene repeats) and a polymeric polyisobutylene-succinic amide (PIBSA) of mean molecular mass of 1200

g mol–1 from a solution in toluene. The toluene solution is directly spread on an aqueous surface to produce the homogenous oil layer. This mixed oil-water surface layer has a well-defined surface pressure-surface area isotherm (measured on a Langmuir trough) and reflects X-rays strongly - indicating a smoothness of a few Ångstroms at most.

The figure below shows the X-ray reflectivity (R) multiplied by the fourth power of the vertical momentum transfer (Q_4) as a function of Q. The fringe pattern contains information on the density and thickness of both the oil over-layer and the surfactant at the oil-water interface. The scattering length density profile of these layers from entry into the oil layer from the air and into the underlying water is shown in the inset. *(With D J McGillivray, J Zank)*



X-ray reflecometry from a layer of oil, ~90Å thick, on a pure water subphase. The layer is stabilised by the use of a monolayer of PIBSA surfactant.

High Internal Phase Emulsions (SANS and USANS Analysis)

Small angle neutron scattering (SANS) and ultra small angle neutron scattering (USANS) measurements have continued from high internal phase emulsions (90% aqueous phase/10% oil phase). The focus has been to understand the role of reverse micelles and co-surfactants - synthesised by the RAFT method - on emulsion stability and viscosity. Very large changes in both properties, important for practical applications, have been found. The scattering experiments, especially using neutron contrast variation by swapping deuterium for hydrogen in the oil, surfactant and aqueous phases, continue to be quite fruitful in arriving at a molecular mechanistic understanding of bulk properties. *(With K Baranyai, A J Jackson, D J McGillivray, J Mata, P A Reynolds, A J Scott, J Zank, and J Barker [NIST, USA])*

High Internal Phase Emulsions – Reactions to Stress

In a long-standing collaboration with Orica Australia Ltd, we have been looking at high internal phase emulsions with industrial applications. As part of this work, we have been investigating the mechanisms by which these emulsions remain stable when exposed to environmental stresses such as shear fields or temperature changes, or to aging. *(With D J McGillivray, J P Mata, K Baranyai, A J Jackson, P A Reynolds, A J Scott, J Zank, and J Barker [NIST, USA])*

RSC reflectometer and Dairy Innovation Australia collaborators

VISITING FELLOWS (POST RETIREMENT)

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

Emeritus Professor Athelstan L J Beckwith AO BSc *WA* DPhil *Oxford*, FRACI, FAA, FRS (retired 1996)

During 2006 – 2007 Professor Beckwith continued work on the factors thought to control the structure, stability and reactions of organic free radicals. In an extension of earlier collaborative work in Freiburg with Rüchardt and Brocks on the utility of ESR spectroscopy for the estimation of the stabilisation energy of carbon–centred radicals, approximate relationships between ESR hyperfine splitting constants and experimental and theoretical indices of radical reactivity and stability have been observed. In view of recent publications questioning the validity of the concept of 'radical stabilisation' the work is now being extended to cover a much wider range of substituted radicals. Also, an extensive ESR database has been collected and published as a major chapter in the Landoldt–Börnstein series. It comprises 256 pages containing ESR parameters, kinetic data, methods of generation and other relevant information for more than 1500 carbon–centred free radicals, including some derived from complex peptides and other biologically active compounds.

Collaborative work conducted with Dr K U Ingold during 2006 and 2007 included an examination of the kinetics and mechanisms of chain reactions involving relatively stable radical intermediates, a topic of considerable importance for the development of new polymerisation procedures. Also, a major invited paper was published with Dr Ingold as co–author in a special issue of *Helvetica Chimica Acta* honouring the life and achievements of Professor Hanns Fischer. Not only does this paper summarise Professor Fischer's seminal contributions, but it also shows how some of the methods and approaches he developed are applicable to modern radical chemistry. It also includes kinetic methods and data now published for the first time.

Other activities included acting as a referee for *J Am Chem Soc* and *J Org Chem*, and serving as an advisor to the Australian Foundation for Science, the ARC, and the Australian Academy of Science.

Emeritus Professor Martin A Bennett BSc PhD DIC DSc *London*, ARCS, FRACI, FAA, FRS (retired 2000)

Professor Bennett has been involved in three collaborative research projects during the past two years:

(1) With Professor Suresh Bhargava, RMIT University, Professor Vivian Yam, University of Hong Kong, and Professor Alan Bond, Monash University, on the chemistry, electrochemistry and luminescence behaviour of various dinuclear complexes of gold and platinum. This has entailed detailed supervision of a research assistant and two PhD students at RMIT;

(2) With Dr Masafumi Hirano at the Tokyo Institute of Agriculture and Technology, on the stoichiometric dimerisation of butadiene and substituted butadienes at a ruthenium centre. This work stems from research carried out by a PhD student, Wang Xian–qi, in this School (PhD Thesis, ANU, 1992); and

(3) With Dr Fabian Mohr at the University of Wuppertal, Germany, on a new class of dinuclear, luminescent gold complexes based on a bridging 1,8–bis(naphthyl) unit.

Professor Bennett has contributed to the writing–up of results from the first project and is also preparing papers based on his earlier work in the School.

Dr Richard Bramley MSc *Sydney* PhD *London*, MRACI (retired 1997)

Dr Bramley has continued consultations with the Laser Physics Group, RSPhysSE, 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)

During 2006 – 2007, two projects were undertaken. The first was the preparation of the first book devoted entirely to the naphthyridines. These six isomeric heterocyclic systems display fascinating chemistry and contain many individual derivatives of considerable interest as medicinal (eg. antimalarial) and agrochemical agents. Such a detailed review process involved the critical evaluation of more than 1500 original research papers in half a dozen languages. The book* was eventually published as a volume in the Wiley series "Chemistry of Heterocyclic Compounds", already embracing more than 100 comprehensive compilations.

The second project was the preparation of a cumulative index to systems covered in the above–mentioned series. This sorely needed aid has long been avoided by potential authors because of the very time–consuming difficulties associated with the use of a standardised nomenclature for more than 2300 systems already covered in the series. However, this forthcoming book will provide relatively easy access to all such reviews, many of which have been all but impossible to find. (*D J Brown "The Naphthyridines", Wiley, New York, 2007 pp 423 + xxi)

Dr John K MacLeod BSc PhD *Queensland*, FRACI (retired 1999)

The past two years have resulted in the publication of two landmark papers by Professor John Williams and Dr John McLeod in *Photosynthesis Research*, confirming the role of octulose phosphates in the photosynthetic carbon reduction cycle (known as the Calvin Cycle) in spinach. This has necessitated a modification to the Calvin Cycle to accommodate the intermediacy of these C_8 sugar phosphates.

Two other papers that appeared during this period relate to collaborative research carried out (1) with Dr Murali Nayudu (BoZo) on the identification of gluconic acid as the biological control agent produced by the *Pseudomonas* strain AN5 against the take–all fungal root disease of wheat and (2) with a group from the Garvan Institute of Medical Research, Sydney, on the role of the avocado leaf component, persin, on lactating mammary epithelium and its possible use in the treatment of breast cancers.

Emeritus Professor Rodney W Rickards, BSc *Sydney* FRACI, FAA (retired 1999)

Emeritus Professor Rickards is a Visiting Fellow in the RSC and a Visiting Scientist at CSIRO Entomology. Collaboration continued with Dr Geoffrey Smith in the Division of Biochemistry and Molecular Biology (BaMBi), Faculty of Science, 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. 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 that 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.

The Research School of Chemistry notes with great sadness that Rod passed away on the 17th of December 2007.

Emeritus Professor Alan M Sargeson BSc PhD DipEd *Sydney*, FRACI, FAA, FRS (retired 1996)

A cage has been developed to contain radioactive copper tightly so that the radiation can be used to image organs in biological systems. The copper does not escape the cage and ties have been added to the cage periphery so that it may be linked to a monoclonal antibody, which then targets specific sites in the biological system. Depending on the level of radioactivity, the system may be used to irradiate sites for therapeutic purposes or merely used as a detection or diagnosis device. This technology has the potential for wide use in biological systems and in a recent publication it has been used to image neuroblastoma and melanoma.

Structural analyses of pentamethyl–tricosane cages containing zinc, cadmium and mercury have been carried out using both X–ray and NMR spectroscopic analyses. The structures vary from approximately octahedral to trigonal prismatic with these divalent metal ions. The study has exposed the influences from the metal and the ligand when these structures are compared with those of the strong and weak field transition metal complexes already established.

Aqueous cyclic voltammetry of the Cu(II)pentamethyl–tricosane cage complex is reversible. This implies a stable Cu(I) state that resists dissociation from the cage. The chemistry is very unusual since Cu(I) compounds are usually very labile and it is brought about by the ability of the cage to encapsulate the metal ion and accommodate both smaller and larger ions.

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

HONOURS AND AWARDS

Professor M G Banwell was awarded:

- the University of Toronto's 2007 *Boehringer–Ingelheim Lectureship*, and
- the UK Royal Society of Chemistry's 2008 *Australasian Lectureship.*
- He was a *Leibniz Award–funded Visiting Professor* at The University of Munich from January 1 – February 28, 2006, and
- presented the 2006 *G I Feutrill Memorial Lecture* of the Melbourne University Chemical Society on 29 March, 2006.

Miss E Barrett was awarded the 2005 *Dean's Prize for the Best Publication by a PhD Student.*

Miss G Bojase–Moleta was awarded the *Best Student Lecture prize* at the RACI NSW Organic Chemistry Group 27th Annual One–Day Symposium 2006, Canberra, 27 November, 2006.

Miss L Carpinelli was awarded the *Best Student Lecture prize* at the 22nd Royal Australian Chemical Institute Organic Conference (22RACIOC) and the 6th RACI Conference on Physical Chemistry (CPC2007), Adelaide, 28 January – 2 February, 2007.

Dr M L Coote received:

- the *Royal Australian Chemical Institute Rennie Medal*, 2006, and
- the *Australian Journal of Chemistry Prize*, 2007.

Dr R E Dawson received the *Encouragement Award* of the 4th Asian Cyclodextrin Conference, Kyoto, Japan, 18–20 May 2007 for his poster (with C J Easton, S F Lincoln and H Onagi) – "Stilbene and a–cyclodextrin as the basis of a light driven molecular muscle".

Dr R Dewhurst was awarded the 2005 *Dean's Prize for the Best PhD Thesis.*

Professor N E Dixon was awarded:

- the *Foundation for Inorganic Chemistry Lectureship* at the University of Sydney for 2007, and
- was appointed to the ARC College of Experts in 2007.

Professor C J Easton

- was elected President–elect of The Society for Free Radical Research (Australasia) 2007, and
- his joint publication "Some Guidelines for Radical Reactions", A L J Beckwith, C J Easton and A K Serelis, *J. Chem. Soc., Chem. Commun.*, 1980 (11), 482, was ranked the 31st most cited article in the 40 years of publication of the journal.

Professor D J Evans was appointed as Scientific Chair of Statphys 24 (to be held in 2010).

Dr K Fairweather was the joint winner of the 2006 *Dean's Prize for the Best PhD Thesis.*

Mr T Fallon was awarded the *Best Student Poster prize* at the 22nd Royal Australian Chemical Institute Organic Conference (22RACIOC) and the 6th RACI Conference on Physical Chemistry (CPC2007), Adelaide, 28 January – 2 February, 2007.

Dr D J Goossens won the *2006 Australian Institute of Nuclear Science and Engineering (AINSE) Research Fellowship,* which he took up in November 2006. This was one of two such Fellowships awarded nationally, and is approximately equivalent to an ARC QEII Fellowship. Darren is now a 50% split with the Department of Physics at ANU, where he is a teaching academic.

Ms K Hasse was awarded a *Daimler–Benz Foundation Scholarship* to support her PhD studies at the ANU.

Ms J L Hodgson received the 2006 *CRC for Polymers Prize.*

Dr C Y Lin received the *Poster Prize* at the International Congress of Quantum Chemistry in Kyoto, May, 2006.

Dr E H Krenske received:

- an *Australian Academy of Science Travelling Fellowship*, 2007, and
- a *Fulbright Fellowship*, 2007.

Miss S Maniam received the *Best Poster prize* of the 4th Asian Cyclodextrin Conference, Kyoto, Japan, 18–20 May, 2007 for her poster (with S F Lincoln and C J Easton) – "Three–stationed molecular switches".

Dr D J McGillivray won the *2007 Australian Institute of Nuclear Science and Engineering (AINSE) Research Fellowship*. He will take this up at the University of Auckland in 2008.

Miss E L Pearson was awarded the *Best Student Lecture prize* at the Centre of Excellence For Free Radical Chemistry and Biotechnology Winter Symposium, Canberra, 5–6 June, 2006.

Dr G Sandala was the joint winner of the 2006 *Dean's Prize for the Best PhD Thesis.*

Associate Professor E M Sevick's work was chosen as an *Institute of Physics (IOP) SELECT Article:* an article chosen by IOP Editors for the "novelty, significance and potential impact on future research".

Associate Professor M S Sherburn was awarded:

- the *Le Fèvre Memorial Prize 2006* of the Australian Academy of Science. This is a prestigious award for "outstanding basic research in chemistry by scientists under 40 years", and
- was the *Merck Frosst Visiting Professor 2007,* at the University of Toronto, Canada.

Dr J Wagler was awarded the *Post Doctoral Research Fellowship Deutscher Akademischer Austausch Dienst (DAAD).*

Dr Z Watts received the *Young Investigator Award* of the 4th Joint Meeting of the Society for Free Radical Research (SFRR) Australasia and Japan, Kyoto, Japan, 1–5 December, 2007, for his lecture (with D K Jordan and C J Easton) – "Synthesis of peptides incorporating non–proteinogenic amino acids produced through radical functionalisation of proteinogenic analogues".

Professor J W White was awarded:

- the *Victorian Institute of Chemical Sciences Distinguished Fellowship* and gave a series of lectures in August, 2007 at Monash University, University of Melbourne, Latrobe University and at the Royal Australian Chemical Institute, and
- was made a *Distinguished Friend of Oxford University* in October, 2007. This was in recognition of work done for the Oxford Australia Scholarship Fund, whose Selection Committee is chaired by Professor White. In the last 10 years, 45 young Australians have been sent to Oxford University on scholarships from this Fund.

PUBLICATIONS

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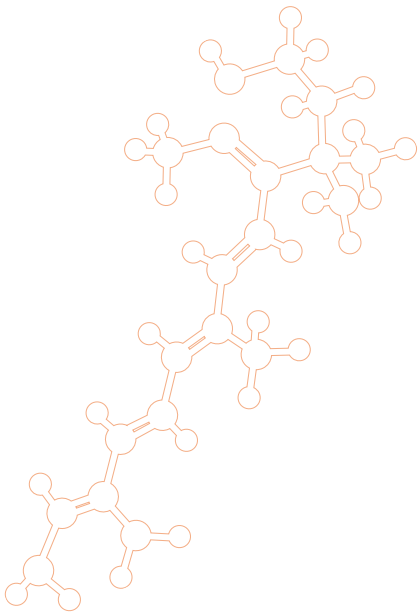

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Adjunct Professors

Professor Roger D Amos

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Professor Veronica J James

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Professor Leo Radom

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Visiting Fellows (Post-retirement)

Professor Athelstan L J Beckwith

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Professor Martin A Bennett

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Dr Desmond J. Brown

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Dr Richard Bramley

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Professor Rodney W Rickards

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Professor Alan M Sargeson

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Professor John F Williams

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NATIONAL AND INTERNATIONAL LINKS

Collaborative Research Projects with Universities, CSIRO and Other Institutions

Biological Chemistry

Protein Structure and Function – N E Dixon

Cell free protein synthesis. *(With M J Headlam, K V Loscha, S Noor, K Ozawa, I Ugwumba, G Otting, and Z Xu, S E Brown [CSIRO Entomology, Canberra])*

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

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

Mechanisms of termination of DNA replication. *(With M D Mulcair, P M Schaeffer, A J Oakley, and D C Neylon [U Southampton, UK], T M Hill [U North Dakota, USA])*

Single molecule studies of DNA replication. *(With S Jergic, P M Schaeffer, E Sevick, G Wang, and N A Tanner, S M Hamdan, A M van Oijen [Harvard Medical School, USA])*

Small molecule sensor proteins. *(With Y Pham, and P Hendry [CSIRO Molecular and Health Technologies])*

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])*

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

Structures and functions of the *Bacillus subtilis* DnaC helicase and DnaI proteins. *(With G Otting, P M Schaeffer, X–C Su, K V Loscha, and C Ioannou, P Soultanas [U Nottingham, UK])*

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 [Ecole Normale Superieure de Lyon, France], T Huber [U Queensland])*

Nuclear Magnetic Resonance – M A Keniry

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

Structural Biology – A J Oakley

Cofactor free oxygenases. *(With R Qi, and S Fetzner [U Oldenburg, Germany])*

Termination of DNA replication in bacteria. *(With N E Dixon, M D Mulcair, P M Schaeffer [U Wollongong])*

Human omega–class glutathione S–transferases and glutathione metabolism. *(With P G Board [JCSMR, ANU])*

Protein Crystallography and Engineering – D L Ollis

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

Structure and function studies with organophosphate degrading enzymes. *(With G Schenk [School of Microbial Sciences, U Queensland])*

Biomolecular NMR – G Otting

Development of a lead compound against the West Nile virus and dengue virus NS2B/NS3 proteases. *(With S–P Lim, S Vasudevan [Novartis Institute of Tropical Diseases, Singapore])*

Structural biology of *E. coli* DNA polymerase III. *(With N E Dixon [U Wollongong])*

Inorganic Chemistry

Synthetic Organometallic and Coordination Chemistry – A F Hill

An integrated synthetic and NMR spectroscopic study of photochemical organometallic bond activation. *(With G E Ball [U New South Wales])* 2007

Investigations of metal silicon dative bonding *(With J Wagler [U Freiberg])*

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

Hydrometallation of poly ynes *(With P Low [Durham U])* 2006

Migratory insertion reaction of thiocarbonyl ligands (*With J D E T Wilton-Ely [U Oxford]*)

Inorganic Stereochemistry and Asymmetric Synthesis – S B Wild

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

Inorganic Materials Chemistry – R L Withers

Precise diffraction studies of temperature and composition induced structural phase changes. *(With A-K Larsson, and C J Howard [ANSTO, Sydney], B J Kennedy, S Schmid [U Sydney])*

Coupled structural and elastic response studies of the phase transformation behaviour of environment-friendly, lead-free electroceramics. *(With Y Liu, and B J Kennedy, S Schmid [U Sydney], C J Howard [ANSTO, Sydney], M Carpenter [U Cambridge, UK])*

A coupled electron microscopy, XRD and *ab initio* energy minimisation study of local order and its relationship to the ferroelectric/pyroelectric behaviour of $BaAl_2O_4$ and $SrAl_2O_4$. *(With A-K Larsson, and J M Perez-Mato [U of the Basque Country, Spain], J D Fitzgerald [RSES, ANU])*

A reverse Monte Carlo approach to the real space refinement of electron diffuse scattering and application to disordered bi-based pyrochlores. *(With Y Liu, N B Nguyen, and A L Goodwin [U Cambridge, UK])*

Tailoring the microwave dielectric properties of promising electroceramics for use in wireless telecommunication components and devices. *(With Y Liu, and R Taylor, J Barry, T Yamashita [Microwave and Materials Designs Pty Ltd, Brisbane])*

Enhancing the performance of mobile wireless telecommunications systems by exploiting the properties of high temperature superconductors and new ceramic materials. *(With Y Liu, and R Taylor, J Barry, T Yamashita [Microwave and Materials Designs Pty Ltd, Brisbane], M Bick [CSIRO Materials Science and Engineering])*

Organic Chemistry

Synthesis and Mechanism – M G Banwell

Biotransformation. *(With G M Whited [Genencor International Inc., Palo Alto, USA])*

The development of chemoenzymatic methods for the selective elaboration of polyfunctionalised therapeutic agents to oligomers with improved efficacy. *(With M 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 Augustine, A Stewart [Cryptopharma Pty Ltd, Melbourne])*

The development of novel-carbohydrate-like drugs. *(With D Offermann, C Bluechel, and V Ferro [Progen Industries Ltd, Brisbane])*

The total synthesis of biologically active marine alkaloids from the Great Barrier Reef. *(With D Dauge, Z Yi-Jun, and M Garson [U Queensland])*

The synthesis of chelator-lipids that promote stable binding of His-tagged proteins to membranes. *(With D Offermann, B Leita, and J Altin [BaMBi, ANU], N White [Lipotek Pty Ltd])*

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 [Purdue U, USA], J Nester [Sam Houston State U, USA])*

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

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

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

Experimental–computational investigations into Diels–Alder sequences. *(With R Tripoli, D Robinson, T N Cayzer, A Longshaw, E L Pearson, L C H Kwan, W Lording, and M N Paddon–Row [U New South Wales])*

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

Physical and Theoretical Chemistry

Theoretical Chemical Physics – M A Collins

Chemical reaction dynamics. *(With D H Zhang [Chinese Academy of Science, China])*

Nonabiabatic dynamics and coupled potential energy surfaces. *(With D Yarkony [John Hopkins U, USA], D H Zhang [Chinese Academy of Science, China])*

Approximate *ab initio* quantum chemistry. *(With R Bettens [National U Singapore, Singapore], M Gordon [Iowa State U, USA])*

Chemically accurate theoretical approaches to chemistry in the solid state. *(With M Jordan [U Sydney], M Gordon [Iowa State U, USA])*

Computational Quantum Chemistry, Polymer Chemistry – M L Coote

Mechanism and kinetics of dithiobenzoate–mediated RAFT polymerisation by the IUPAC Working Party on RAFT Kinetics and Mechanism. *(With C Barner–Kowollik [U New South Wales], M Buback, P Vana [Georg–August–Universität Göttingen, Denmark], B Charleux [Université Pierre et Marie Curie, France], M Drache [Technische Universität Clausthal, Denmark], A Goto, T Fukuda [Kyoto U, Japan], B Klumperman [Eindhoven U of Technology, Netherlands], A B Lowe [U Southern Mississippi, USA], J B McLeary, R D Sanderson [U Stellenbosch, South Africa], M P Tonge [U Sydney], G Moad [CSIRO Molecular Science], M J Monteiro, [U Queensland])* 2006

Controlling free radical polymerisation with thioketone spin traps. *(With E I Izgorodina, and A Ah Toy, C Barner–Kowollik, H Chaffey–Millar, T P Davis, M H Stenzel [U New South Wales])* 2006

Reactions catalysed by vitamin B12. *(With L Radom, G Sandala, and D Smith [Rudjer Boskovic Institute, Zagreb, Croatia], B T Golding [U Newcastle upon Tyne, UK])* 2006

Hydrogen atom transfer in peptide radicals. *(With L Radom, C J Easton, R Jacob, D Brittain, and D Moran, G P F Wood [U Sydney], R A O'Hair [U Melbourne] M J Davies [Heart Research Institute and U Sydney])* 2006

Computational and experimental studies of electro–chemistry. *(With M Namazian, and H R Zare, M R Noorbala, S Siahrostami, F Kalantary–Fotoh [Yazd U, Iran])*

Computational and experimental studies of radical mediated reactions. *(With C J Easton, and S Zard [Ecole Polytechnique, France])*

Valence bond theory studies of hydrogen atom abstraction. *(With R Harcourt [Melbourne U], K Shaefer [Ludwig–Maximilians–Universität München, Germany])*

Ab initio kinetic modelling of free radical polymerisation. *(With E I Izgorodina, E H Krenske, and M Busch [Technische Universität Darmstadt], H Chaffey–Millar, C Barner–Kowollik [U New South Wales] S Perrier [U Sydney], E Chernikova [Moscow State U, Moscow])*

Structure–reactivity in atom transfer radical polymer–isation. *(With C Y Lin, and K Matyjaszewski [Carnegie Mellon U, USA], R Poli [Toulouse U, France])*

Computer–aided design of nitroxide antioxidants. *(With J L Hodgson, M Namazian, and S E Bottle [Queensland U of Technology])*

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, G M Wang, and D J Searles [Griffith U])*

Theoretical Quantum Chemistry – P M W Gill

Q–Chem 3.0 software package. *(With various groups including M Head–Gordon [U Berkeley, USA], A I Krylov [U Southern California, USA], H F Schaefer III [U Georgia, USA])*

New density functional for transition metal clusters. *(With M A Addicoat, G F Metha, M A Buntine [U Adelaide])*

Models for DNA damage. *(With M W George [U Nottingham, UK])*

Structure and Magnetism of Materials – D J Goossens

Development of neutron diffuse scattering at Australia's OPAL reactor. *(With A J Studer [ANSTO, Sydney])* 2007

Neutron diffuse scattering from optimally doped high–temperature superconductor HgBa2CuO4+δ. *(With M J Gutmann [ISIS, UK])* 2007

Neutron diffuse scattering from CePdSb. *(With M J Gutmann [ISIS, UK])* 2007

Magnetic structures of rare–earth intermetallic compounds. *(With W D Hutchison [UNSW@ADFA])*

Magnetic structures of layered magnetic materials: the (MM')PS3 family. (M, M' = Mn, Fe, Ni...) *(With T J Hicks [Monash U])*

Phase formation in metal injection moulding through in situ neutron diffraction. *(With K–D Liss, A J Studer [ANSTO, Sydney])*

Microstructure of horseshoe nails using neutron diffraction. *(With Z Stachurski [CSEM, ANU], A J Studer [ANSTO, Sydney])* 2006

Laser and Optical Spectroscopy – E Krausz

Spectroscopy of photosynthetic protein sub–assemblies. *(With M Seibert [NREL, USA])*

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

Magneto–optical spectroscopy of cytochrome b6f. *(With S Peterson Årksöld, J F Allen, J Ström [U Lund, Sweden])*

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

Tyrozine oxidation and secondary donor pathways in Photosystem II. *(With A W Rutherford, A Boussac [CNRS, CEA Saclay France])*

Polymers and Soft Condensed Matter – E M Sevick

Single molecule studies of replisomal function. *(With N E Dixon [U Wollongong], A M Van Oijen, S Hamdan [Harvard Medical School, USA])*

Stretching DNA–protein complexes using optical tweezers. *(With N E Dixon [U Wollongong])*

Molecular Electrochemistry – R D Webster

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

Disordered Materials – T R Welberry

Disorder in pentachloronitrobenzene, $C_6Cl_5NO_2$: A diffuse scattering study. *(With D J Goossens, A P Heerdegen, and C C Wilson, L H Thomas [U Glasgow, UK], J M Cole [U Cambridge, UK], M J Gutmann [ISIS, Rutherford Appleton Laboratory, UK], S J Teat [Daresbury Laboratory, UK], P L Lee [Advanced Photon Source, Argonne, USA])*

Chemical origin of nanoscale polar domains in $PbZn_{1/3}Nb_{2/3}O_3$. *(With D J Goossens, and M J Gutmann [ISIS, Rutherford Appleton Laboratory, UK])*

Crystal chemistry on a lattice: The case of BZN and BZN–related pyrochlores. *(With Y Liu, R L Withers, and H Wang, H Du [Electronic Materials Research Laboratory, Xian Jiaotong U, PR China])*

Structural phase transition in deuterated benzil $C_{14}D_{10}O_2$: Neutron inelastic scattering. *(With D J Goossens, and M E Hagen, J A Fernandez–Baca [Oak Ridge National Laboratory, USA])*

Simultaneous fitting of X–ray and neutron diffuse scattering data. *(With D J Goossens, A P Heerdegen, and M J Gutmann [ISIS, Rutherford Appleton Laboratory, UK])*

Deformed model sets and distorted Penrose tilings. *(With B Sing [Fakultät für Mathematik, Universität Bielefeld, Germany])*

Deformed Penrose tilings. *(With B Sing [U Bielefeld, Germany])*

Solid State Molecular Science – J W White

Conformation of proteins at interfaces. *(With M J Henderson, and S A Holt [Rutherford Appleton Laboratory, 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], Dr A R Rennie [U Uppsala, Sweden])*

Nanostructure of milk membranes 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, B Ladewig [U Queensland])*

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

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

Interface structure in water and surface movement of splendipherin, the aquatic male sex pheromone of the tree frog *litoria splendida***.** *(With A W Perriman, and M W Rutland [Royal Institute of Technology, Sweden]), J H Bowie, M A Apponyi [U Adelaide])*

Academic Visitors

The Birch Lecturer

2006

Professor Michael Graetzel, Swiss Federal Institute of Technology, Lausanne, Switzerland.

2007

Professor Richard R Shrock, Massachusetts Institute of Technology, Cambridge, USA.

The David Craig Lecturer

2006

Professor Kenneth Jordan, University of Pittsburgh, USA.

2007

Professor Stephen G Boxer, Camille and Henry Dreyfus Professor of Chemistry, Standford University, California, USA.

Visiting Fellows

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

Abell, Professor Chris, U Cambridge, UK, 2006–2007

Barriault, Associate Professor Louis, U Ottawa, Canada, 2007

Besley, Dr Nicholas A, U Nottingham, 2007

Bettens, Assistant Professor Ryan, National U Singapore, 2006

Bichoutskaia, Dr Elena, U Nottingham, 2007

Billeter, Professor Martin, U Gothenburg, Sweden, 2007

Clark-Walker, Emeritus Professor George Desmond, Research School of Chemistry, 2006–2007

Goodwin, Dr Andrew, Cambridge University, UK, 2006–2007

Gordon, Professor Mark, Iowa State U, USA, 2007

Gutmann, Dr Matthias, ISIS, Rutherford Appleton Laboratory, UK, 2007

Hill, Dr Justine, U Queensland, 2006

Ho, Dr Felix, U Uppsala, Sweden, 2006

Jux, Dr Norbert, U Erlangen, Germany, 2007

Low, Dr Paul, Durham U, UK, 2006

Morris, Dr Jonathan, U Adelaide, 2006

Perez-Mato, Professor Manuel, U of the Basque Country, Spain, 2007

Pintacuda, Dr Guido, Ecole Normale Superieure de Lyon, France, 2007

Proffen, Dr Thomas, LANSCE, Los Alamos, New Mexico, USA, 2006

Rutherford, Professor Bill, Saclay, France, 2006–2007

Storey, Dr John, U Aberdeen, UK, 2006–2007

Styring, Professor Stenbjorn, U Uppsala, Sweden, 2006

Van Beijeren, Professor Henk, Utrecht U, Netherlands, 2007

Von Nagy-Felsobuki, Professor Ellak, U Newcastle, 2006

Wagler, Dr Jörg, U Freiberg, Germany, 2006–2007

Weber, Dr Thomas, ETH, Switzerland, 2006

Research Seminar Speakers

The following were short-term visitors to the School. They presented invited lectures or research seminars and held discussions with academic staff and students:

2006

Bottle, Dr Steven, Queensland U Technology

Charleux, Professor Bernadette, Université Pierre et Marie Curie, Paris, France

Harding, Professor Margaret, U New South Wales

Hutton, Dr Craig, U Melbourne

Makha, Dr Mohamed, U Western Australia

Masters, Associate Professor Anthony, U Sydney

Rendina, Dr Lou, U Sydney

Stephenson, Dr Richard, U East Anglia, UK

Wedd, Professor Anthony, U Melbourne

Wills, Professor Martin, U Warwick, UK

Young, Associate Professor Charles, U Melbourne

2007

Alvarez, Dr Rebecca, U Manchester, UK

Bohme, Professor Diethard, York U, Toronto, Canada

Casey, Professor Charles, U Wisconsin, USA

Chernikova, Professor Elena, Moscow State U, Moscow

Dove, Professor Martin, U Cambridge, UK

Edmonds, Dr Michael, Christchurch Polytechnic Institute of Technology, New Zealand

Galy, Professor Jean, CNRS, France

Hamdan, Dr Samir, Harvard Medical School, USA

Hashmi, Professor Stephen, U Stuttgart, Germany

Holt, Dr Steven, ISIS, Rutherford Appleton Laboratory, UK

Hultzsch, Dr Kai, Friedrich-Alexander U Erlangen-Nuremberg, Germany

Kepert, Professor Cameron, U Sydney

Koeper, Dr Ingo, Max-Planck Institute for Polymer Research, Mainz, Germany

Matyjaszewski, Professor Kris, Carnegie-Mellon U, USA

Moore, Dr Evan, U California, USA

Porter, Professor Ned, Vanderbilt U USA

Richmond, Dr Michael, U North Texas, USA

Roach, Dr Gerald, Extraction Technology, Alcoa World Aluminium

Sharrad, Dr Clint, U Manchester, UK

Svergun, Dr Dimitri, European Molecular Biology Lab, Germany

Whitmire, Professor Kenton, Rice U, USA

Woodward, Dr Patrick, Ohio State U, USA

Conference Presentations

Biological Chemistry

31st Lorne Conference on Protein Structure and Function, Lorne, VIC, 5–9 February 2006. The following invited lecture was presented:

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

The following poster was also presented:

A-Y Park, S Hamdan, M J Headlam, P D Carr, D L Ollis and N E Dixon: *Structural and kinetic analysis of substrate specificity of the 3'–5' exonuclease proofreading exonuclease subunit of* E. coli *DNA polymerase III*

Keystone Symposium on Nucleic Acid Enzymes, Taos, New Mexico, USA, 11–16 February 2006. The following invited lecture was presented:

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

ANZMAG 2006 Conference, Murramarang National Park, NSW, 12–16 February 2006. The following invited lecture was presented:

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

The following posters were also presented:

N Mitic, A-Y Park, N Dixon, G Hanson and G Schenk: *Substrate analogue-induced formation of a binuclear centre in the proofreading 3'–5' exonuclease (e) subunit of* Escherichia coli *DNA polymerase III*

G Pintacuda, A Y Park, M Keniry, N E Dixon and G Otting: *3D structures of protein-protein complexes by lanthanide labelling*

M Rosenberg, L Hekimian, K Ozawa, P Board, N E Dixon and M Casarotto: *Expressing the virus ion channel, VPU, for NMR studies*

P Wu, K Ozawa, S Jergic, X-C Su, N E Dixon and G Otting: *New quick-fit nuts and bolts for the toolbox of NMR spectroscopists*

Experimental Biology 2006 Conference, San Francisco, USA, 1–5 April 2006. The following invited lecture was presented:

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

Experimental NMR Conference (ENC), Asilomar, California, USA, 23-28 April 2006. The following invited lecture was presented:

G Otting: *Lanthanide labelling for structure determinations of protein-ligand complexes*

5th East Coast Bacillus Meeting, University of Technology, Sydney, NSW, 23 June 2006. The following invited lecture was presented:

N E Dixon: *Termination of bacterial DNA replication*

International Congress of Plant Molecular Biology, Adelaide, SA, 20–25 August 2006. The following poster was presented:

P M Chandler, C A Harding, A R Ashton, M Mulcair, N E Dixon and L N Mander: *Gibberellin receptor mutants in barley* Hordeum vulgare (L.)

XXII ICMRBS, Göttingen, Germany, 20-25 August 2006. The following invited lecture was presented:

G Otting: *Fast structure determination of protein-protein and protein-ligand complexes by paramagnetic lanthanide labelling*

17th International Mass Spectrometry Conference, Prague, Czech Republic, 27 August – 1 September 2006. The following invited lecture was presented:

J L Beck, T Urathamakul, S J Watt, M M Sheil, P M Schaeffer and N E Dixon: *Electrospray ionisation mass spectrometry of non-covalent macromolecular complexes of the* E. coli *replisome*

The following poster was also presented:

T Urathamakul, L L Jessop, A-Y Park, N E Dixon, M M Sheil and J L Beck: *Study of interactions of protein and metals in* E. coli *DNA polymerase III using electrospray ionisation mass spectrometry*

ComBio 2006 Conference, Brisbane, QLD, 24–28 September 2006. The following posters were presented:

L L Jessop, S Jergic, M M Sheil, N E Dixon and J L Beck: *Mass spectrometric investigations of the interaction between DNA polymerase III subunits alpha and tau*

K Ozawa, S Jergic, G Otting and N E Dixon: *Cell-free protein expression shows that the q subunit of* Escherichia coli *DNA polymerase III acts as a chaperone for the e proofreading subunit*

C Schmitz, M John, A-Y Park, N E Dixon, G Otting, G Pintacuda and T Huber: *ECHIDNA - fully automatic, structure-based NH assignment of paramagnetic proteins*

Queensland NMR Network Symposium, Brisbane, QLD, 26 September 2006. The following invited lecture was presented:

G Otting: *Structural biology by NMR spectroscopy the quick way*

6th East Coast Bacillus Meeting, University of Newcastle, NSW, 10 November 2006. The following invited lecture was presented:

N E Dixon: *Single-molecule studies of DNA replication*

National Japanese NMR Meeting, Kyoto, Japan, 22-24 November 2006. The following invited lecture was presented:

G Otting: *Lanthanide labelling for structure determination of protein-ligand complexes*

Joint Annual Meeting of (I3) EU-NMR and (CA) NMR-LIFE, "Advances and Management of NMR in Life Sciences", Florence, Italy, 18-20 January 2007. The following invited lecture was presented:

G Otting: *Structure determination of protein-ligand complexes by lanthanide labelling*

32nd Lorne Conference on Protein Structure and Function, Lorne, VIC, 4–8 February 2007. The following invited lectures were presented:

N E Dixon, M D Mulcair, P M Schaeffer and A J Oakley: *A molecular mousetrap determines polarity in termination of DNA replication*

G Otting: *High-yield cell-free protein production and analysis by NMR*

The following poster was also presented:

G Otting, G Pintacuda, M John, X Su, K Ozawa, P S C Wu, A Park, M Headlam, M A Keniry, C Schmitz, T Huber and N E Dixon: *New fast methods for structural biology by NMR spectroscopy*

Conference on Perspectives on Stable Isotope Aided NMR Methods for Protein Structure Analysis, Osaka, Japan, 30-31 March 2007. The following invited lecture was presented:

G Otting: *Protein samples for NMR: Cell-free protein synthesis and lanthanide labelling*

FASEB Summer Research Conference on Helicases & NTP-Driven Nucleic Acid Motors, Indian Wells, USA, 23–28 June 2007. The following poster was presented:

C Ioannou, P M Schaeffer, N E Dixon and P Soultanas: *The loading of the helicase in* Bacillus subtilis

4th East Coast Protein Meeting, Coffs Harbour, NSW, 12–14 July 2007. The following plenary lecture was presented:

N E Dixon: *A molecular mousetrap determines polarity in termination of DNA replication*

The following invited lectures were also presented:

C Ioannou, P M Schaeffer, N E Dixon and P Soultanas: *The loading of the helicase in* Bacillus subtilis

C Schmitz, M John, A-Y Park, N E Dixon, G Otting and T Huber: *Automatic NMR resonance assignment of methyl groups using paramagnetic lanthanides*

ComBio 2007 Conference, Sydney, NSW, 22–26 September 2007. The following invited lectures were presented:

N E Dixon, M D Mulcair, P M Schaeffer and A J Oakley: *A molecular mousetrap determines polarity in termination of DNA replication*

C Ioannou, P M Schaeffer, N E Dixon and P Soultanas: *The loading of the helicase in* Bacillus subtilis

M John, X-C Su, P S C Wu, K Ozawa, C Schmitz, T Huber, N E Dixon and G Otting: *New fast methods for structural biology by NMR spectroscopy*

N A Tanner, S M Hamdan, N E Dixon and A M van Oijen: *Single-molecule studies of the* E. coli *replication machinery*

The following poster was also presented:

S Jergic, X-C Su, K Ozawa, D D Scott, G Otting and N E Dixon: *An intrinsically-unstructured region of the tau subunit interacts with the alpha subunit of DNA polymerase III*

16th Conference for the International Society of Magnetic Resonance (ISMAR), Kenting, Taiwan, 14-19 October 2007. The following invited lecture was presented:

G Otting: *Labelling with paramagnetic lanthanides for accelerated structure analysis*

International Symposium on Drug Discovery and Design by NMR, RIKEN, Yokohama, Japan, 22 October 2007. The following invited lecture was presented:

G Otting: *New fast methods for structural biology by NMR spectroscopy*

Annual Meeting of the Spectroscopical Society of Japan, Tokyo, Japan, 12-14 November 2007. The following invited lecture was presented:

G Otting: *New fast methods for structural biology by NMR spectroscopy*

Symposium on New NMR in Structural Biology, Frankfurt, Germany, 16-17 November 2007. The following invited lecture was presented:

G Otting: *Lanthanide labelling for studies of protein-ligand interactions*

Queensland Protein Expression Symposium, Brisbane, QLD, 22-23 November 2007. The following invited lecture was presented:

G Otting: *Cell-free protein synthesis for structural biology*

Inorganic Chemistry

30th Australian Institute of Physics, Condensed Matter and Materials Meeting, Wagga Wagga, NSW, 7-10 February 2006. The following lecture was presented:

L Norén, J Christensen, S Lidin, S Schmid and R L Withers: *The $Sn_{1-x}Sb_{1+x}$, x~0.5, solid solution: The relationship between α and β*

The following posters were also presented:

Y Liu and R L Withers: *New electrical field-tunable dielectric materials – structurally frustrated ferroelectric relaxors*

W Somphon, V Ting, Y Liu and R L Withers: *Structure and dielectric properties of $Bi_2(MNb)O_7$ ($M = Fe^{3+}$, In^{3+})*

Supramolecular Chemistry Symposium, held in Honour of Professor Len Lindoy, University of Sydney, NSW, 27 February 2006. The following lecture was presented:

S B Wild: *Inorganic asymmetric synthesis of two-bladed propellor, octahedral, metal complexes*

The following poster was also presented:

N L Kilah, J W Wielandt, A C Willis and S B Wild: *Self-assembly of square-planar complexes of phosphine-stabilised stibenium salts*

10th Reactive Organometallics Symposium (ROMS 10), University of New South Wales, Sydney, NSW, 30 June 2006. The following lectures were presented:

R J Abernethy, A F Hill and A C Willis: *Novel reactions of coordinated $[H_2B(pz)_2]^-$: A not-so-innocent ligand*

A F Hill, I R Crossley and A C Willis: *Coordinative activation of carbon monosulfide*

M L Weir and S B Wild: *The asymmetric synthesis of ethylene-bridged chiral diarsines*

American Crystallographic Association (ACA) Annual Meeting, Honolulu, Hawaii, USA, 22–27 July 2006. The following poster was presented:

W Somphon, K J Haller and A D Rae: *Variable low-temperature data collection and hierarchical refinement to study an order-disorder phase transition*

Gordon Research Conference on Solid State Chemistry, Colby Sawyer College, New London, New Hampshire, USA, 23–28 July 2006. The following invited lecture was presented:

R L Withers: *Local crystal chemical 'rules', inherent structural flexibility and their characteristic diffraction signatures*

XXII International Conference on Organometallic Chemistry, Zaragoza, Spain, 23–28 July 2006. The following invited lectures were presented:

A F Hill: *Organometallic chemistry of poly(methimazolyl)borates and boranes: Metallaboratrane formation*

S B Wild: *New approach to the asymmetric synthesis of tertiary arsines via phosphine-stabilised arsenium salts*

X-El, Satellite Workshop of ECM 23 on Electron Crystallography and X-ray Powder Diffraction, EMAT, The University of Antwerp, Belgium, 1–4 August 2006. The following invited lecture was presented:

R L Withers: *Electron diffraction and the structural characterisation of modulated and aperiodic structures*

23rd European Crystallographic Meeting, Leuven, Belgium, 6-11 August 2006. The following lecture was presented:

A D Rae: *Prototype structures and structure factor algebra as an aid to the refinement of problem structures*

R L Withers: *The use of electron diffraction for the structural characterisation of modulated and aperiodic structures*

37th International Conference on Coordination Chemistry, Cape Town, South Africa, 13–18 August 2006. The following invited leture was presented:

A F Hill: *Tricarbido complexes: Delivering carbon in packets of three*

Aperiodic 2006, Zao, Miyagi Prefecture, Japan, 17–22 September 2006. The following invited lecture was presented:

R L Withers: *Structured diffuse scattering, local crystal chemistry and metal ion ordering in the* $(1-x)MgS.(^{x}/_{3})Yb_2S_3$, $0 \leq x \leq \sim 0.45$, *'defect' NaCl system*

9th Brisbane Inorganic Chemistry Symposium (BICS-IX), University of Southern Queensland, Toowoomba, QLD, 25 September 2006. The following invited lecture was presented:

A F Hill: *Tricarbido complexes: Delivering carbon in packets of three*

8th International Symposium on Supercritical Fluids, International Conference Hall, Kyoto, Japan, November 2006. The following lecture was presented:

I A Cade, N J Long and A J P White: *Catalytic isomerisation of alkyl and aryl formates*

Theoretical Crystallography and Materials Science, Satellite Conference of the AsCA'06/CrSJ Meeting, Tsukuba, Japan, 18–19 November 2006. The following invited lecture was presented:

A D Rae: *The need for coexisting symmetrised components to rationalise the description and refinement of problem structures*

Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Epochal, Tsukuba, Japan, 20–23 November 2006. The following posters were presented:

P Naumov, G Jovanoski, O Grupce, B Kaitner, A D Rae and S W Ng: *Small imperfection causes a very small molecule to pack in a very large cell: Sodium saccharinate 1.875 hydrate with unit cell of 15.6nm*^{3}

A D Rae: *Prototype structures and structure algebra as an aid to the refinement of problem structures*

Singapore-Australia Collaborative and Co-operative Chemistry Symposium (SAuCCCS), Singapore, 22–23 November 2006. The following invited lecture was presented:

R L Withers: *Local crystal chemistry, inherent structural flexibility and its consequences*

11th Reactive Organometallics Symposium (ROMS 11), University of New South Wales, Sydney, NSW, 24 November 2006. The following lectures were presented:

R L Cordiner, P J Low and F Hartl: *Synthesis and electrochemistry of novel cyanoacetylide compounds*

J Wagler: *Hypercoordinate silicon complexes with bidentate (ON) and tetradentate (ONNO) ligand systems*

IC07, Hobart, TAS, 4–8 February 2007. The following posters were presented:

N L Kilah, S B Wild: *Deracemisation of chiral phosphines by asymmetric transformation*

J Wagler and D Gerlach: *Hypercoordinate silicon complexes of the dianion of pyrrole-2-N-(o-hydroxyphenyl)-carbaldimine*

M L Weir, N L Kilah, A C Willis and S B Wild: *Asymmetric syntheses of chiral diarsines via bis(phosphine-stabilised) diarsenium salts*

31st Australian Institute of Physics, Condensed Matter and Materials Meeting, Wagga Wagga, NSW, 6-9 February 2007. The following lectures were presented:

A-K Larsson, A M Carnerup, S T Hyde and J D Fitzgerald: *Crystallography of biomimetic silica carbonate precipitates*

Y Liu, R L Withers and T R Welberry: *The superstructure phase of microwave dielectric* $(Bi_{1.5}Zn_{0.5})(Ti_{1.5}Nb_{0.5})O_7$ *pyrochlore*

The following posters were also presented:

L Norén, A-K Larsson, R L Withers and H Rundlöf: *Te for two, II: A neutron powder diffraction study of the structure of the* 'Ni_3InTe_2' *solid solution*

R L Withers, Y Liu, X Wei and J D Fitzgerald: *Structured diffuse scattering and polar nano regions in the* $Ba(Ti_{1-x}Sn_x)O_3$ *relaxor ferroelectric system*

SCANZ 2007 Conference – Crystal XXV, Hunter Valley, NSW, 10-13 April 2007. The following lecture was presented:

A D Rae: *A false minimum in the refinement of a 9x superstructure. A problem with commensurately modulated structures with a cell volume (2N+1) that of a parent structure.*

The following posters were also presented:

B Nguyen: *The local crystal chemistry and dielectric properties of the cubic pyrochlore phase in the* Bi_2O_3-M^2+O-Nb_2O_5 (M^2+ = *Ni and Mg) systems*

A C Willis and A D Rae: *A pseudo cubic structure with weak extra reflections: The structures of* $[M\{N(CH_2CH_2P(ipr)_2)_3\}CO](BPh_4)$ *M=Rh, Ir*

R L Withers, Y Liu, X Wei and J D Fitzgerald: *Structured diffuse scattering and polar nano regions in the* $Ba(Ti_{1-x}Sn_x)O_3$ *relaxor ferroelectric system*

Materials and Austceram 2007, Sydney, NSW, July 4–6 2007. The following lecture was presented:

Y Liu, R L Withers, B Nguyen, L Norén and A-K Larsson: *Towards the development of high performance, frequency agile, RF/microwave dielectric ceramics based on nanoscale structural analysis*

American Crystallographic Association (ACA), 2007 Annual Meeting, Salt-Lake City, USA, 21-26 July 2007. The following invited lecture was presented:

A D Rae: *Problem structures: Attempts to rationalise their description and refinement*

12th Reactive Organometallics Symposium (ROMS 12), University of New South Wales, Sydney, NSW, 24 July 2007. The following lectures were presented:

I A Cade: *Borabenzenes – synthesis and reactivity*

J Wagler: *Atranomania – metallaboratranes and more*

24th European Crystallographic Meeting, Marrakech, Morocco, 22–27 August 2007. The following poster was presented:

A D Rae: *Problem structures: Attempts to rationalise their description and refinement*

4th European Silicondays, Bath, UK, September 2007. The following lecture was presented:

J Wagler: *Silicon complexes of dianionic tridentate (ONO) and (NNO) chelating ligands*

The following poster was also presented:

J Wagler and A F Hill: *Novel penta- and hexacoordinate silicon complexes via templated ligand synthesis from benzoxazolin-2-one*

The Cowley-Moodie Symposium: Celebrating 50 Years of Multislice, Brighton Savoy Hotel, Melbourne, VIC, 6 November 2007. The following lecture was presented:

R L Withers: *Local crystal chemistry, inherent structural flexibility and the consequences for materials chemistry*

13th Reactive Organometallics Symposium (ROMS 13), Australian National University, Canberra, ACT, 27 November 2007. The following lectures were presented:

I A Cade, A F Hill and J Wagler: *M→B bonding in late transition metallaboratranes*

R L Cordiner, L M Caldwell, A F Hill and A C Willis: *The incorporation of selenium into unsaturated carbon chains*

Organic Chemistry

Supramolecular Chemistry Symposium, held in Honour of Professor Len Lindoy, University of Sydney, NSW, 27 February 2006. The following invited lecture was presented:

C J Easton: *Cyclodextrin molecular reactors and nanoscale devices*

The following posters were also presented:

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

R E Dawson, C J Easton, A Herlt and S F Lincoln: *Cyclodextrins with ditopic axles as the basis of molecular shuttles*

Indirubin, The Red Shade Of Indigo, Dordogne, France, 8-13 April 2006. The following invited lecture was presented:

C J Easton: *A molecular reactor for the synthesis of indirubin and related compounds*

13th International Cyclodextrin Symposium, Torino, Italy, 14-17 May 2006. The following invited lecture was presented:

C J Easton: *Cyclodextrin molecular reactors and nanoscale devices*

Centre of Excellence For Free Radical Chemistry and Biotechnology Winter Symposium, Canberra, ACT, 5-6 June 2006. The following lectures were presented:

L Carpinelli and M S Sherburn: *The intramolecular radical carboxyarylation reaction: Scope and application to natural product synthesis*

I Li: *Free radical reactions for the regulation of peptide hormones*

E L Pearson and M S Sherburn: *Towards the total synthesis of viridin* **for which E Pearson was awarded the Best Student Lecture Prize**

Y-C Tsai: *Oxidative processing of amino acid derivatives*

Joint International Symposium on Macrocyclic and Supramolecular Chemistry, Vancouver, Canada, 25-30 June 2006. The following poster was presented:

S Maniam: *Towards three-stationed molecular shuttles*

Southern Highlands Conference on Heterocyclic Chemistry, Moss Vale, NSW, 27-29 August 2006. The following posters were presented:

M G Banwell, A Bissember and A C Willis: *Dichlorocarbene adducts of enamines as precursors to pyrroles*

O Kokas, M G Banwell: *A chemoenzymatic approach to the montanine alkaloids*

4th Sino-Australia Organic Chemistry Symposium, Beijing, China, 26-28 September 2006. The following invited lecture was presented:

M G Banwell: *Chemoenzymatic methods for the assembly of biologically active natural products*

RACI NSW Branch Natural Products Group Symposium, Wollongong, NSW, 29 September 2006. The following lecture was presented:

N A Miller and M S Sherburn: *Total synthesis of triptolide*

10th European Panel Products Symposium, Wales, UK, 11-13 October 2006. The following invited lecture was presented:

A Philbrook, S Earnshaw, C J Easton and T R Webber: *Novel amino resins*

2nd Pacific Symposium on Radical Chemistry, Daejeon, Korea, 5-8 November 2006. The following posters were presented:

I Li: *Free radical reactions for the regulation of peptide hormones*

Y-C Tsai: *Oxidative processing of amino acid derivatives*

Singapore-Australia Chemistry Collaborative and Cooperative Symposium, National University of Singapore, Singapore, 22-23 November 2006. The following invited lecture was presented:

M G Banwell: *A little bit of strain can be good for you: Gem-Dihalogenocyclopropanes as building blocks for chemical synthesis*

RACI NSW Organic Chemistry Group 27th Annual One-Day Symposium 2006, Canberra, ACT, 27 November 2006. The following lectures were presented:

G Bojase-Moleta and M S Sherburn: *Synthesis and reactions of the dendralenes* **for which G Bojase-Moleta was awarded the Best Student Lecture Prize**

D Padmakshan, S A Bennett, G Otting and C J Easton: *Stereocontrolled synthesis of (S)-γ-fluoroleucine*

The following posters were also presented:

S Maniam: *Three-stationed rotaxane molecular switches*

A Philbrook: *Demonstration of co-polymerisation in melamine-urea-formaldehyde resins*

15th Annual Conference of the Society for Free Radical Research (Australasia), Perth, WA, 1-4 December 2006. The following invited keynote lecture was presented:

C J Easton and Z I Watts: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions*

New Zealand Institute of Chemistry Conference, Rotorua, New Zealand, 2-6 December 2006. The following keynote lecture was given:

C J Easton and Z I Watts: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions*

The following poster was also presented:

A Philbrook, S Earnshaw and C J Easton: *Novel amino resins*

RACI Organic Chemistry Division Annual Synthesis Symposium, Flinders University, Adelaide, SA, 4 December 2006. The following invited lecture was presented:

M G Banwell: *Chemoenzymatic methods for the assembly of biologically active natural products*

2nd International Conference on Heterocyclic Chemistry, Jaipur, India, 16-19 December 2006. The following invited lecture was presented:

M G Banwell: *New processes for the synthesis of biologically relevant heterocycles*

22nd Royal Australian Chemical Institute Organic Conference (22RACIOC) and the 6th RACI Conference on Physical Chemistry (CPC2007), Adelaide, SA, 28 January – 2 February 2007. The following invited Le Fèvre Award lecture was presented:

M S Sherburn: *Everything you always wanted to know about synthesis*

The following invited keynote lecture was also presented:

C J Easton and Z I Watts: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions – why peptides were the original biopolymers*

The following lectures were also presented:

T Bradford and M S Sherburn: *Controlling domino sequences*

L Carpinelli and M S Sherburn: *The good, the bad and the ugly - new frontiers for radical intramolecular carboxyarylation* **for which L Carpinelli was awarded the Best Student Lecture Prize**

S Maniam, S F Lincoln and C J Easton: *Three-stationed rotaxane molecular switches*

H Onagi, R J Coulston, S F Lincoln and C J Easton: *Molecular machines and switches at work*

The following posters were also presented:

S K Bowen, C J Easton, S F Lincoln and H Onagi: *Cyclodextrins as molecular reactors*

G Bojase-Moleta and M S Sherburn: *Practical synthesis and cycloaddition reactions of [5]dendralene*

A Buchan, and C J Easton: *Enzyme catalysis of non-biological reactions*

S Chand, C J Easton and I Li: *Inhibition of peptidylglycine α-amidating monooxygenase*

R J Coulston, H Onagi, S F Lincoln and C J Easton: *Harnessing the energy of molecular recognition in a molecular machine having a photochemical on/off switch*

R E Dawson, C J Easton, S F Lincoln and H Onagi: *Stilbene and cyclodextrins as the basis of a light driven molecular muscle*

T Fallon and M S Sherburn: *Furano-dendralenes* **for which T Fallon was awarded the Best Student Poster Prize**

J E Hennessy and C J Easton: *Post-translational chemical modification of enzyme active sites*

S A Ivanic, G P F Wood, G B Bacskay, C J Easton and L Radom: *Thermodynamic and kinetic indications of radical stability*

N Kanizaj and M S Sherburn: *Superbowl molecules*

L C H Kwan, M N Paddon-Row and M S Sherburn: *Enantioselective catalysis of IMDA reactions*

A I Longshaw, W J Lording, M S Sherburn and M N Paddon-Row: *The intramolecular Diels–Alder reaction of ether tethered trienes*

W J Lording, M N Paddon-Row and M S Sherburn: *A deeper understanding of the intramolecular Diels-Alder reaction*

I Louis, M Norret and M S Sherburn: *Synthetic studies towards Nic-10*

N A Miller and M S Sherburn: *A concise formal total synthesis of triptolide*

T V Nguyen, D S Sinclair and M S Sherburn: *Synthesis and properties of aryl cavitand hosts*

D Padmakshan, S A Bennett, C J Easton and G Otting: *Stereocontrolled synthesis of (S)-γ-fluoroleucine*

A D Payne, M S Sherburn and A C Willis: *Dendralenes: No longer chemical curiosities*

A D Payne, M S Sherburn and A C Willis: *Polycyclic molecules from acyclic molecules using the Diels-Alder reaction*

E L Pearson and M S Sherburn: *Towards the total synthesis of viridin*

A Philbrook, S Earnshaw and C J Easton: *Novel amino resins*

D Robinson and M S Sherburn: *Investigations into the double Diels-Alder reactions of linear conjugated tetraenes*

G Statham and C J Easton: *Photocleavable amino acids for use in peptide hormone prodrugs*

4th Asian Cyclodextrin Conference, Kyoto, Japan, 18-20 May 2007. The following invited lectures were presented:

C J Easton, R J Coulston, H Onagi and S F Lincoln: *Cyclodextrin molecular machines at work*

S F Lincoln, B L May, P D Truc, C J Easton, R K Prud'homme, X Guo, A A Abdala and S A Khan: *Cyclodextrin interactions in aqueous polymeric systems*

The following posters were also presented:

R E Dawson, C J Easton, S F Lincoln and H Onagi: *Stilbene and α-cyclodextrin as the basis of a light-driven molecular muscle* **for which R E Dawson received the Encouragement Award**

S Maniam, S F Lincoln and C J Easton: *Three-stationed molecular switches* **for which S Maniam was awarded the Best Poster Prize**

Gordon Conference on Physical Organic Chemistry, Plymouth, USA, 24-29 June 2007. The following poster was presented:

C J Easton (Session Chair), R J Coulston, H Onagi and S F Lincoln: *Harnessing the energy of molecular recognition in a molecular machine having a pH dependent on/off switch*

Gordon Research Conference on Radicals and Radical Ions in Chemistry and Biology, Plymouth, USA, 1–6 July 2007. The following plenary invited lecture was presented:

M S Sherburn: *New domino radical sequences and their application in target synthesis*

4th Conference on Mechanism and Synthesis: Reactive Intermediates and Unusual Molecules, Heron Island, QLD, 7-14 July 2007. The following invited lectures were presented:

M G Banwell: *Base-promoted reactions of the dihalocarbene adducts of enol ethers and enamines – useful routes to furans and pyrroles*

C J Easton: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions – why peptides were the original biopolymers*

L N Mander: *Enabling strategies for the assembly of complex natural products: A retrospective*

21st International Conference on Heterocyclic Chemistry, University of New South Wales, Sydney, NSW, 15-20 July 2007. The following invited lecture was presented:

M G Banwell: *New processes for the synthesis of biologically relevant heterocycles*

The following posters were also presented:

T Fallon and M S Sherburn: *Furano-dendralenes*

C Gray, L C H Kwan and M S Sherburn: *A double intramolecular Diels-Alder approach to tetracycles*

20th International Symposium: Synthesis in Organic Chemistry, University of Cambridge, UK, 16–19 July 2007. The following plenary invited lecture was presented:

M S Sherburn: *Synthesis inspired by efficient domino reactions*

The following poster was also presented:

W J Lording, M N Paddon-Row and M S Sherburn: *A deeper understanding of the intramolecular Diels-Alder reaction*

41st IUPAC Congress, Torino, Italy, 5-10 August 2007. The following invited lecture was presented:

C J Easton: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions – why peptides were the original biopolymers*

234th Meeting of the American Chemical Society, Boston, USA, 19-23 August 2007. The following lecture was presented:

A Philbrook, S Earnshaw and C J Easton: *Fluorescent tags for amino resins*

12th Asian Chemical Congress, Kuala Lumpur, Malaysia, 23-25 August 2007. The following keynote lecture was presented:

C J Easton: *Resistance of the α-amino acid and peptide structural motifs towards radical reactions – why peptides were the original biopolymers*

Centre of Excellence For Free Radical Chemistry and Biotechnology Spring Symposium, Melbourne, VIC, September 2007. The following lectures were presented:

D Brittain: *Tunnelling in 1,4- and 1,5-hydrogen shifts in peptide radicals*

S Chand: *Kinetic isotope effects and hydrogen atom transfer in radical species*

T V Nguyen and M S Sherburn: *Functionalisations and host-guest binding studies with superbowl molecules*

E L Pearson and M S Sherburn: *Towards the total synthesis of viridin*

Z Watts: *Functionalisation of unactivated amino acid C-H bonds*

The following posters were also presented:

A Buchan and C J Easton: *Enzyme catalysis of non-biological reactions*

R J Coulston, H Onagi, N Spilman, C J Easton and S F Lincoln: *Harnessing the energy of molecular recognition in a molecular machine having a pH dependent on/off switch*

R E Dawson, C J Easton, S F Lincoln and H Onagi: *Stilbene and α-cyclodextrin as the basis of a light-driven molecular muscle*

S A Ivanic, M Taylor, G P F Wood, G B Bacskay, C J Easton and L Radom: *Abstraction reactions associated with model peptides*

A Longshaw, M Carland, E Krenske, M Coote and M S Sherburn: *Tris(Trimethylsilyl)methane is not an effective mediator of radical reactions*

S Maniam, S F Lincoln and C J Easton: *Three-stationed rotaxane molecular switches*

D Padmakshan, S A Bennett, C J Easton and G Otting: *Stereocontrolled synthesis of (S)-γ-fluoroleucine*

E Wiadrowski and M S Sherburn: *Stretching the boundaries of the radical carboxyarylation reaction*

Training Workshop, Monash University Centre for Green Chemistry, Melbourne, VIC, 29-30 November 2007. The following invited lecture was presented:

M G Banwell: *Green chemistry - how can industry and the public sector be better engaged by the Centre?*

4th Joint Meeting of the Society for Free Radical Research (SFRR) Australasia and Japan, Kyoto, Japan, 1-5 December 2007. The following plenary lecture was presented:

C J Easton: *The role of radicals in peptide and protein evolution*

The following lectures were also presented:

S Chand, C K Barlow, D Brittain, M L Coote, R A J O'Hair, L Radom and C J Easton: *1,4- and 1,5-hydrogen atom transfer in amino acid and peptide radicals*

Z Watts, D K Jordan and C J Easton: *Synthesis of peptides incorporating non-proteinogenic amino acids produced through radical functionalisation of proteinogenic analogues* **for which Z Watts received the Young Investigator Award**

The following poster was also presented:

D Padmakshan, C J Easton, S A Bennett and G Otting: *Stereocontrolled synthesis of (S)-γ-fluoroleucine*

RACI Organic Chemistry Division One-day Symposium, Macquarie University, Sydney, NSW, 5 December 2007. The following invited lectures were presented:

T Fallon and M S Sherburn: *Furano-dendralenes*

T V Nguyen and M S Sherburn: *Functionalisations and host-guest binding studies with superbowl molecules*

T Reekie: *Bacteria, microwaves and light: An enantioselective total synthesis of (-)-phellodonic acid*

32nd Annual Synthesis Symposium, University of Melbourne, VIC, 7 December 2007. The following plenary invited lecture was presented:

M S Sherburn: *Total synthesis inspired by efficient domino reactions*

Annual Synthesis Symposium, University of Adelaide, SA, 10 December 2007. The following plenary invited lecture was presented:

M S Sherburn: *Total synthesis inspired by efficient domino reactions*

International Symposium on Catalysis and Fine Chemicals, Nanyang Technological University, Singapore, 17-21 December 2007. The following invited lectures were presented:

M G Banwell: *Chemoenzymatic methods for the assembly of biologically active natural products*

C J Easton: *Cyclodextrin molecular reactors and nanoscale devices*

Physical and Theoretical Chemistry

Australia – Japan Consultation on Materials Science, University of Queensland, Brisbane, QLD, 23 January 2006. The following invited lecture was presented:

J W White: *Chemistry at interfaces*

28th Australasian Polymer Symposium, Rotorua, NZ, February 2006. The following invited lecture was presented:

M L Coote, E I Izgorodina and E H Krenske: *CRAFT: A computer-aided approach to RAFT agent design*

The following lectures were also presented:

H Chaffey-Millar, L-A Carmody, T P Davis, M H Stenzel, M L Coote, C Barner-Kowollik: *Star polymers produced by the RAFT process: Design criteria, kinetics and simulations*

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

E I Izgorodina and M L Coote: *Propagation rate coefficients: Prediction in the frames of quantum theory*

A Theis, C Gudipati, M L Coote, M H Stenzel, T P Davis, C Barner-Kowollik: *RAFT agent design strategies: F-RAFT and recent R-group advances*

The following poster was also presented:

H Chaffey-Millar, A Ah Toy, T P Davis, M H Stenzel, E I Izgorodina, M L Coote and C Barner-Kowollik: *Using thioketone spin traps as mediating agents for free radical polymerisation processes: Theory and practice*

The Australian and New Zealand Institute of Physics 30th Annual Condensed Matter and Materials Meeting, Wagga Wagga, NSW, 7-10 February 2006. The following lecture and poster was presented:

D J Goossens, M E Hagen, X Wu and T R Welberry: *The structural phase transition in deuterated benzil,* $C_{14}O_2D_{10}$

J W White, M J Henderson, A Gibaud, A Rennie and A Hawley: *Titania and zirconia film formation at interfaces*

First Australian-Italian Workshop On Statistical Physics: Statistical Systems Out Of Equilibrium: Random Systems and Complex Fluids, Goldcoast, QLD, 12-15 February 2006. The following invited lecture was presented:

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

Principles of the Dynamics of Non-Equilibrium Systems, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, 10-31 March 2006. The following invited lecture course was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

American Physical Society, March Annual Meeting, Baltimore, USA, 13-17 March 2006. The following lecture was presented:

D J McGillivray: *Charge inversion near modulated interfaces by multivalent counterion*

Work, Dissipation & Fluctuations in Nonequilibrium Physics, Brussels, Belgium, 22-25 March 2006. The following invited lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

The Biotechnology Industry Organization, Bio 2006, Chicago, USA, 9-12 April 2006. The following invited lecture was presented:

D J McGillivray: *Neutrons and biology*

MM2006, Perth, WA, 19 April 2006. The following invited lecture was presented:

P M W Gill: An optimal point charge model for molecular electrostatic potentials

APS User Meeting, Argonne, USA, May 2006. The following invited lecture was presented:

T R Welberry: *Diffuse scattering and models of disorder: New opportunities for diffuse X-ray and neutron scattering*

Dairy Ingredients and Emulsions, Food Science Australia, Werribee, VIC, 5 May 2006. The following invited lecture was presented:

J W White and A Jackson: *Empirical practice & nanoscale formulation*

International Congress of Quantum Chemistry, Satellite Meeting, Tokyo, Japan, 18 May 2006. The following invited lecture was presented:

P M W Gill: *Dispersion energies from intracules*

The XIIth International Congress of Quantum Chemistry (ICQC), Kyoto, Japan, 21-26 May 2006. The following poster was presented:

C Y Lin, M L Coote, R Poli and K Matyjaszewski: *Penultimate unit effects in atom transfer radical polymerisation* **for which C Y Lin was awarded the Poster Prize**

89th Canadian Chemistry Conference, Halifax, Canada, 27-31 May 2006. The following lectures were presented:

P M W Gill: *New ways of thinking about London forces and dispersion*

B Viswanathan, D R B Brittain, E I Izgorodina, and M L Coote: *Application of DFT methods to the thermochemistry of organic chemistry reactions: Advisable?*

Dairy Ingredients Group, Melbourne, VIC, 29 May 2006. The following invited lecture was presented:

J W White: *Denaturation of proteins at interfaces at the nanometer scale*

Free Radical Winter Carnival, Inaugural Symposium for Members and Friends of the ARC Centre of Excellence for Free Radical Chemistry and Biotechnology, Canberra, ACT, 5-6 June 2006. The following lectures were presented:

M L Coote, E H Krenske, E I Izgorodina, M Busch and C Barner-Kowollik: Ab initio *polymerisation: Modelling the initialisation period in RAFT polymerisation*

E H Krenske, M L Coote, M S Sherburn and K L Goh: *Hypophosphorous acid as a radical chain carrier – quantum chemical investigations*

The following posters were also presented:

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

C Y Lin, M L Coote, R Poli, and K Matyjaszewski: *Penultimate unit effects in atom transfer radical polymerisation*

Seventh Liblice Conference on the Statistical Mechanics of Liquids, Czech Republic, 11-16 June 2006. The following plenary lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

American Conference of Neutron Scattering, Illinois, USA, 18-22 June 2006. The following lecture was presented:

D J McGillivray: *Magnetic underlayer contrast for neutron reflectometry*

Ninth International Conference on Hole Burning, Single Molecule and Related Spectroscopies: Science and Applications, Paul Langevin Centre, Aussios, France, 24-29 June 2006. The following poster was presented:

J Hughes, L Debono, R Steffen and E Krausz: *Spectral 'hole blasting' and 'trench digging' in photosynthetic assemblies*

Gordon Photosynthesis Conference, Bryant University, Smithfield, Rhode Island, USA, 2-7 July 2006. The following invited lecture was presented:

Elmars Krausz: *Photosynthesis limbo: How low can you go to make oxygen?*

The following poster was also presented:

N Penwin, F Ho, R Stefan, N Cox, P J Smith, J Hughes, L Debono, E Krausz, S Styring, R J Pace: *Cryogenic*

illumination (<20K) of photosystem II: Demonstration of a tyrosine-manganese exchange coupled 'split signal' interaction

London Mathematical Society Durham Symposium, Dynamical Systems and Statistical Mechanics, Durham, UK, 3-9 July 2006. The following invited lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

International Workshop on Mesoscale and Multiscale Description of Complex Fluids (IWMMCOF 2006), Monash University, Prato Centre, Italy, 5- 8 July 2006. The following invited lecture was presented:

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

The following lecture was also presented:

R Prabhakar: *Coarse-graining of hydrodynamic and excluded volume interactions in polymer chains*

Physical Chemistry of Foods, Adelaide, SA, 8 July 2006. The following invited lecture was presented:

J W White: *Protein structure in thin films*

EUCHEM Conference on Organic Free Radicals, Bergen, Norway, 9-13 July 2006. The following poster was presented:

E H Krenske, M S Sherburn and M L Coote: *Hypophosphorous acid as a radical chain carrier: Computational investigations*

FOMMS 2006, Foundatons of Molecular Modelling and Simulation, Blaine, USA, 9-14 July 2006. The following plenary lecture was presented:

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

7th Girona Seminar, Girona, Spain, 12 July 2006. The following invited lecture was presented:

P M W Gill: *A new way to calculate dispersion energies*

Meeting of the American Crystallographic Association, Honalulu, Hawaii, USA, 22-27 July 2006. The following lectures were presented:

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

D J McGillivray: *Grazing Incidence Small-Angle Neutron Scattering (GISANS): Techniques and applications to bilayer membranes*

23rd European Crystallography Meeting, Leuven, Belgium, August 2006. The following lectures were presented:

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

T R Welberry, A G Beasley and B Sing: *Deformed Penrose tilings*

16th Symposium on Thermophysical Properties Conference, Boulder, Colorado, USA, 30 July – 4 August 2006. The following plenary lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

Macro Group UK International Conference on Polymer Synthesis, Warwick UK, 31 July - 3 August 2006. The following lectures were presented:

C Barner-Kowollik, M H Stenzel, M L Coote, H Chaffey-Millar, T P Davis, Z Szablan, A Ah Toy and J Chiu: *Designing new controlling protocols for free radical polymerisation – designing new polymer structures*

H Chaffey-Millar, M H Stenzel, T P Davis, M L Coote and C Barner-Kowollik: *Design criteria for star polymer formation processes via living free radical polymerisation (RAFT)*

Sagamore 2006, Warwick, UK, 14 August 2006. The following invited lecture was presented:

P M W Gill: *Calculating dispersion energies from the Wigner distribution*

Symposium on Nonlinear Dynamics of Nanosystems, Chemnitz, Germany, 28-30 August 2006. The following lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

American Chemical Society Conference, San Francisco, USA, September 2006. The following invited lecture was presented:

M A Collins: *Diabatic potential energy matrices for nonadiabatic dynamics*

Nonequilibrium Thermodynamics and Complex Fluids, Rhodes, Greece, 3-7 September 2006. The following lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

Aperiodic 2006, Zao, Miyagi Prefecture, Japan, 17–22 September 2006. The following invited lectures were presented:

T R Welberry and B Sing: *Deformed Penrose tilings*

Centre Europeen de Calc Atomique et Moleculaire (CECAM) Workshop: Theory of Single Molecule Force Experiments and Simulations, Lyon, France, 26-29 September 2006. The following invited lectures were presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

DICP Symposium on Molecular Dynamics, Dalian, China, October 2006. The following invited lecture was presented:

M A Collins: *Diabatic potential energy matrices for nonadiabatic dynamics*

Theory of Molecular and Macromolecular Kinetics: A Symposium held in Honour of Professor Bob Gilbert's 60th Birthday, University of Sydney, NSW, October 2006. The following lecture was presented:

M A Collins: *Molecular potential energy surfaces and matrices for chemical reaction dynamics*

AMSI Workshop: Mathematical Formulation of Micro and Macro Thermodynamics, Melbourne University, VIC, 10 October 2006. The following invited lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

2nd Pacific Symposium on Radical Chemistry, Daejeon, Korea, 5-8 November 2006. The following lecture was presented:

E H Krenske, M S Sherburn and M L Coote: *Hypophosphorous acid as a radical chain carrier: Computational investigations*

The following poster was also presented:

E H Krenske and M L Coote: *Hydrogen and chlorine transfer reactions relevant to PVC degradation*

Singapore-Australia Chemistry Symposium, Singapore, 22-23 November 2006. The following lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

Ninth International Conference on Surface X-ray and Neutron Scattering, Taipei, Taiwan, 29 November 2006. The following invited lecture was presented:

R Garrett and J W White: *Reflectometry to study layer by layer growth of protein-inorganic films*

Australian Synchrotron Users Meeting, Melbourne, VIC, 29 November - 1 December 2006. The following lecture was presented:

D J McGillivray: *Anomalous X-ray reflectivity from charged surfaces*

17th Biennial Congress of the Australian Institute of Physics, Brisbane, QLD, December 2006. The following lecture was presented:

T R Welberry, D J Goossens and M J Gutmann: *The mechanism behind the polar nano-domain structure in relaxor ferroelectric* $Pb(Zn_{1/3}Nb_{2/3})O_3$, *PZN*

New Zealand Institute of Chemistry Conference, Rotorua, New Zealand, 2-6 December 2006. The following invited lectures were presented:

P M W Gill: *Electron correlation: Back to basics*

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

AIP Congress, Brisbane, QLD, 3-8 December 2006. The following lectures were presented:

R Prabhakar: In silico *demonstration of Crooks relation for a Brownian particle in a time-dependent harmonic trap*

G M Wang: *Demonstration of Fluctuation Theorem in a viscoelastic solution using optical tweezers*

AirUCI Workshop, University of Canterbury, New Zealand, 11 December 2006. The following plenary lecture was presented:

J W White: *Energy from water and sunlight*

AINSE/ANSTO Neutron Scattering Symposium, Sydney, NSW, 11-13 December 2006. The following lectures were presented:

D J Goossens, A G Beasley and M J Gutmann: *Neutron diffuse scattering in para-terphenyl, $C_{18}D_{14}$*

W D Hutchison, D J Goossens, B Saensunon, G A Stewart, M Avdeev and K Nishimura: *Magnetic order studies of $RNiAl_4$*

D J McGillivray: *The effects of high-pressure treatments on milk proteins*

Society of Photo-Optical Instrumentation Engineers (SPIE), Adelaide, SA, 12 December 2006. The following invited lecture was presented:

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

Physical and Chemical Aspects of Molecular Biology, Joint NSF-Mexico Workshop, Puebla, Mexico, 4-6 January 2007. The following lecture was presented:

D J McGillivray: *Toxin interactions with tethered bilayer lipid membranes*

Laue2007: International Workshop on Advanced Laue Diffraction in Frontier Science, Grenoble, France, 23-27 January 2007. The following lecture was presented:

D J Goossens: *Laue diffuse scattering with X-rays and neutrons*

6th RACI Organic and Physical Chemistry Conference, Adelaide, SA, 28 January - 2 February 2007. The following invited lectures were presented:

M A Collins: Ab initio *molecular energies by fragmentation: A feasible strategy for reaction dynamics and molecular and crystal properties*

P M W Gill: *Van der Waals interactions: Can't live with 'em, can't live without 'em!*

J L Hughes and E Krausz: *Electrochromic hole-blasting in photosystem II cores: Identifying the players and tracking charge transfer*

E M Sevick: *Experimental demonstrations of new theorems in non-equilibrium thermodynamics*

The following lectures were also presented:

M L Coote, E H Krenske and M S Sherburn: *Hypophosphorus acid as a radical chain carrier – quantum chemical investigations*

M L Coote, E I Izgorodina and C Y Lin: *Energy-directed tree search: An efficient systematic algorithm for finding the lowest energy conformation of oligomeric molecules*

M L Coote, J L Hodgson and K A Green: *Radical addition to P=S versus C=S double bonds: Are phosphorus-centred radicals really more stabilised than carbon-centred radicals*

The following posters were also presented:

D R B Brittain, M L Coote, A T B Gilbert, P M W Gill, E I Izgorodina and B Viswanathan: *Limitations of Density Functional Theory*

A Dick, M Riley, E Krausz, G Schenk, L Gahan, G Hanson and A Neves: *Magnetic circular dichroism studies into a series of biomimetic analogues for red kidney bean purple acid phosphatase*

J L Hodgson, M L Coote and S E Bottle: *Biological protection from oxidative damage by nitroxide antioxidants*

J Hughes, B Conlan, R Razeghifard, A Oakley, T Wydrzynski and E Krausz: *Chlorophyll-chrolophyll and chlorophyll-protein interactions studied by persistent spectral hole-burning of a protein tetramer binding two excitation-coupled chlorophylls*

C Y Lin, M L Coote, R Poli and K Matyjaszewski: *Penultimate unit effects in atom transfer radical polymerisation*

Australian Colloid and Interface Symposium, Sydney, NSW, 4-8 February 2007. The following lecture was presented:

D J McGillivray: *Structure of functional toxin pores in tethered bilayers: Membrane association of a-hemolysin*

The Australian and New Zealand Institute of Physics 31st Annual Condensed Matter and Materials Meeting, Wagga Wagga, NSW, 6-9 February 2007. The following lectures were presented:

P A Altin and D J Goossens: *Diffuse X-ray scattering from optically pure ibuprofen*

D J Goossens and A P Heerdegen: *ZMC: A program for modelling short-range order in molecular crystals*

D J Goossens and K F Wilson: *Improving student engagement in third year CMP: A case study*

W D Hutchison, D J Goossens, B Saensunon, G A Stewart, M Avdeev and K Nishimura: *Magnetic order studies of $ErNiAl_4$*

29th Australasian Polymer Symposium, Hobart, Tasmania, 11-15 February 2007. The following invited keynote lectures were presented:

M Busch, M Roth, K Becker, C Barner-Kowollik, M L Coote: *Kinetics and simulation of polymerisation reactions*

M L Coote, E H Krenske, E I Izgorodina, M Busch, C Barner-Kowollik: Ab initio *kinetic modelling free radical polymerisation*

The following lectures were also presented:

H Chaffey-Millar, E I Izgorodina, C Barner-Kowollik and M L Coote: *A quantum-chemical approach to polymerisation design: Thioketone mediated polymerisation*

T Junkers, M L Coote, T P Davis, M H Stenzel and C Barner-Kowollik: *Using spin traps in radical polymerisation: A new approach to achieve controlled polymerisation characteristics*

The following poster was also presented:

J L Hodgson, S E Bottle and M L Coote: *Structure reactivity trends in nitroxide mediated polymerisation*

Materials with Designed Functions JSPS – DST Asian Academic Seminar, Pune, India, 23 February 2007. The following plenary lecture was presented:

J W White: *Hydrogen from water and sunlight*

American Physical Society Meeting, Denver, USA, 6 March 2007. The following invited lecture was presented:

P M W Gill: *Resolutions of the Coulomb operator*

Crystal 25, Meeting of the Society of Crystallographers in Australia and New Zealand, Hunter Valley, NSW, April 2007. The following invited lectures were presented:

A G Beasley: *Disorder in polymorphic systems*

T R Welberry, L H Thomas, D J Goossens and A P Heerdegen: *Disorder in pentachloronitrobenzene, $C_6Cl_5NO_2$: A diffuse scattering study*

Nonlinear Dynamics Meets Stochastic Dynamics Workshop, Erwin Schroedinger Institute, Vienna, Austria,18-20 April 2007. The following lecture was presented:

D J Evans: *The fluctuation & nonequilibrium free energy theorems, theory & experiment*

Royal Society/Novartis Foundation Discussion Meeting, London, UK, 25 April 2007. The following invited lecture was presented:

E Krausz: *Revealing how nature uses sunlight to split water: What is and where is the primary oxidant PSII?*

International Symposium on Theory of Atomic and Molecular Clusters, Richmond, USA, 14 May 2007. The following invited lecture was presented:

P M W Gill: *Resolutions of the Coulomb operator*

Southeastern Theoretical Chemistry Association 2007, Blacksburg, USA, 18 May 2007. The following invited lecture was presented:

P M W Gill: *Foundations of intracule functional theory*

Molecular Quantum Mechanics, Budapest, Hungary, 30 May 2007. The following invited lecture was presented:

P M W Gill: *Electron correlation: A Hungarian dance in three movements*

***IX QRS* Workshop on Quantum Reactive Scattering,** University of Cambridge, UK, July 2007. The following invited lecture was presented:

M A Collins: *Molecular potential energy surfaces constructed from interpolation of systematic fragment surfaces*

Mathematical Challenges in Quantum Chemistry, Warwick, UK, 17 July 2007. The following invited lecture was presented:

P M W Gill: *Accurate computation of electronic energies via the Wigner distribution*

American Crystallographic Association (ACA), 2007 Annual Meeting, Salt-Lake City, USA, 21-26 July 2007. The following invited lectures were presented:

A G Beasley, T R Welberry, D J Goossens and A P Heerdegen: *A study at 150K and 295K of the disorder in the polymorphic system p-methylbenzylidene-p-methylaniline*

T R Welberry, D J Goossens, A G Beasley and A P Heerdegen: *Diffuse scattering as a probe of nanoscale structure and function*

14th International Congress of Photosynthesis, Glasgow, Scotland, 22-27 July 2007. The following posters were presented:

N Cox, J Hughes, R Steffen, P Smith, A Rutherford, E Krausz and R Pace: *The primary electron acceptor of photosystem II is weakly coupled to the accessory chlorophyll and the plastoquinone Q*

J Hughes, R Steffen, N Cox, P Smith, R Pace, A Rutherford and E Krausz: *What is the origin of the highly dispersive quantum efficiencies for secondary donor oxidation at low temperature in photosystem II?*

R Steffen, J Hughes, N Cox, P Smith, R Pace, A Rutherford and E Krausz: *Secondary donors in low-temperature optical spectroscopy of photosystem II*

Society of Photo-Optical Instrumentation Engineers (SPIE), San Diego, USA, 26 August 2007. The following invited lecture was presented:

E M Sevick: *Fluctuation theorems: Demonstrations using optical tweezers*

16th Canadian Symposium on Theoretical Chemistry, St. John's, Newfoundland, Canada, 9 August 2007. The following lecture was presented:

P M W Gill: *Electron correlation through the lens of the omega intracule*

Free Radical Spring Carnival, Melbourne, VIC, 4-5 September 2007. The following lectures were presented:

D R B Brittain, S Chand, C Easton, M L Coote, C Barlow and R O'Hair: *Tunnelling in 1,4- and 1,5-hydrogen shifts in peptide radicals*

J L Hodgson, S E Bottle and M L Coote: *One-electron oxidation and reduction potentials of nitroxide antioxidants: A theoretical study*

The following poster was also presented:

M Namazian and M Coote: *Calculation of absolute one-electron redox potentials of some para-quinone derivatives in acetonitrile*

2nd Japan-Australia Symposium, Matsumoto, Japan, 19-23 September 2007. The following poster was presented:

J Mata: *Block copolymer nanoaggregates: Their characterisation and use in different applications*

3rd Asia-Pacific Conference on Theoretical and Computational Chemistry, Beijing, China, 23 September 2007. The following invited lecture was presented:

P M W Gill: *Electron correlation models based on the morph operator*

Dairy Ingredients Group, Melbourne, VIC, 28 September 2007. The following invited lecture was presented:

A W Perriman, J W White and D J McGillivray: *Casein assembly at the air-water interface*

AMSI: Concepts of Entropy and their Applications Workshop, Melbourne University, VIC, 28-30 November 2007. The following keynote lecture was presented:

D J Evans, D J Searles and L Rondoni: *Nonlinear response theory and the fluctuation theorem*

AICHE: American Institute of Chemical Engineers Annual General Meeting, Salt Lake City, USA, 4-9 November 2007. The following lecture was presented:

D J Evans: *On the fluctuation theorem and its connection with response theory*

AINBSE/ANBUG Neutron Scattering Symposium, Sydney, NSW, December 2007. The following lecture was presented:

T J Hicks, T Keller, A R Wildes, Pygor and D J Goossens: *Magnetic dipole splitting of magnon bands in a 2-dimensional antiferromagnet*

The following poster was also presented:

J Mata: *Scattering techniques for nanoaggregates of soft matter*

Australian Physiological Society & Australian Society for Biophysics Joint Meeting, Newcastle, NSW, 2-5 December 2007. The following invited lecture was presented:

E Krausz, J L Hughes, A Oakley, B Conlan and T Wydrzynski: *Water-soluble single-chlorophyll-binding proteins (WSCP's) as well-defined systems by which to probe and modify chlorophyll-chlorophyll and chlorophyll-protein interactions*

The following poster was also presented:

P J Smith, N Cox, R Steffen, J L Hughes, E Krausz and R J Pace: *Seasonality of chlorophyll β presence in core complexes of photosystem II from higher plants. A role of photoprotection?*

Plenary and Invited Lectures

Professor M G Banwell

Chemoenzymatic methods for the assembly of biologically active natural products, U Marburg, Germany, 13 February 2006; U Munich, Germany, 21 February 2006; BASF, Ludwigshafen, Germany, 23 February 2006; U Munster, Germany, 24 February 2006

A little bit of strain can be good for you: Gem–dihalogenocyclopropanes as building blocks for chemical synthesis, Free U of Berlin, Germany, 14 February 2006; Clausthal U of Technology, Germany, 17 February 2006; U Freiburg, Germany, 22 February 2006; U Munich, Germany, 27 February 2006; Nanyang Technological U, Singapore, 3 March 2006; U Adelaide, SA, 1 May 2006; U Western Australia, Perth, WA, 1 June 2007; U Sydney, NSW, 2 June 2006; CSIRO Division of Molecular and Health Technologies, VIC, 26 June 2006

Why I chose a career in chemical research, CSIRO Double Helix Club Careers in Science Presentation, CSIRO Discovery, Canberra, ACT, 24 May 2007

Australian Research Council – Discovery, Linkage and Fellowship applications, ANU College of Science Research Office Sponsored Presentation on ARC DP'09 grant applications, ANU, Canberra, ACT, 20 November 2007

Professor M A Collins

Molecular energies and energy surfaces: A feasible strategy for theoretical chemical dynamics, U Sydney Chemistry Society, Sydney, NSW, May 2006; Centre for Molecular Simulation, Swinburne U of Technology, Melbourne, VIC, August 2006

Dr M L Coote

Ab initio *polymerisation,* School of Molecular and Microbial Sciences Seminar Series, U Queensland, Brisbane, QLD, 6 March 2006; School of Chemistry and Physics Seminar Series, U Adelaide, SA, 27 March 2006; School of Chemistry Seminar Series, U Melbourne, VIC, 11 August 2006

Hypophosphorous acid as a radical chain carrier: Computational investigations, École Polytechnique, Palaiseau, France, 5 July 2006. (E H Krenske, M L Coote, M S Sherburn, K L Goh)

Computational investigations of the MADIX/RAFT process at the Australian National University, Industry presentation to Rhodia Recherches, Aubervilliers, France, 7 July 2006. (E H Krenske, M L Coote)

Computational radical polymerisation, School of Chemistry Flagship Seminar Series, U Sydney, NSW, 21 September 2007

Professor N E Dixon

Protein interactions in bacterial DNA replication, U Wollongong, NSW, 15 May 2006

A new kind of protein–DNA interaction in replication termination, Monash U, Melbourne, VIC, 19 June 2006; CSIRO Molecular and Health Technologies, Sydney, NSW, 12 September 2006; Institute for Biomedical Science, U Wollongong, NSW, 15 September 2006; Sydney Protein Group, Sydney, NSW, 8 December 2006

DNA replication: The end of the story, Monash U, Melbourne, VIC, 21 June 2006

A molecular mousetrap in termination of DNA replication, La Trobe U, VIC, 6 September 2006

A new kind of protein–DNA interaction in replication termination, Flagship Seminar, U Sydney, NSW, 4 May 2007

Role of structural disorder in function of a multiprotein machine – the E. coli *replisome,* U Queensland, Brisbane, QLD, 17 September 2007

Professor D J Evans

Nonlinear response theory and the fluctuation theorem, Henri Poincare Institute, France, 17 September – 17 October 2007

Professor P M W Gill

A new way to think about Van der Waals forces, Melbourne U Chemical Society, Melbourne, VIC, 14 June 2006

Calculating London forces and dispersion energies, ETH, Zurich, Switzerland, 29 June 2006

Gridless density functional theory, National U Singapore, Singapore, 27 February 2007

Resolutions of the Coulomb operator, U Bonn, Germany, 3 July 2007

Dr D J Goossens

The mechanism behind the polar nano–domain structure in relaxor ferroelectric $Pb(Zn_{1/3}Nb_{2/3})O_3$, PZN, Argonne National Laboratory, Chicago, USA, October 2006

Diffuse scattering in PCNB, Bragg Institute, ANSTO, Sydney, NSW, 22 November 2007

Diffuse scattering, AINSE/ANSTO/IAEA Summer School on Neutron Diffraction, Sydney, NSW, 3 December 2007

Professor E Krausz

Photosynthesis limbo: How low in energy can you go to make oxygen? U Melbourne, VIC, 24 August 2006

The engine room of life: A new and unexpected low, U Wollongong, NSW, 20 July 2007; U Geneva, Switzerland, 19 June 2007; U Bern, Switzerland, 20 June 2007

Associate Professor E M Sevick

Experimental demonstrations of new theorems in non–equilibrium thermodynamics, U Hong Kong, Hong Kong, 29–30 August 2006; Hong Kong U Science and Technology, Hong Kong, 30 August 2006; NZIC, New Zealand, 2–6 December 2006; MacDiarmid Institute for Advanced Materials and Nanotechnology Institute of Fundamental Sciences, Massey U, New Zealand, 7 December 2006; SPIE, Adelaide, SA, 12 December 2006

Optical Tweezers: What can you pluck, pull or tease with light? ANU's Annual PhB Student Retreat, Kioloa, NSW, 16–18 February 2007

Stretching a single DNA molecule: Optical Tweezers and the Fluctuation Theorems, ANU's Outreach Campaign, Wellington, New Zealand, 15 August 2007; Millenium Hotel, Christchurch, New Zealand, 16–17 August 2007

Fluctuation Theorems: Demonstrations using Optical Tweezers, SPIE, San Diego, USA, 26 August 2007

Associate Professor M S Sherburn

Efficient chemical synthesis of complex, natural, non–natural and big structures, Eskitis Institute, Griffith U, NSW, 29 May 2006; U Toronto, Ontario, Canada, 22 February 2007; U Waterloo, Ontario, Canada, 26 February 2007; Universite de Montreal, Quebec, Canada, 23 March 2007; Merck Frosst Centre for Therapeutic Research, Montreal, Quebec, Canada, 26 March 2007; U Ottawa, Ontario, Canada, 27 March 2007; U Sydney, Flagship Seminar, Sydney, NSW, 11 May 2007; Merck & Co., Inc., New Jersey, USA, 29 June 2007; U York, UK, 20 July 2007; U Manchester, UK, 24 July 2007; U Sheffield, UK, 25 July 2007; Université Pierre et Marie Curie, Paris, France, 17 December 2007; Université Paris–Sud 11, France, 18 December 2007

Everything you always wanted to know about synthesis, Queen's U, Ontario, Canada, 23 February 2007

Professor T R Welberry

Introduction to crystallography, AINSE/ANSTO/IAEA Summer School on Neutron Diffraction, Sydney, NSW, December 2007

Professor J W White

Understanding soft matter by contrast variation, Craig/Leighton Lecture, U Sydney, NSW, February 2006; University of Otago, New Zealand, March 2006

Australian nuclear energy debate, AINSE Winter School, Sydney, NSW, 1 July 2006

Australian Institute of Nuclear Science and Engineering, ANSTO Board, Sydney, NSW, August 2006

Making hydrogen from water and sunlight, Flagship Lecture, U Sydney, NSW, August 2006; Victorian Institute of Chemical Sciences Fellowship Lecture, RMIT, Melbourne, VIC, 29 August; La Trobe U, VIC, 5 September 2007

Stem cell science and ethics, ANU medical students, Canberra, ACT, September 2006

The ethical questions in stem cell research, ANU, Canberra, ACT, September 2006

Issues in stem cell science, Scientific Soiree, Australian Academy of Science, Canberra, ACT, September 2006

(1) The Lockhart Review; (2) Stem cells, science and politics; (3) Ethics from different perspectives, L'Abri Fellowship Meeting, Camden, NSW, 18 November 2006

British stem cell science and stem cell science questions, Oxford U, UK, November 2006

Belief in science, Founders Lecture, Oxford U, UK, May 2007; Victorian Institute of Chemical Sciences Fellowship Lecture, Royal Australian Chemical Institute, Melbourne, VIC, 3 September 2007

The structure of proteins at interfaces, Australian Institute for Bio–Engineering and Nano Technology, Institute Lecture, U Queensland, Brisbane, QLD, June 2007; Victorian Institute of Chemical Sciences Fellowship Lecture, Monash U, Melbourne, VIC, 20 August 2007

X–rays, neutrons and scattering, Victorian Institute of Chemical Sciences Fellowship Lecture, Monash U, Melbourne, VIC, 20 August 2007

Ionic liquids, Victorian Institute of Chemical Sciences Fellowship Lecture, Monash U, Melbourne, VIC, 30 August 2007

Casein assembly at the air–water interface, Dairy Innovation Group, Melbourne, VIC, September 2007

Structure of emulsions, Victorian Institute of Chemical Sciences Fellowship Lecture, Melbourne U, VIC, 6 September 2007

Professor S B Wild

Inorganic and organometallic asymmetric synthesis, U Toronto, Canada, 5 August 2007; U Freiberg, October 2007

Chiral arsines and phosphines: Resolutions and asymmetric syntheses, Ludwig–Maximillian U, Munich, Germany, September 2007; U Liepzig, Germany, November 2007

Inorganic asymmetric synthesis, U Liepzig, Germany, November 2007

Service to External Organisations

Service covers 2006 and 2007 unless otherwise stated

Professor M G Banwell:

Chair, Editorial Advisory Committee, *Australian Journal of Chemistry,* 2007; Member, Panel reviewing the Department of Chemistry, U Tasmania, 18–20 June 2007; Chair, PCG Panel, ARC College of Experts, 2007; Member, Advisory Board, Monash U Centre for Green Chemistry, 2007; Member, New Zealand PBRF Panel of Experts Evaluating Chemistry

Professor M A Collins:

Committee member, Physical Chemistry Division, RACI

Dr M L Coote:

Secretary, Physical Division, RACI; Treasurer, ACT Branch, RACI; Standing Committee Member, Polymer Division, RACI; Member, IUPAC Working Party on RAFT Kinetics; Intreader, Australian Research Council, 2006; Reviewer of Grant Applications for National Science Foundation (USA), 2007, and Research Corporation (USA), 2006; Marker of PhD theses for U Melbourne, 2006; Reviewer of Journal Articles for *Journal of the American Chemical Society, Macromolecules, Journal of Physical Chemistry, Chemical Physics Letters, Journal of Chemical Physics, Chemical Physics, ChemPhysChem, Physical Chemistry Chemical Physics, Theochem, Journal of Polymer Science, Polymer, Progress in Polymer Science, Macromolecular Chemistry and Physics, Macromolecular Theory and Simulation, Macromolecular Rapid Communication, Australian Journal of Chemistry, Journal of Photochemistry and Photobiology, Tetrahedron Letters, Organic Letters, Journal of Organic Chemistry, Journal of Physical Organic Chemistry*

Professor C J Easton:

Chair, Australian Delegation, 41st IUPAC General Assembly, 2007; Member, Board, Asian and Oceanian Cyclodextrin League; Member, Academic Advisory Board, School of Chemistry and Physics, University of Adelaide; Chair, National Committee for Chemistry, Australian Academy of Science (AAS); Member, Sectional Committee (Chemistry), AAS; Member, International Programs Committee, AAS; Chair, Organising Committee, 10th International Symposium on Organic Free Radicals and 3rd Pacific Symposium on Radical Chemistry, to be held in 2008; Member, Scientific Advisory Committee, 21st International Congress for Heterocyclic Chemistry, 2007; Member, Editorial Advisory Boards, *Journal of the Chemical Society, Chemical Communications; ARKIVOC; Current Organic Chemistry; Mini Reviews in Organic Chemistry; Letters in Organic Chemistry; Open Organic Chemistry Journal*; Member, United Kingdom EPSRC Peer Review College; Deputy Director, ARC Centre of Excellence in Free Radical Chemistry and Biotechnology; Foreign Reviewer, Department of Chemistry, Quaid-i-Azam University, Pakistan; Member, International Advisory Board, 2nd Pacific Symposium on Radical Chemistry, Dajeon, Korea, 2007.

Professor D J Evans:

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; 2007–2010 Scientific Chair of Statphys XXIV, (IUPAP)

Professor P M W Gill:

President, US software company *Q-Chem, Inc.*; International Panel (SPP 1145) of the *Deutsche Forschungsgemeinschaft;* Advisory Board of *Physical Chemistry Chemical Physics*; Advisory Board of Asia–Pacific Association of Theoretical & Computational Chemists

Dr D J Goossens:

Reviewer for *Journal of Physics: Condensed Matter, Journal of Applied Crystallography* and *Journal of Physics D;* Member, Organising Committee for the Australian and New Zealand Institute of Physics 31st Annual Condensed Matter and Materials Meeting, 2007; Member, Instrument Advisory Panels for the Wombat diffractometer, the Taipan three axis spectrometer and the Pelican polarisation analysis spectrometer at the Bragg Institute, ANSTO, 2006; Lecturer, AINSE/ANSTO/IAEA Summer School on Neutron Diffraction, AINSE, 2007

Professor A F Hill:

Member, International Advisory Board, International Conferences on Organometallic Chemistry; Member, Referee Panel, *Chemical Communications;* Editor, *Advances in Organometallic Chemistry* (Academic Press); Assessor: ARC, EPSRC, PRF, NSF grant applications; Member, Editorial Advisory Board, *Organometallics,* 2006; *Member, International Editorial Advisory Board, Dalton Transactions,* 2006; Member, EPSRC (UK) Peer College Review

Professor E R Krausz:

Member, RACI Physical Chemistry Committee; Assessor DOE, NSF & ARC Ozreader research grant applications; Member, Spectroscopy Committee, AAS; ANU 'Emerging Energy Sources' presentation to Parliament; National television 'New Inventors' presentation on Artificial Photosynthesis; Asia Pacific Network on Energy Technology (APNet) Workshop, Government Initiative

Emeritus Professor L N Mander:

Member, Finance and Audit Committee, AAS; Member, Editorial Advisory Boards, *Current Organic Chemistry, Dictionary of Organic Compounds, Heterocycles, Natural Product Reports, Synthesis,* and *Synlett*; Member, Board of Consulting Editors, *Tetrahedron, Tetrahedron Letters*; Assessor, Royal Society, ARC, PRF and NSF grant applications

Professor D L Ollis:

Assessor, ARC and NHMRC grant applications; Editorial Board, Protein Engineering Design and Selection (PEDS)

Professor G Otting:

President, Australian and New Zealand Magnetic Resonance Society (ANZMAG); Member, Editorial Board of the *Journal of Biomolecular NMR*; Assessor: ARC and NHMRC grant applications

Associate Professor E M Sevick:

Referee for several journals including *Physical Review, Physical Review Letters, and Journal of Chemical Physics*

Associate Professor M S Sherburn:

Member, RACI; President, ACT Branch, RACI; Treasurer, Organic Division, RACI; Chair, RACI NSW Organic Chemistry Group, 2006; Chair and Organiser, RACI NSW Organic Chemistry Group 27th Annual One-Day Symposium 2006; Co-Chair and Organiser, Free Radical Symposium, 22nd RACI Organic Conference (22RACIOC) and the 6th RACI Conference on Physical Chemistry (CPC2007); Co-Chair, 9th International Symposium on Organic Free Radicals, Heron Island, to be held August 2008; Grant application reviewer: Australian Research Council (International Reader), American Chemical Society Petroleum Research Fund, Science Foundation Ireland, National U Singapore, NSERC Canada Discovery Grants; Journal manuscript reviewer: *Science, Journal of the American Chemical Society, Angewandte Chemie, Chemistry: A European Journal, Chemical Communications, Journal of Organic Chemistry, Organic Letters, European Journal of Organic Chemistry, Synlett, Tetrahedron Letters, Tetrahedron, Australian Journal of Chemistry, Journal of Molecular Structure,* and *Advanced Functional Materials;* Member, American Chemical Society

Professor T R Welberry:

Participant, TOPAZ Working Group Meeting for the (SNS) Spallation Neutron Source, Oak Ridge, Tennessee, May 2006; Member, Nominations Committee of SCANZ (Society of Crystallographers in Australia and New Zealand); Co-editor, *Journal of Applied Crystallography*; Co-editor of Crystallography Reviews; Member, Journals Commission of the International Union of Crystallography

Professor J W White:

Chairman, International Advisory Committee, J-PARC Project, Japan; Member, International Advisory Committee, Bragg Institute, ANSTO, Sydney; Member, Instrument Advisory Team for Platypus at OPAL, ANSTO; Member (with D J McGillivray), Instrument Advisory Committee, Small Angle Scattering Instrument, Bragg Institute, ANSTO; Member, Program and Review Board, Australian Synchrotron Research Program; Member, Board of Governors, CARS Consortium, Advanced Photon Source, Argonne, Chicago; Chairman, Sectional Committee 3, AAS; Convenor, Working Party on Nuclear Matters, AAS; Member, Working Party on Nuclear Physics, OECD; Member, International Advisory Committee, Central Laboratory of the Research Councils, UK; AINSE, Immediate Past President; Member of the AINSE Executive, Member of the AINSE Council (ANU Councillor)

Professor S B Wild:

Member, North American Exchange Committee, AAS, 2006; Consulting Editor, *Tetrahedron Asymmetry*; Guest Professor, PhD Program, University of Leipzig; Member, RACI, Professional Assessment Committee

Professor R L Withers:

Chairman, Aperiodic Commission of the International Union of Crystallography (IUCr); Member, Editorial Advisory Board, *Journal of Solid State Chemistry*; Member, National Committee for Crystallography of the AAS; Member, Executive Committee of the Australian Microscopy and Microanalysis Society (AMMS); Member of Council, Society of Crystallographers in Australia and New Zealand (SCANZ); Member; International Advisory Board for the International Conference Aperiodic 2006; Member, Organising Committee and Chair of the Program Committee for the 31st Condensed Matter and Materials Meeting, 2007; Member; International Program Committee for the 21st Congress of the International Union of Crystallography (IUCr XXI) to be held in 2008; OzReader, ARC

External Lectures and Courses

Dr M L Coote:

Computational radical chemistry, Graduate Lecture Course, University of Melbourne, August 8, 14 and 16 2006

A quantum chemical approach to polymer science, Lecture Course at the 8th Australasian Polymer Summer School, Geelong, Victoria, 6-9 February 2007

Professor N E Dixon:

Structure and chemistry of metalloenzymes, Foundation for Inorganic Chemistry Lecture Series, School of Chemistry, University of Sydney (6 lectures at Honours level), 2007

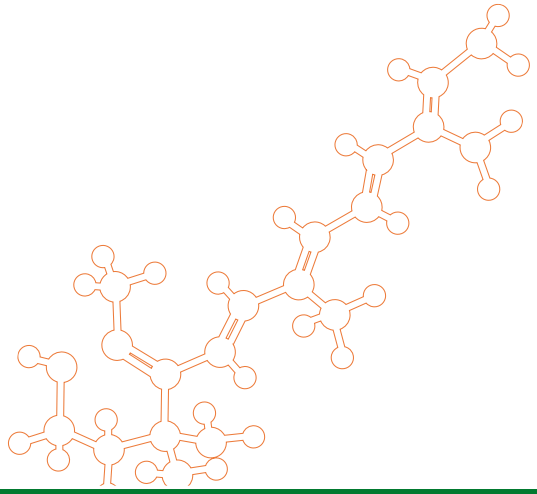
Associate Professor E M Sevick:

Stretching a single DNA molecule: Optical Tweezers and the Fluctuation Theorems, Wellington, New Zealand, 15 August 2007; Christchurch, New Zealand, 16 and 17 August 2007

Optical Tweezers: What can you pluck, pull or tease with light? ANU's Annual PhB Student Retreat, Kiola NSW, 16-18 February 2007

Associate Professor M S Sherburn:

Radicals and pericyclics in synthesis, Department of Chemistry, University of Toronto, Canada (12 hour graduate lecture course), February - March 2007



Outreach Activities

Conference Organisation

Professor C J Easton, Dr M L Coote and Associate Professor M S Sherburn organised a Free Radical Symposium as part of the 22nd Royal Australian Chemical Institute Organic Conference and 6th Royal Australian Chemical Institute Conference on Physical Chemistry, Adelaide, SA, 28 January – 2 February 2007.

Professor G Otting organised and lectured at the 3rd Wollongong Workshop on Biomolecular NMR, 4-8 December 2006.

Australian Institute of Nuclear Science and Engineering (AINSE)

Professor J W White, President, implemented the AINSE Tenure-Track Research Fellowship scheme in 2006. From an excellent group of 15 candidates, two were selected. One of the Fellowships went to Dr Darren J Goossens, of the Research School of Chemistry, and the other to Dr Daniel Riley, Melbourne University. In 2007 the scheme continued and two further excellent candidates were selected from extremely strong field, one of whom was Dr Duncan J McGillivray from the Research School of Chemistry. He will take up his Fellowship at the University of Auckland in New Zealand in 2008.

In 2006, Professor White also started the process of organising an AINSE National Nuclear School. This was subsequently funded at $12.5M by the Government for implementation starting in 2007.

Australian National University's Outreach Campaign to New Zealand

In 2007 Associate Professor E M Sevick represented the ANU College of Science during the Australian National University's outreach campaign to attract New Zealand students. She presented her talk on *Optical Tweezers* in Wellington and Christchurch.

Australian School Innovation in Science, Technology and Mathematics

Since 2006, Associate Professor M S Sherburn has been the Project Coordinator for the Australian School Innovation in Science, Technology and Mathematics funded project "Cool Chemistry: Creating Curious Chemistry Students in ACT Primary Schools".

Big Day of Chemistry – Questacon 2007

Drs H Onagi, A Philbrook, R Dawson, Z Watts, M Gresser, and Mr R Coulston and many other members of the Easton research group organised the "Big Day of Chemistry" at Questacon, the National Science and Technology Centre in Canberra. Visitors to Questacon on the day had the opportunity to make their own latex balls, build molecular models, play with glow sticks, make vitamin E cream and hear about the importance of chemistry in our everyday lives.

Big Day of Chemistry 2007

National Youth Science Forum, 2006/2007

In January, Professor A F Hill, Mr H Neumann, and members of the Inorganic research group, hosted the National Youth Science Forum. After attending an engaging introductory lecture given by Professor Hill and Dr Crossley, the students prepared various transition metal complexes and characterised them by infrared spectroscopy. The students enjoyed their time at the Research School and benefited their Year 12 study by having an opportunity to try hands-on chemistry.

Oxford–Australia Scholarship Scheme

Professor J W White continues to chair the Selection Committee for the Oxford Australia Scholarship Scheme. In the last ten years, 45 Australians, who were selected from a top cohort of graduates of all Australian universities, have gone from Australia to Oxford under this scheme. In October 2007, Professor White was presented with a *Distinguished Friend of Oxford* award for his work during the past ten years.

Royal Australian Chemical Institute (RACI)

Associate Professor M S Sherburn is President of the ACT Branch of the Royal Australian Chemical Institute, which organises the joint RSC-RACI seminar series, the cornerstone of the RACI's professional activities in the ACT. The ACT Branch Committee comprises members of the RSC, the Department of Chemistry and the University of Canberra. Other important activities include running the ACT Schools Titration Competition (expertly coordinated by Dr Mark Ellison), assisting and promoting the teaching of chemistry in local schools, and careers information sessions. A number of social events are held each year, including a Christmas dinner, a midwinter Chemistry Ball, lake cruise, and a Paintball event. All events were well attended and social events were expertly organised by RSC PhD students Tanya Bradford and Nathan Kilah, and Department of Chemistry postdoctoral fellow Dr Rachel Roberts.

Big Day of Chemistry 2007

POSTGRADUATE CAREER DEVELOPMENT, EDUCATION AND TRAINING

The David Craig Lecture Series

The 2006 Craig Lecture was entitled *Excess electrons and protons in water: A cluster perspective*. Other lectures in the series were: *Rings, cages, prisms and cubes: The myriad forms of water clusters, On the role of electrostatics, dispersion and polarisation in water force fields; Connections between potential energy landscapes and thermodynamics of clusters,* and *Potential energy surfaces and vibrational properties of conformationally flexible biomolecules.* The series was delivered by Professor Kenneth Jordan, University of Pittsburgh, USA.

The 2007 Craig Lecture was entitled *Imaging and reaction dynamics in model membranes: Soft nanoscience.* Other lectures in the series were: *Electrostatics and dynamics in proteins; Ultra-fast dynamics in green fluorescent protein (GFP),* and *Re-engineering photosynthetic reaction centers.* The series was delivered by Professor Stephen G Boxer, Camille and Henry Dreyfus Professor of Chemistry, Stanford University, California, USA.

The Arthur Birch Lecture Series

The 2006 Birch Lecture was entitled *Light and energy, mimicking natural photosynthesis.* Other lectures in the series were: *Dynamics of interfacial and cross-surface electron transfer reactions in mesoscopic systems*, and *Solar generation of hydrogen from water.* The series was delivered by Professor Michael Graetzel, Swiss Federal Institute of Technology, Lausanne, Switzerland.

The 2007 Birch Lecture was entitled *The discovery and development of alkene and alkyne metathesis reactions.* Other lectures in the series were: *Applications of modern olefin metathesis catalysts for organic and polymer chemistry and recent developments in synthetic chemistry,* and *Catalytic reduction of dinitrogen to ammonia at room temperature and one atmosphere with protons and electrons.* The series was delivered by Professor Richard R Shrock, Massachusetts Institute of Technology, Cambridge, USA.

Graduate Program in Chemistry – Lectures

Associate Professor M S Sherburn presented an Honours course of eight lectures in 2006: *Radicals and pericyclic reactions*

Professor J W White presented a guest lecture in a Physics Honours course in 2007

Degrees Awarded and Present Employment of Graduates

For the Degree of Doctor of Philosophy

2006

Dr Daniel Antony Speedie Beck BSc *RMIT*

Stereoselective Intramolecular Michael Addition Reactions of Pyrrole and their Application to Natural Product Syntheses
Supervisor: Professor M G Banwell
Currently: Internship, Novartis, Switzerland

Dr David Michael Carberry BSc BEng Hons *ANU*

Optical Tweezers: Experimental Demonstrations of the Fluctuation Theorem
Supervisor: Assoc Professor E M Sevick
Currently: Research Associate, U Bristol, UK

Dr Marta Maria Cieslinski BSc *Adelaide*

Cyclodextrin-based Supramolecular Assemblies
Supervisor: Professor C J Easton
Currently: Project Officer – Scientist, Victorian Government, Melbourne

Dr Rian David Dewhurst BSc *Canterbury NZ*

Synthesis and Reactivity of Polymetallic Complexes Containing Tricarbido (C_3) Ligands
Supervisor: Professor A F Hill
Currently: Postdoctoral Fellow, Department of Chemistry, U California, Riverside, USA

Dr Christian Ralph Evenhuis BSc *Tasmania*

Interpolation of Diabatic Potential Energy Surfaces
Supervisor: Professor M A Collins
Currently: Postdoctoral Fellow, Universität Bielefeld, Germany

Dr Kelly Ann Fairweather BSc *Auckland NZ* Hons *ANU*

A Formal Total Synthesis of the Marine Diterpenoid Diisocyanoadociane
Supervisor: Professor L N Mander
Currently: EFPL SB ISIC LGSA, Lausanne, Switzerland

Dr Michael John Harvey MSc *Waikato NZ*

Towards the Assembly of the Binary Vinca Alkaloids: Strategies for the Synthesis of the Indole–Indoline Core of (+)–Vinblastine
Supervisor: Professor M G Banwell
Currently: Development chemistry position, Shasun Pharma Solutions, Newcastle, NSW

Dr Joseph Lee Hughes BSc *ANU*

Magneto–Optic and Selective Spectroscopies of Natural Photosystems
Supervisor: Professor E R Krausz
Currently: Postdoctoral Fellow, iBiTecs–S, CNRS, CEA Saclay (Gif–sur–Yvette) France

Dr Heather Joy Kitto BSc *Canterbury NZ*

Conformational Control in Dinuclear Metal Helicates and Related Complexes Containing Tetra(tertiary phosphines)
Supervisor: Professor S B Wild
Currently: Institute for Molecules and Materials, Nijmegen, The Netherlands

Dr Ching–Yeh Lin App Chem *National Chiao Tung, Taiwan*

Computational Methods in Vibrational Spectroscopy
Supervisor: Professor P M W Gill
Currently: Postdoctoral Fellow, RSC

Dr Karin Loscha BSc MSc *Göttingen*

Structures and Functions of Primosomal Proteins in Bacterial DNA Replication
Supervisor: Professor N Dixon
Currently: Postdoctoral Fellow, RSC

Dr Mark Donald Mulcair BSc *Monash*

Mechanism of DNA Replication Termination in Escherichia coli
Supervisor: Professor N E Dixon
Currently: Research Scientist, Apollo Life Science, Sydney, NSW

Dr Ah Young Park BSc *Victoria U Wellington*

Structure and Function of the Proofreading Exonuclease Subunit of E. coli *DNA Polymerase III and Related Enzymes*
Supervisor: Professor N E Dixon
Currently: Postdoctoral Fellow, Department of Chemistry, U Cambridge, UK

Dr Amy Philbrook BSc *Maine*

^{15}N NMR Correlation Spectroscopy: Co–Polymerisation in Melamine– and Melamine Replacement–Urea–Formaldehyde Resins
Supervisor: Professor C J Easton
Currently: Postdoctoral Fellow, RSC

Dr Gregory M Sandala BSc *Windsor*

Theoretical Studies of Adenosylcobalamin–dependent Enzymes
Supervisor: Professor L Radom
Currently: Research Associate, U Sydney, NSW

Dr Bradley James Stevenson BSc *Lincoln NZ*

Directed Evolution of Pyruvate Decarboxylase for In Vitro *Glycolysis*
Supervisor: Professor D L Ollis
Currently: Postdoctoral Fellow, Institute for Tropical Diseases, Liverpool, UK

Dr Never Tshabang BSc *Botswana* MSc *Sussex*

The Chemistry of Poly(methimazolyl)borate Complexes
Supervisor: Professor A F Hill
Currently: Lecturer, U Botswana, South Africa

Dr Rebecca Jayne Warr BSc *Canterbury NZ*

Inorganic Asymmetric Synthesis: Stereoselective Synthesis of Two–bladed Propeller, Octahedral Metal Complexes
Supervisor: Professor S B Wild
Currently: Postdoctoral Fellow, U Nottingham

Dr Zachary Ivan Watts BApplSc *RMIT*

Studies into Hydrogen Atom Abstraction from Amino Acids and Peptides
Supervisor: Professor C J Easton
Currently: Postdoctoral Fellow, RSC

2007

Dr Lorraine Margaret Caldwell BSc *UQ*

Synthesis and Reactivity by Organochalcogen Complexes
Supervisor: Professor A F Hill
Currently: Postdoctoral Fellow, School of Chemistry, Trinity College, Dublin, Ireland

Dr Ryan Edward Dawson BSc *Adelaide*

Cyclodextrins as the Basis of Molecular Devices
Supervisor: Professor C J Easton
Currently: Postdoctoral Fellow, RSC

Dr Martin Peter Friend BSc *Murdoch*

Chemoenzymatic Manipulation of an Aminoglycoside Scaffold: Site-selective Refunctionalisation of Tobramycin for the Purposes of its Attachment to Dendrimers
Supervisor: Professor M G Banwell
Currently: Research Scientist, Institute of Drug Technology (IDT) Australia Ltd, Melbourne, VIC

Dr Colin John Jackson BSc *Otago* NZ

Enzymatic Catalysis of Phosphate Ester Hydrolysis
Supervisor: Professor D L Ollis
Currently: Postdoctoral Fellow, Entomology, CSIRO

Dr Slobadan Jergic AssocSc *La Guardia Coll* NY BSc *Belgrade*

Structure and Function of Escherichia Coli *DNA Polymerase III Holoenzyme*
Supervisor: Professor N E Dixon
Currently: U Wollongong, NSW

Dr Jasmine Clare Jury BSc *Massey*

Studies Directed Towards the Synthesis of (+)-Tricholomenyn B
Supervisor: Professor M G Banwell
Currently: Postdoctoral Fellow, U Wollongong, NSW

Dr Maria Elizabeth Kubik BA *UQ* BAppSc *Canberra*

The Use of Non-sampling Spectroscopic Techniques in Conservation: Improved Methodologies for Pigment Identification
Supervisor: Professor E R Krausz
Currently: Art Gallery of Western Australia – Conservation, Perth, WA

Dr Ching Hei Laurence Kwan BSc/BCA *Victoria U Wellington* NZ MSc *LSE* UK

Towards an Enantioselective O → ABCD Synthesis of Steroids
Supervisor: Assoc Professor M S Sherburn
Currently: Scientist, Jean-Tech Chemicals, Hong Kong

Dr Iris Hin Wah Li BSc *Auckland* NZ

Investigations of Factors Affecting Binding Affinity with Peptidylglycne α-Amidating Monooxygenase (PAM)
Supervisor: Professor C J Easton
Currently: Australian Academy of Science, Canberra, ACT

Dr Natalie Anne Miller BSc *Sydney*

New Synthetic Applications of the Diels-Alder Reaction
Supervisor: Assoc Professor M S Sherburn
Currently: U Cambridge, UK

Dr Emma Louise Pearson BSc *WA*

Applications of Domino Sequences to Natural Products Synthesis
Supervisor: Assoc Professor M S Sherburn
Currently: Postdoctoral Fellow, RSC

Dr Adam Willis Perriman BSc *James Cook*

Chemical Denaturation of Proteins at an Interface
Supervisor: Professor J W White
Currently: Postdoctoral Fellow, U Bristol, UK

Dr James C Reid BSc LLB *Victoria U Wellington* NZ

Fluctuations of Dynamic Systems
Supervisor: Assoc. Professor E M Sevick
Currently: Postdoctoral Fellow, U Calgary, Canada

Dr Pauline Carol Stanislawski BSc *Monash*

Enantioselective Total Syntheses of (-)-ent-Erythramine and (+)-3-epi-Erythramine
Supervisor: Professor M G Banwell
Currently: Johnson & Johnson, Medicinal Chemistry, Belgium

Dr Valeska P Ting BSciTech *Victoria U Wellington* NZ

Structural Studies of the Photocatalytic A_2InNbO_6 and $A_3CoNb_2O_9$ (A = Ba, Sr and Ca) Compounds
Supervisor: Professor R L Withers
Currently: Postdoctoral Researcher, U Southampton, UK

For the Degree of Master of Philosophy

2006

Ms Leonie Yin Fan Chow BSc *Melbourne*

β-Nitro-α-amino Acids: Scope, Limitations and Applications
Supervisor: Professor C J Easton
Currently: Scientist, Australian Pesticides and Veterinary Medicines Authority, Canberra, ACT

Postdoctoral Fellows, Research Fellows and Fellows – Completions and Destinations

The Research School of Chemistry provides one of the very best environments for the education and 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 forty years ago, many of our alumni now occupy senior positions in academia, government and industry, both in Australia and overseas.

* left in 2006
ˆ left in 2007

Dr Margit Apponyi took up a position as a Scientist at Biotech Company, Adelaide *

Dr Lorraine Axford took up a position as a Research Scientist at Argenta Discovery Ltd, Essex, UK *

Dr Michael Backes took up a position as a Laboratory Leader at Symrise GmbH & Co. Holzminder, Germany *

Dr Lorna Barr took up a Postdoctoral Fellowship at the University of Notre Dame, Indiana, USA *

Dr Akkattu Biju took up a position as a Postdoctoral Fellow at Taiwan National University, Taipei ˆ

Dr Christian Bluechel took up a position as a Research Scientist at the School of Engineering, Temasek Polytechnical High School, Singapore ˆ

Dr Muriel Bonnet took up a position at ICES in Singapore, working with Dr Christina Chai *

Dr David Carberry accepted a Research Associate position at the University of Bristol *

Dr Marta Cieslinski accepted a position as a Project Officer, Scientist with the Victorian Government in Melbourne *

Dr Ian Crossley took up a position at Monash University *

Dr Delphine Dauge concluded her Postdoctoral Fellowship *

Dr Elise Dumont concluded her Postdoctoral Fellowship ˆ

Dr Jonathan Foot took up a position as a Research Scientist at Pharmaxis, Sydney *

Dr Oded Godsi concluded his Postdoctoral Fellowship ˆ

Dr Madeleine Headlam took up a position as a Research Officer at the Queensland Institute of Medical Research, Brisbane *

Dr Mark Henderson accepted an appointment at the University of Maine, France *

Dr Joseph Hughes took up a position as a iBiTecs-S, CNRS, CEA Saclay, Gif-sur-Yvette, France ˆ

Dr Ekaterina Izgorodina commenced a position at Monash University, VIC *

Dr Mario Knoke took up a position at BASF in Ludwigshafen, Germany *

Dr Elizabeth Krenske commenced a position at UCLA ˆ

Dr Peter Mahon took up a position at Monash University ˆ

Dr Stephen Martin concluded his Postdoctoral Fellowship ˆ

Dr Stephen McAteer returned to the UK *

Dr Duncan McGillivray won the Australian Institute of Nuclear Science and Engineering (AINSE) Fellowship for 2007, which he took up at Auckland University, NZ ˆ

Dr Mark Mulcair took up a position as a Research Scientist at Apollo Life Science, Sydney *

Dr Heather Netzloff took up a position at Aimes Laboratory, IOWA, USAˆ

Dr Daniel Offerman took up a position as a Postdoctoral Fellow at Imperial College, London, UK ˆ

Dr Ah Young Park took up a Postdoctoral Fellowship at Cambridge University ˆ

Dr Pavel Prosselkov took up a Research Fellowship at Max-Planck-Institut, Germany *

Dr Prabhakar Ranganathan took up a position as a Postdoctoral Fellow at the ARC Centre of Excellence for Free Radical Chemistry & Biotechnology, Melbourne ˆ

Dr Diane Robinson is now working with the ARC Centre of Excellence for Free Radical Chemistry and Biotechnology in Melbourne ˆ

Dr Ken Robinson took up a position as an Evaluator with the Australian Pesticides and Veterinary Medicines Authority in Canberra *

Dr Andrew Scott commenced as a Trainee Patent Attorney with Davis Collison Cave in Melbourne *

Dr Shane Simonsen left at the end of his appointment to return to Queensland *

Dr David Sinclair took up a position as an Evaluator at OTC Medicines Section, Therapeutic Goods Administration, Canberra *

Dr Joerg Steinbach took up Studies in Coatings Engineering, Germany *

Dr Balakrishnan Viswanathan concluded his Postdoctoral Fellowship *

Dr Jorg Wagler left to resume work at the Institut für Anorganische Chemie, Technische Universität Bergakademie Freiberg ^

Dr Richard Webster left to commence a position as Assistant Professor at Nanyang Technological University in Singapore *

Dr Johann Zank left to take up an appointment with Orica, Kurri Kurri, NSW *

PhD Scholars

Australian Postgraduate Award = APA
Australian Postgraduate Award (Industry) = APA(I)
ANU Graduate School Scholarship = GSS
Co-funded ANU Graduate School/Research School of Chemistry = GSS/RSC
ANU PhD Stipend Scholarship = ANU PhD
International Postgraduate Research Scholarship = IPRS
University-Industry Linkages in Chemistry = UnIChe
RSC Tuition Fee Scholarship = RSCT
CSIRO Postgraduate Studentship = CSIRO
CSIRO Tuition Fee Scholarship = CSIROT
CSIRO Emerging Sciences = CSIRO EM
Daimler-Benz Foundation Fellowship = Daimler-Benz
candidature ended in 2006
+ candidature started in 2007
* scholarship ceased in 2006

Abernethy, Robyn J BSc *Massey* BSc Hons *ANU* – ANU PhD

Arthur, Isaac N MSc *TU Braunschweig* – CSIRO EM

Austin, Kerrie A B BSc *Auckland* NZ – APA

Baranyai, Krisztian J* BSc MSc *Monash* – ANU PhD

Beasley, Andrew G BSc Dip Ed BSciTech *WA* – APA

Beck, Daniel A S# BSc *RMIT*

Beeren, Sophie R# BSc *UNSW* – GSS

Bernard, Yves A+ DipEng *EngSchool Geneva* BSc MScChemPhysics *Geneva* – ANU PhD

Bilski, Tomasz BSc Chem *Curtin UT* – APA(I)

Bissember, Alexander C BSc *ANU* – APA

Bojase-Moleta, Gomotsang BSc MSc *Botswana* – U Botswana

Bowen, Saara K BSc Hons *New England* – ANU PhD

Bradford, Tanya A BA *UQ* BSc *UQ* BSc *ANU* – APA

Brittain, David R B BSc *Adelaide* – APA

Brock, Joseph S+ BMedSci *ANU* – ANU PhD

Buchan, Alexander MChem *Aberdeen* – ANU PhD/CSIROT

Caldwell, Lorraine M# BSc *UQ* – GSS/RSC

Carpinelli, Lucinda L BSc *Melbourne* – ANU PhD

Chien, Siu-Hung BSc *USciTech Hong Kong* MPhil *Chinese U Hong Kong* – ANU PhD/RSCT

Coulston, Roger J BMedSci *ANU* – APA

Dawson, Ryan E* BSc *Adelaide* – ANU PhD

Debono, Lesley* BSc *New South Wales* – ANU PhD

Deev, Vitali BSc *Canterbury* NZ – GSS/RSC

Dietinger, Christine MSc *Helsinki* – ANU PhD

Fairweather, Kelly A# BSc *Auckland* NZ Hons *ANU* – APA

Fallon, Thomas+ BTech *Flinders* BSc Hons *ANU* – ANU PhD

Fearnside, Luisa# BSc *Melbourne* BSc Hons *UQ* – APA(I)

Foo, Jee L BSc *Nat U Singapore* – ANU PhD/Orica & UnIChe Tuition Fee

Friend, Martin P BSc *Murdoch* – APA(I)

Goodwin, Shelley K# BSc *Griffith* – ANU PhD

Gray, Catherine A+ BBMedSc *Victoria U Wellington* NZ – ANU PhD

Harvey, Michael J# MSc *Waikato* NZ

Hasse, Katrin Diploma Chemistry *Philipps-University Marburg* – Daimler-Benz

Hennessy, James E MChem *Aberdeen* – ANU PhD

Hodgson, Jennifer L BSc Hons *ANU* – APA

Hughes, Joseph L# BSc *ANU* – GSS/RSC

Jackson, Colin J# BSc *Otago* NZ – GSS/RSC

Jergic, Slobodan# AssocSc *La Guardia Coll NY* BSc *Belgrade* – ANU PhD/IPRS

Jia, Xinying+ BSc *Peking* PhD *Shanghai Institute of Organic Chemistry* – ANU PhD

Jones, Matthew T BSc *La Trobe* – APA

Jury, Jasmine C* BSc *Massey* NZ – 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

Kokas, Okanya J BBiotech *UQ* – ANU PhD

Kubik, Maria E# BA *UQ* BAppSc *Canberra* – GSS

Kwan, Ching H L BSc/BCA *Victoria U Wellington* NZ MSc *LSE UK* – GSS

Lapalikar, Gauri V+ BSc MSc *Nagpur* – CSIRO EM

Lehmann, Anna L BSc *Auckland* NZ – ANU PhD

Li, Iris H W BSc *Auckland* NZ – ANU PhD

Lin, Andrew+ BMedChem *Monash* – APA

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

Maniam, Subashani BSc *Kebangsaan Malaysia* – ANU PhD

Matveenko, Maria BSc *Victoria U Wellington* NZ – APA

Miller, Natalie A# BSc *Sydney* – ANU PhD

Mohd Hashim, Amalia B+ BEng *Tokyo* – Govt of Malaysia

Mortimer, Adam J# BSc *Wollongong*

Nguyen, Hai B BE (Chemical Engineering) *Sydney* – ANU PhD

Nguyen, Thanh V BSc *UNSW* – ANU PhD

Noor, Sajid BSc MSc *Karachi* – CSIRO EM

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

Pham, Yen H BSc *RMIT* MSc *UNSW* – CSIRO EM

Phillis, Andrew T BSc MSc *Waikato* NZ – ANU PhD

Pinkerton, David M BSc *ANU* – ANU PhD

Reid, James C# BSc LLB *Victoria U Wellington* NZ – GSS

Sandala, Gregory M# BSc *Windsor* – ANU PhD/IPRS

Sedgwick, Kathryn J+ BForensicSc *Deakin* – APA

Smith, Michael H# BSc *Melbourne* Hons *Sydney*

Stanislawski, Pauline C BSc *Monash*

Statham, Georgina M+ BSc *ANU* – APA

Stevenson, Bradley J# BSc *Lincoln* NZ – GSS/VC

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

Ugwumba, Isaac N BPharm *Lagos* – CSIRO EM

Valizadeh, Sanaz F+ BSc *Tabriz*

Wanty, Christopher J BSc *Canterbury* NZ – APA

Watson, Morgan A BSc Biochem *Canterbury* NZ – GSS/RSC

Watts, Zachary I# BApplSc *RMIT* – ANU PhD

Weir, Michelle L B Biotech *ANU* – ANU PhD

Wells, Kerrina BSc *ANU* – ANU PhD

Wiadrowski, Emma+ BSc *Adelaide* – APA

Wu, Nan+ BEng Meng *Northeastern* China – CSIRO EM

Wu, Peter S BAppSc *QUT* BSc Hons *ANU* – APA/VC

Yip, Sylvia H C BSc *National University of Malaysia* – CSIRO EM

Visiting Scholars

As part of the recruitment program the Research School of Chemistry hosts international and Australian scholars for a visit of two to six months to undertake research projects with individual staff members. In most instances the project formed part of their course requirements and the scholars were supported by their home institution:

2006

Foster, Simon PhD *UC* - S B Wild

Du Preez, Franco PhD *University of Stellewbosch* - D L Ollis

Kar, Gopa PhD *RMIT* - A F Hill / M A Bennett

Mirzadeh, Nedaossadat PhD *RMIT* - A F Hill / M A Bennett

2007

Chainok, Kittipong PhD *Suranaree UT* - A D Rae

Halliday, Jill PhD *Syd* - M D McLeod

Horsch, Philipp Prediploma *Philipps U Marburg* - M G Banwell

Jordan, Deborah PhD *Otago* - C J Easton

Kar, Gopa PhD *RMIT* - A F Hill / M A Bennett

Kemp, Daniel PhD *Iowa State* - M A Collins

Mirzadeh, Nedaossadat PhD *RMIT* - A F Hill / M A Bennett

Muirhead, Kirsty MChem *Aberdeen* - C J Easton

Mullin, Jonathan PhD *Iowa State* - M A Collins

Nicoll, Sarah MChem *Aberdeen* - C J Easton

Njegic, Bosiljka PhD *Iowa State* - M A Collins

Pertici, Francesca MSc *Pisa* - C J Easton

Ray, Paramita MSc *Indian IT Kharagpur* - M G Banwell

Tayati, Ponlawat BSc *ANU* - E M Sevick

Wilkinson, Shane PhD *Syd* - M D McLeod

Zanzoni, Serena PhD *Verona* - G Otting

Zorn, Deborah PhD *Iowa State* - M A Collins

Honours Scholars

The following students undertook Honours projects within the School:

2006

Basutto, José *RMIT* - M G Banwell

Brock, Joseph *ANU* - A J Oakley

Fallon, Thomas *Flinders* - M S Sherburn

Holden, Kate *ANU* - M G Banwell

Sharp, Phillip Patrick *ANU* - M G Banwell

2007

Reekie, Tristan *ANU* - M G Banwell

Sharp, Phillip Patrick *ANU* - M G Banwell

Yue, Chung–Yen (Ascar) *ANU* - D L Ollis

Summer Scholar Program

Summer Research Scholarships, of eight to eleven weeks duration, were awarded to undergraduate students from Australia and New Zealand from November to February. In 2006, twenty–four scholarships were awarded by the Research School of Chemistry. In 2007 the Research School of Chemistry combined with the Department of Chemistry and, in total, 30 scholarships were awarded. All students were involved in research projects with individual staff members:

2006

Andrews, Cecily *Swinburne UT*	M G Banwell
Ang, Joo *Melbourne*	E R Krausz
Chen, Simon *UQ*	J W White
Cheng, Mei Hsia *Wellington NZ*	C J Easton
Clements, Brodee *New England*	L Mander
Deng, Jia *NSW*	P M W Gill
Deplazes, Evelyne *Curtin*	P M W Gill
Downs, James *RMIT*	R L Withers
Fallon, Thomas *Flinders/ANU*	M S Sherburn
Gao, Renyu *Auckland NZ*	A J Oakley
Gray, Catherine *Wellington NZ*	M S Sherburn
Lin, Andrew *Monash*	M G Banwell
Lu, Di *ANU*	S B Wild
Lucas, Pradeep *RMIT*	A J Oakley

Moodie, Lindon *Otago NZ*	M S Sherburn
Nielsen, Kresten *UQ*	J W White
Reid, David *Wellington NZ*	M Keniry
Ridgewell, Jay *QUT*	D L Ollis
Spindler, Xanthe *Newcastle*	M L Coote
Stockton, Keiran *New England*	A F Hill
Thida, Mya *ANU*	A F Hill
Wong, Michael *ANU*	G Otting
Wu, Yue *Sydney*	L Mander
Zhang, Amy *Canterbury NZ*	C J Easton

2007

Ang, Joo *Melbourne*	J W White
Ban, Kung *La Trobe*	M G Banwell
Bon, David *Auckland NZ*	M G Banwell
Bulbrook, Michelle *ANU*	G Salem
Davis, Catherine, *Victoria NZ*	M S Sherburn
Deane, Karen *ANU*	R Barrow
Eyles, Matthew *ANU*	M G Banwell
Gupta, Vivek *ANU*	R Barrow
Hoekstra, Rafael *Canterbury NZ*	M S Sherburn
Hoskins, Dwain *Sydney*	M McLeod
Hudson, Sean *Adelaide*	C J Easton
Jennaway, Mark *ANU*	M Humphrey
Jin, Lu *ANU*	R Pace
Jones, Bronwyn *UWA*	A F Hill
Lechte, Thomas *Canterbury NZ*	G Otting
Lee, Hwi Young *ANU*	C J Easton
Lu, Di *ANU*	R L Withers
Lu, Belinda *Sydney*	M McLeod
Ng, Amelia *ANU*	M S Sherburn
Nguyen, Kelly *ANU*	D L Ollis
Nhu, Duong *La Trobe*	M McLeod
Shang, Rong *Canterbury NZ*	A F Hill
Shepherd, Jessica *ANU*	G Salem
Smith, Natalie *UWA*	M A Collins
Sun, Eric *UQ*	C J Easton
Tayati, Joe *ANU*	E M Sevick
Teng, Ruth *Waikato NZ*	M S Sherburn
Wang, Mark *Waikato NZ*	E R Krausz
Wu, Yue *Sydney*	J W White
Xu, Peng *Sydney*	P M W Gill

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

CHEM2101 Introduction to Crystallography – 8 lectures (T R Welberry, 2007)

CHEM2203 Chemical Structure and Reactivity – Organotransition Metal Chemistry – 10 Lectures (A F Hill, 2007)

CHEM2203 Chemical Structure and Reactivity – Inorganic and Materials Chemistry – 8 Lectures (R L Withers, 2007)

CHEM 2203 Chemical Structure and Reactivity – Inorganic and Materials Chemistry – Invited Lecture (Y Liu, 2007)

CHEM2204 Environmental Chemistry – one quarter of course lectures (E M Sevick, 2007)

CHEM 3101 Concepts in Medicinal Chemistry – DNA and DNA–Drug Interactions – 3 lectures (M Keniry, 2006)

CHEM 3101 Concepts in Medicinal Chemistry – 9 lectures (L N Mander, 2007)

CHEM 3101 Concepts in Medicinal Chemistry (A J Oakley, 2006)

CHEM3102 Applied Physical Chemistry – one half of course lectures (E M Sevick, 2007)

CHEM3105 Quantum Mechanics – 10 lectures (M A Collins and A T B Gilbert, 2006)

CHEM3105 Quantum Mechanics – 10 lectures (G Otting, 2006–07)

CHEM3105 Quantum Mechanics – 10 lectures (M A Collins and D L Crittenden, 2007)

CHEM 3107 Bioorganic and Natural Products Chemistry – 6 lectures (D L Ollis, 2006)

CHEM 3107 Bioorganic and Natural Products Chemistry – 12 lectures (D L Ollis, 2007)

The following research students undertook demonstrating and marking in the Department of Chemistry:

2006 – 1st Semester

CHEM1101 – P Sharp and M Weir

CHEM2104 – J Basutto, J Brock, R Coulston, T Fallon, and D Pinkerton

CHEM 3101 – O Kokas and C Wanty

CHEM3102 – J Antony

2006 – 2nd Semester

CHEM1201 – J Hodgson, O Kokas, D Pinkerton, P Sharp and C Wanty

CHEM2103 – M Weir

2007 – 1st Semester

CHEM1101– T Reekie and P Sharp

CHEM2202 – J Brock, R Coulston, J Jury, N Kanizaj and C Wanty

CHEM3101 – N Kanizaj and O Kokas

CHEM3103 – M Weir

2007 – 2nd Semester

CHEM1201 – C Gray, K Sedgwick, P Sharp and C Wanty

CHEM2203 – J Brock, R Coulston and M Weir

Division of Biochemistry and Molecular Biology, Faculty of Science

BIOL2171 Biochemistry of the Cell – 12 lectures (D L Ollis, 2006-07)

BIOL3181 Current Topics in Developmental and Molecular Biology (A J Oakley, 2006 – 07)

BIOL3181 Current Topics in Developmental and Molecular Biology – 2 lectures (G Otting, 2006–07)

BIOL3181 Current Topics in Developmental and Molecular Biology – 1 lecture (D L Ollis, 2007)

Division of Engineering, Faculty of Science

ENGN 4601 Engineering Materials – Invited lecture (Y Liu, 2007)

Division of Medicine, Faculty of Science

MEDI – Guest lecture to Medical students (J W White, 2006)

Division of Physics, Faculty of Science

PHYS3032 Condensed Matter Physics – 12 lectures, 12 hours of laboratory work (D J Goossens, 2006)

PHYS3032: Condensed Matter Physics – Convenor, 28 lectures, 21 hours of laboratory work (D J Goossens, 2007)

PHYS3032 Condensed Matter Physics – Invited lecture (Y Liu, 2007)

PHYS2013 Quantum Mechanics – Guest lecture (D J Goossens, 2007)

University Service

Professor M G Banwell:

Deputy Dean, RSC, 2007; Member, Major Equipment Committee, 2007; Member, ANU College of Science New Buildings Committee

Dr M L Coote:

Mentor in the PhB program and gave a guest lecture on Computational Chemistry at the induction weekend for new PhB students (Kiola Campus, February 17-19, 2006)

Professor C J Easton:

Deputy Dean, RSC, 2006; Convenor, Graduate Studies Committee in Chemistry; Member, Major Equipment Committee, 2006

Professor D J Evans:

Convener, ANU College of Science; Vice Chancellor's Science Laboratory Delegate; Member, Academic Board; Consultative Committee; Chair, Centre for the Science and Engineering of Materials (CSEM); Member, Chemistry Discipline Promotions (ANU College of Science); Member, Board of the Centre for Complex Systems; Chair, Supercomputer Time Allocation Committee, ANU Supercomputer Faculty (ANUSF); Member, Appointment Committees, including: Dean of ANU College of Science and General Manager of ANU College of Science

Profesor P M W Gill:

Member, Divisional Information Committee SHE; Member, ANU College of Science Advisory Board; Member, Strategic Group for New ANU College of Science Building

Professor A F Hill:

Forum of the Institute of Advanced Studies; Coordinator National Youth Science Forum

Professor E Krausz:

Member, Board CSEM; OHS Radiation Safety Committee; ANU College of Science Building Committee

Emeritus Professor L N Mander:

Member, ANU College of Science New Buildings Committee

Professor A D Rae:

Member, Radiation Safety Sub-committee - Occupational Health and Safety Policy

Associate Professor E M Sevick:

Member, Tenure Review Committee RSPHYSSE; Member, C-D Promotions Committee (Maths and Environmental) 2007

Associate Professor M S Sherburn:

Management representative, ANU Occupational Health and Safety Policy Committee; Member, New Synthetic Chemistry Building "Chemistry Strategic Group"

Professor J W White:

Member, University Staff Consultative Committee (USCC)

Professor S B Wild:

Chairman, Chemistry Promotions Committee, ANU College of Science, 2006

Professor R L Withers:

Member, ANU College of Science Higher Degree Research Committee

INTERNAL MANAGEMENT

Administrative Support Structure

The management of the School is coordinated through the Business Office. During 2006 and 2007 the School underwent a change management process, which is ongoing. Existing positions are currently being re-developed for the benefit of the School. The senior administrative staff in 2006 and 2007 comprised:

- the School Manager (K Jackson 2006, G Deeble 2007): who is responsible for the administrative staff and the non-academic functions in the School, including business management, financial and budgetary matters, occupational health and safety, security/cleaning, and the supervision and well-being of the technical support staff;
- 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 Welling): who is responsible for the maintenance and operation of laboratory facilities, and oversees the control of hazards in all of the School's laboratories;
- the Finance 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.
- the Student and Marketing Officer (S Meharg 2006 – July 2007, S Neulinger [Acting] August 2007 -); who is responsible for matters pertaining to students, particularly admissions, scholarships, current rules, regulations and practises, and is the focus for outreach and marketing activities. The Student and Marketing Officer acts as the Secretary to the RSC Prizes and Awards Committee, and provides advice and administrative assistance to the Dean/Director.

Technical Support and Research Services

The capacity of the School to undertake leading-edge research is underpinned by highly skilled technical staff, whose skills and expertise complement those of the academic staff.

Technical staff are attached to individual groups and support and contribute to the research work of experimental groups in the RSC. 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 group. Technical staff provide continuity within particular groups, although their expertise is also made available to other groups. In addition, the technical staff assist the School Manager in implementing and monitoring safety policy within the groups.

Staff of the Research Services section provide 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 2006, the Unit completed a total of 2024 analyses on samples submitted by 166 individuals, most of which (77%) were for CHN analyses. 41% of requests originated in the RSC.

In 2007, the Unit completed a total of 1487 analyses on samples submitted by 153 individuals, most of which (75%) were for CHN analyses. 34% of requests originated in the RSC.

External institutions requesting analyses (40% of total requests in 2006 and 36% in 2007) include the Australian Defence Force Academy, James Cook University, Newcastle University, University of New South Wales, Sydney University, Sydney Grammar School, Deakin University, University of Western Australia, University of Western Sydney, University of Wollongong, University of Technology (Sydney), Kent State University (USA) and University of British Columbia (Canada). Significant requests continue to come from commercial and

government sources (11% in 2006 and 24% in 2007). These clients included the Institute for Drug Technology, CSIRO (Energy Technology), Boron Molecular, Siemens Water Technology, Prana Biotechnology, Museum of Victoria, Epichem, Radpharm Scientific, Advanced Molecular Technologies, Dyesol, ANSTO, and the Museum of Victoria.

External earnings for 2006 were $56,451.50. External earnings for 2007 were $46,946.

The instrumentation within the Unit has been enhanced by the arrival of a EuroVector Elemental Analyser 3022. This will be used for CHN analyses. A new 7-figure balance has also been received to operate alongside the EA. To compensate for our position in the building and the ongoing construction work, the balance now rests upon a specially constructed anti-vibration table.

Unfortunately, the flood in February 2007 necessitated the closure of the unit for nearly 4 weeks. We are grateful to our academic supervisor (Professor Martin Banwell), Lee Welling (OHS unit) and the many other services, which facilitated our return to work so rapidly.

The new EA3000 instrument is operating well and up to specifications. It will complement the faithful CE1106 for CHN analyses. Our new balance tables are also proving extremely valuable and ensure that the two Mettler 7-figure balances operate to the high level of accuracy and precision as demanded by our work in the Unit.

Reet Bergman was again able to contribute both her time and expertise to the running of the Unit, returning on a casual basis to work whenever absences of the regular staff necessitated it.

Details of instrumental techniques used and the procedures for the submission of samples can be found on the website. *(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 RSC. The School uses workstations running several varieities of Linux/Unix. These Linux/Unix computers are used for a variety of purposes including data-reduction, desktop use and a small amount of computation. Macintosh computers are used as the desktop systems for most staff and students. In addition, PCs mainly running Microsoft Windows are used for controlling experimental and data collection equipment. Printing services are provided by mono laser printers and laser, thermal and 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, as well as 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 in the School. Archives and backups of the School's computers are now done to hard disk. The backup servers are currently located in the Department of Chemistry and the School of Mathematical Sciences.

The School's web page is administered by Chris Blake. *(P R Cohen, C D Delfs, G A Lindsell, H Macarthur Onslow, E Mittag)*

http://rsc.anu.edu.au/~rsccu/index.html

Single Crystal X–ray Diffraction Unit

The Unit performs crystal structure analyses on samples provided by various groups within the RSC and Department of Chemistry. 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.

In total, 312 data sets were collected and 221 final reports produced for the year. External work was performed for the University of New South Wales, the South Australian Museum, RMIT University and the Australian Defence Force Academy. *(A C Willis)*

Source of Crystal	Data Sets Collected	Reports Completed
ANU (performed by unit)	139	78
ANU (performed by others)	149	134
Others (performed by unit)	24	9
TOTAL	**312**	**221**

http://rsc.anu.edu.au/facilities/index.php

Mass Spectrometry Service

In 2006 Professor Ellak von Nagy-Felsobuki, who was on sabbatical leave from the Chemistry Department of the University of Newcastle, conducted a research project on our Bruker Apex 3 FTICR Mass Spectrometer. John Allen assisted him for 5 months on a Project Quantification and Characterisation of Metallothioneins Proteins using Bruker Apex 3.

A total of 6881 measurements were made throughout 2006 on the five different mass spectrometers in the Unit. The majority of samples were run for the School.

In 2007 John Allen attended the Biannual *ANZSMS21 Mass Spectrometry Conference* at the University of Canterbury, New Zealand.

A total of 5658 measurements were made in 2007 on the five different mass spectrometers in the Unit. The majority of samples were run for the School. 277 were run for the Department of Chemistry, ANU. *(J M Allen, G G Lockhart, A Jeyasingham)*

Total samples run through each mass spectrometer are as follows:

Instrument	2006	2007
VG Autospec	2416	2315
VG Quattro	373	78
Micromass ZMD	3104	2335
HP Agilent GC/MS	177	162
Bruker Apex 3 FTICR	811	768
TOTAL	**6881**	**5658**

http://rsc.anu.edu.au/facilities/mass.php

University NMR Centre

The flood in early February was the major event of 2007. All the NMR equipment, except for the Gemini, survived virtually unscathed, although several rooms were flooded. Some components in the Gemini failed when it powered up but the Centre was able to negotiate an upgrade and some assistance from the manufacturer and source spare parts from recently retired Geminis. The Gemini returned to service in May and continues to have an important role in the Centre. Despite this event, consistent reliability of all the instrumentation enabled high productivity for the NMR Centre.

During 2007 the University NMR Centre catered for over 120 users from the RSC, the Research School of Physical Sciences, Research School of Biological Sciences, John Curtin School of Medical Research, the Faculties, University of Sydney, University of NSW and University College UNSW ADFA. 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 M Simmonds)*

http://bloch.anu.edu.au/

RSC Workshops

Workshop staff have been involved in a variety of activities including assisting in the storm recovery, room alterations and refurbishment for the Department of Chemistry, alterations for the McLeod group, alterations for the Administration Area and updating our training to enable us to meet the requirements of the ANU. In addition to this we also provide the services detailed below.

Carpentry and Paint Workshops

These Workshops are well provided for with carpentry, joinery and finishing equipment. The Workshops provide made to order furniture and fitments in addition to room alterations and modifications. *(I Clarke, R O'Brien)*

Cryogenics Unit

This Unit provides cryogens, liquid nitrogen and helium, for the School and the wider ANU community. *(P Devitt, R O'Brien)*

Electrical Unit

This Unit provides services in electrical wiring and modifications, new equipment verification and installation, maintenance safety of electrical research and plant equipment. The mandatory electrical checking of appliances throughout the School is also coordinated by staff in this Unit. *(F Vera, R 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 manufacture. In addition, electronic repair services are provided for the research groups within the School and the instrumentation service units. *(T Davenport - passed away in May 2007, 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 2007 the Unit provided services to research programs within the RSC and the wider ANU community. In addition they undertook work for external clients. *(G Platt - 2 month contract, P Siu, C Tomkins)*

Mechanical Workshops

The Mechanical Workshop is equipped with precision engineering machinery for instrument development, mechanical maintenance and equipment repair. 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 - seconded to RSPSE for 3 months, M J Hill, K L Jackman, R J O'Brien, Anthony Peet - seconded to the RSC for 3 months)*

School Committees, Representatives and Office Bearers

* position ended in 2006
ˆ position taken up in 2007

Dean's Advisory Group

Professor D J Evans, Dean *(Chair) (ex officio)*
Professor C J Easton, Deputy Dean* IF rep, DEC(SHE) *Research Committee rep (ex officio)*
Professor M G Banwell, Deputy Deanˆ
Professor R L Withers, Associate Dean (Students) DEC(SHE) *Education Committee rep (ex officio)*
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 M G Humphreyˆ
Professor E R Krausz *School Integrity Advisor*
Professor L N Mander
Professor D L Ollis *Head, Dept Chemistry*
Professor G Otting
Professor A D Rae
Professor R Strangerˆ
Professor T R Welberry
Professor J W White
Professor S B Wild
Associate Professor E M Sevick
Associate Professor M S Sherburn
Dr R Barrowˆ
Dr M L Coote
Dr M Ellisonˆ
Dr M A Keniry
Dr M McLeodˆ
Dr A J Oakley
Dr R Paceˆ
Dr G Salem *(Dept. Chemistry rep*)*
Dr D J Sinclair* *(Faculty and IF rep)*
Dr R D Webster*
Mr K Cooper
Mr G Deebleˆ
Ms K Jackson*
Ms L Harland*
Secretary: Ms M Baker

Academics–in–Charge

Mass Spectrometry:

Professor C J Easton*
Professor M G Banwellˆ

Microanalytical Unit:

Professor C J Easton*
Professor M G Banwellˆ

Crystallography Unit:

Professor C J Easton*
Professor M G Banwellˆ

UNMRC:

Professor M A Keniry

EPR Facilities:

Dr R D Webster*
Dr R Paceˆ

Advisory Committee on Safety

Professor T R Welberry *(Chair)*
Professor M G Banwell
Professor S B Wild
Dr J-W Liu
Dr M Lynch
Dr R Pace
Dr A J Oakley*
Mr I Clarke^
Mr K Cooper
Mr G Deeble
Mr P A Gugger
Ms K Jackson*
Mr V Lawrence^
Mr H McGlinchey
Mr C J Tomkins
Mr L L Welling (*Secretary*)
Mrs V Withers

ANU Radiation Safety Committee Officers and Licensee for Radiochemicals

Areas of Expertise

1. Radioisotopes
2. Machines Producing Ionising Radiation
3. Lasers
4. Non-ionising Radiations

Professor E R Krausz	3
Professor L N Mander	1
Professor A D Rae	2
Professor T R Welberry	2
Professor J W White	2
Professor D L Ollis	2
Mr L L Welling (Coordinating Officer)	1/4

AQIS Liaison Officer

Professor N E Dixon*
Professor G Otting^

Institutional rDNA Committee Liaison Officer

Professor N E Dixon*
Dr J-W Liu^

Board of Studies of the Graduate Program in Chemistry

Professor C J Easton (*Convenor*)
Professor M G Banwell
Professor M A Collins^
Professor N E Dixon*
Professor A F Hill
Professor R L Withers
Professor Mark Humphrey (*Dept. Chemistry rep*)
*Secretary: Ms S Meharg *, Ms S Neulinger ^*

Chemistry Library Advisory Committee (CHEMLAC)

Professor M G Banwell (*Chair*)
Professor M A Collins
Professor A F Hill
Professor M G Humphrey (*Dept. Chemistry rep*)
Professor G Otting
Dr R Barrow (*Dept. Chemistry rep*)
Dr C Delfs
Mrs J Smith

Chemistry Management Group 2007

Mr G Deeble (*Chair, School Manager*)
Mr N Bayley *(Finance rep*)
Mr I Clarke (*Workshop rep*)
Ms P Cohen (*IT rep*)
Mr K Cooper (*Facilities rep*)
Mr V Lawrence (*Dept rep*)
Mr L Welling (*Secretary, Technical rep*)

Ex-officio Members:
Professor M G Banwell *(Deputy Dean)*
Ms S Neulinger (*A/g Student/Marketing rep*)

Dean's Prize Selection Committee

Professor T R Welberry (*Convenor*)
Professor M G Banwell
Professor C J Easton*
Professor S B Wild^
Secretary: Ms S Meharg

Deanship Liaison Committee 2006

Professor M A Collins (*Chair*)
Professor G Otting
Professor R L Withers
Associate Professor E M Sevick
Associate Professor M S Sherburn
Mr Nathan Kilah
Mrs E O'Toole
Mr C Tomkins

Distinguished Visitors Selection Committee

Professor M G Banwell *(Chair)*
Professor P M W Gill
Professor A F Hill
Professor T R Welberry
Professor S B Wild

IT Committee

Professor T R Welberry *(Chair)*
Professor M G Banwell
Professor E R Krausz
Mr C J Blake
Ms P Cohen

Occupational Safety Liaison Officers

Ms S Neulinger
Mr G Perri

Ombudspersons

Professor C J Easton
Professor R L Withers
Associate Professor E M Sevick
Ms S Meharg

Promotions Committee (Local Area)

Professor A F Hill *(Chair)*
Professor M G Banwell^
Professor E R Krausz
Associate Professor E M Sevick

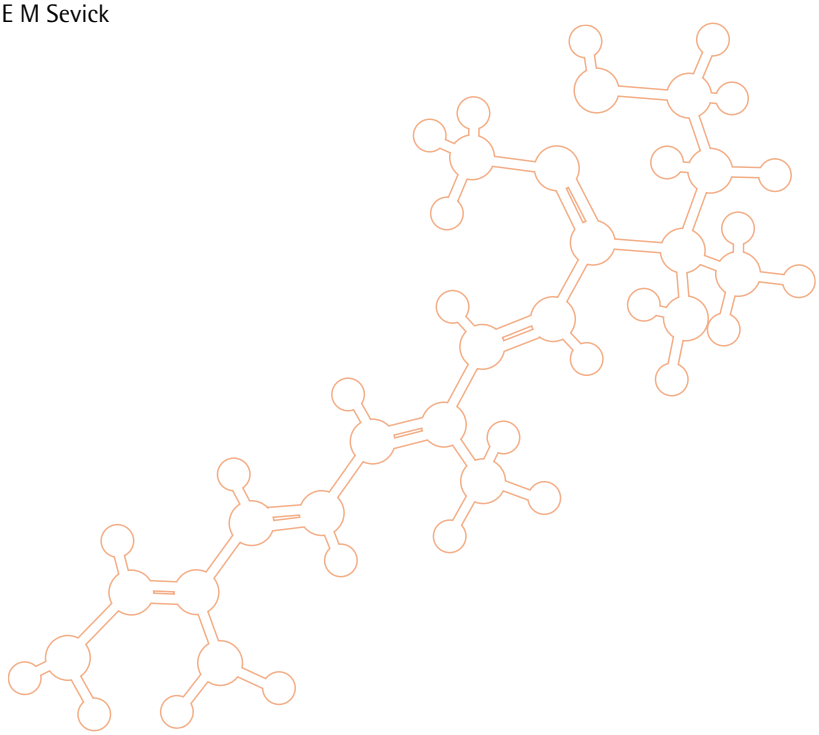
Ex-officio Members
Professor D J Evans

Visitors Grants Committee

Professor T R Welberry *(Chair)*
Professor N E Dixon*
Professor C J Easton
Professor P M W Gill
Professor A F Hill
Professor S B Wild
Secretary: Ms M Baker

WWW Site Committee

Professor E R Krausz *(Chair)*
Mr C J Blake *(Webmaster)*
Ms P Cohen



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 2006 and 2007 was again to be focused on the consolidation and up-grading of resources required to support both new and on-going 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 that occurred in the Birch Building on 5th August 2005.

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 an 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 2006*

*** denotes a new grant in 2007*

Protein Structure and Function

Professor N Dixon *

Molecular interactions in the eubacterial replisome: A paradigm for study of dynamic macromolecular machines
Australian Research Council, Discovery Project, January 2006 – December 2008

Professor N Dixon, Assoc. Professor E Sevick, A M Van Oijen and S Hamdan *

Single molecule studies of replisomal function
Australian Research Council, International Linkage Project, January 2006 – December 2007

Professor N Dixon, G Schenk, L Gahan, G Hanson, L Guddat and M J Riley

An integrated approach towards development of highly specific chemotherapeutics
Australian Research Council, Discovery Project, January 2005 – December 2007

Dr K Ozawa and Professor N Dixon

Subunit contact in a replicative DNA polymerase
Australian Research Council, Linkage Postdoctoral Fellowship (CSIRO), October 2003 – October 2006

Structural Biology

Professor P Board, Dr A Oakley and C Jackson *

Cofactor free oxygenases (GUP 5157)
Australian Nuclear Science & Technology Organisation, and Australian Synchrotron Research Program, November 2006

Dr A Oakley *

Cofactor free oxygenases
Australian Nuclear Science & Technology Organisation, and Australian Synchrotron Research Program, March 2006

Dr A Oakley *

High throughput protein crystallisation
Australian National University, MEC Award, January 2006 – December 2006

Professor P Board, Dr R Baker and Dr A Oakley *

Pharmacogenetic and structural investigation of the omega class glutathione transferases
National Health and Medical Research Council, Project Grant, January 2006 – December 2008

Protein Crystallography and Engineering

Professor D Ollis and E Gillam **

Evolving enzymes to harness the clean energy reserves of nature (led by U Queensland)
Australian Research Council, Discovery Project, January 2007 – December 2009

Professor D L Ollis *

Services agreement CSIRO
Commonwealth Scientific and Industrial Research Organisation, June 2006 – September 2006

Professor D Ollis, G Schenk and L Gahan *

Directed evolution of enzymes for bioremediation: Structure function studies of bimetalloenzymes
Australian Research Council, Discovery Project, January 2006 – December 2008

Biomolecular NMR

Professor G Otting, Dr M Keniry, Professor D L Ollis, Dr A Oakley and Dr R Pace **

New ultracentrifuge for structural biology
Australian National University, MEC, January 2007 – December 2007

Professor G Otting *

The binding mode of inhibitors to dengue NS3/2B by NMR
Novartis Institute for Tropical Diseases Pty Ltd, Industry Project, June 2006 – August 2007

Professor G Otting *

State-of-the-art NMR facilities
Australian National University, MEC and Australian Research Council, Linkage Project, January 2006 – December 2006

Professor G Otting and T Huber *

Fluorine-labelled proteins for NMR spectroscopy
Australian Research Council, Discovery Project, January 2006 – December 2008

Professor G Otting

New methods for structural biology in solution
Australian Research Council, Discovery Project, April 2002 – December 2006 and January 2003 – December 2007

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

Professor T R Welberry, Dr A Heerdegen and Dr E Chan **

Diffuse scattering in disordered and polymorphic materials
Australian Nuclear Science & Technology Organisation, and Australian Synchrotron Research Program, November 2007

Professor T R Welberry **

Understanding prediction and control of polymorphism in pharmaceuticals
Australian Research Council, Discovery Project, January 2007 – December 2009

Dr D Goossens and Professor T R Welberry *

Diffuse scattering from polymorphic materials
Australian Nuclear Science & Technology Organisation, and Australian Synchrotron Research Program, November 2006

Dr D Goossens *

Study of the nature and role of nanoscale order in complex materials
Australian Institute of Nuclear Science and Engineering, November 2006 – November 2009

Dr D Goossens and Dr K Wilson-Goossens *

Exploring the magnetic phase diagram of (Mn Zn) PS3
Australian Institute of Nuclear Science and Engineering, August 2006

Dr D Goossens *

Finding the ferromagnetic direction in $BaPO_3$ using high-magnetic-field neutron powder diffraction
Australian Institute of Nuclear Science and Engineering, August 2006

Professor T R Welberry *

Detector system for diffuse X-ray scattering
Australian National University, MEC Award, January 2006 – December 2006

Professor T R Welberry, Professor R L Withers, C D Ling, R W Robinson and C M Stampfl *

Floating zone crystal growth facility (led by U Sydney)
Australian Research Council, Linkage Project, and Australian Nuclear Science & Technology Organisation, January 2006 – December 2006

Inorganic Stereochemistry and Asymmetric Synthesis

Dr M Coote and Professor S B Wild

Quantum-chemical design of stereoregular polyphosphine for nanowires
Australian Research Council, Discovery Project, January 2005 – December 2007

Synthesis and Mechanism

Professor M G Banwell **

Marine natural products as sources of agrochemicals - the variolins
Australian Research Council, Linkage Project, and BASF Aktiengesellschaft Agricultural Products Division, July 2007 – June 2011

Professor M G Banwell and M J Garson **

Total synthesis and biological evaluation of Australian sponge metabolites
Australian Research Council, Discovery Project, January 2007 – December 2009

Professor M G Banwell and A Stewart *

Cryptopharma Pty Ltd subproject agreement
Cryptopharma Pty Ltd, November 2006 – November 2007

Professor M G Banwell *

Research and development agreement
Progen Industries Ltd, Contract Research, February 2006 – February 2007

Professor M G Banwell *

Organic synthesis and reaction processing facility
Australian National University, MEC Award, January 2006 – December 2006

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

The development of new non-steroidal anti-asthma drugs with novel modes of action
Australian Research Council, Linkage Project, and Cryptopharma Pty Ltd, January 2005 – December 2007

Professor M G Banwell

Chemoenzymatic routes to novel dendritic architectures suitable for pharmaceutical applications
Australian Research Council, Linkage Project, and Starpharma Ltd, March 2004 – December 2006

Professor M G Banwell and 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

Development of chemoenzymatic methods for the selective elaboration of polyfunctional therapeutic agents to oligomers with improved efficacy
Australian Research Council, Linkage Project, and Biota Holdings Ltd, December 2003 – December 2006

Biochemical Reactions and Molecular Recognition

Professor C Easton, Dr M Coote and Associate Professor M Sherburn *

ARC CENTRE OF EXCELLENCE - Centre for Free Radical Chemistry and Biotechnology - (led by U Melbourne)
Australian National University and Australian Research Council, Centres of Excellence, January 2006 – December 2010

Professor C Easton *

Platform technologies for the regulation of peptide hormones
Australian Research Council, Discovery Project, January 2006 – December 2010

Professor C Easton *

Purchase of a carbon hydrogen and nitrogen element analyser
Australian National University, MEC Award, January 2006 – November 2006

Dr M G Casarotto, Professor A Dulhunty and Professor C Easton *

Refinement and delivery of synthetic compounds that specifically alter muscle contraction
Australian National University, Australian Research Council, Linkage Project, and Biotron Ltd, January 2006 – December 2008

Professor C Easton and N Dunlop

Development of optimised processes for manufacturing melamine-urea-formaldehyde type resins and improved resins and reconstituted wood products derived from resins
Australian Research Council, Linkage Project, and ORICA Australia Pty Ltd, December 2005 – December 2008

Professor C Easton and S Lincoln

Supramolecular assemblies as nanoscale devices to control chemical and physical processes
Australian Research Council, Discovery Project, January 2004 – December 2008

Organic Synthesis

Professor R Rickards *

A proprietary molecular signalling system
Commonwealth Scientific and Industrial Research Organisation, National Research Flagship Collaboration Fund, September 2006 – September 2008

Organic Synthesis, Methodology and Host-guest Chemistry

Associate Professor M Sherburn and M Paddon-Row *

Experimental-computational investigations into Diels-Alder sequences
Australian Research Council, Discovery Project, January 2006 – December 2008

Associate Professor M Sherburn

Domino approaches to polycyclic natural products
Australian Research Council, Discovery Project, January 2005 – December 2007

Synthetic Organometallic and Coordination Chemistry

Professor A Hill **

Understanding and harnessing the unique and curious metal boron bond: Unlocking the metallaboratrane
Australian Research Council, Discovery Project, January 2007 – December 2009

Professor A Hill and M Bruce

Towards nano-ciruits: 2 and 3-dimensional carbon-wired nano-architectures
Australian Research Council, Discovery Project, January 2005 – December 2007

Solid State Inorganic Chemistry

Dr Y Liu, Dr Y Chen, Professor T R Welberry, Dr D Goossens, Professor J W White, Professor R L Withers and Dr Z Stachurski **

Facility for polarization characterisation of ferroelectric piezoelectric pyroelectric materials
Australian National University, MEC Award, January 2007 – December 2007

Professor R Elliman, Dr T Senden, Dr Y Chen, Dr J Bradby, Dr L Fu, Dr J Fitz Gerald, Professor R L Withers, Dr S Welch, Professor B Luther-Davies, Professor I Jackson, Dr I Williams, Dr Z Stachurski and Dr K Weber **

Improved understanding of nanoscale materials - structure composition crystallography and defects revealed by electron imaging and analysis at high spatial resolution

Australian National University, MEC Award, and Australian Research Council, Linkage Project, January 2007 – December 2007

Dr Y Liu, S Li, H Liu and P Walls **

Laser flash thermophysical properties analyser for the development of advanced materials food processing technologies and biomedical components (led by UNSW)

Australian Research Council, Linkage Project, January 2007 – December 2007

Professor R L Withers, L Noren, Dr Y Liu and Dr D Goossens *

The structure of the incommensurately modulated solid solution SnSb and the lithium-containing compounds Li_zSnSb (z=0 0.1, 0.5 and 1) and $Li_{[3-x]}Mg_xNbO_{[4-y]}F_x$ (x=0 and 1; y=0 and 1)

Australian Institute of Nuclear Science and Engineering, October 2006

Professor R L Withers and Dr Y Liu *

An integrated approach towards the development of new generation rf/microwave dielectric materials

Australian Research Council, Discovery Project, January 2006 – December 2010

Professor R L Withers, A S Schmid and J C Howard

Understanding phase transitions through precise structural studies

Australian Research Council, Discovery Project, January 2005 – December 2007

Theoretical Chemical Physics

Professor M Collins and Professor P Gill **

Molecular energies and non-bonded interactions

Australian Research Council, Discovery Project, January 2007 – December 2009

Professor M Collins and M Jordan *

The first chemically accurate tools in theoretical materials research (led by U Sydney)

Australian Research Council, Discovery Project, January 2006 – December 2010

Professor M Collins and D H 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 Coote

Computer-aided design of agents for controlling free-radical polymerisation

Australian Research Council, Discovery Project, January 2005 – December 2007

Liquid State Chemical Physics

Professor D Evans and Assoc. Professor E M Sevick*

Experimental demonstrations of new theorems of nonequilibrium thermodynamics

Australian Research Council, Discovery Project, January 2006 – December 2008

Professor D Evans and Dr D Bernhardt

Fluid properties and chaotic dynamics in equilibrium and nonequilibrium states (led by Griffith U)

Australian Research Council, Discovery Project, January 2004 – December 2008

Theoretical Quantum Chemistry

Professor P Gill *

Development and implementation of effective new models for electron correlation

Australian Research Council, Discovery Project, January 2006 – December 2008

Laser and Optical Spectroscopy

Professor E Krausz, Dr J Hughes, A W Rutherford and A Boussac **

Solar energy conversion in the water oxidising enzyme photosystem II: Spectroscopy of primary and secondary electron donors

Commonwealth Department of Education Science and Training, International Sciences Linkages, March 2007 – January 2009

Dr W Hillier, Professor E Krausz, Dr T Wydrzynski, R J Debus, M Sugiura and A Boussac **

The mechanism of water splitting in photosynthesis

Australian Research Council, Discovery Project, January 2007 – December 2009

Polymers and Soft Condensed Matter

Professor B Ninham, Assoc. Professor E M Sevick and Professor D Williams

Salt sugar and sequence: The effect of molecular forces on polymer conformation

Australian Research Council, Discovery Project, January 2004 – December 2006

Solid State Molecular Science

Dr P Reynolds and Professor J W White **

Co-surfactant of oil-soluble and water soluble surfactants in emulsion stabilisation (RB720087). The role of reverse micelles in emulsion stabilisation (RB720088)

Australian Nuclear Science & Technology Organisation, Access to Major Research Facilities Program, October 2007

A Perriman, Dr J Mata and Dr D McGillivray **

Mechanisms of shear stability in emulsion (RB720086): The effect of solution pH on the interaction between poly (silicic) acid and DMPC at the air-water interface (RB720728)

Australian Nuclear Science & Technology Organisation, Access to Major Research Facilities Program, October 2007 – November 2007

Professor J W White, M Palmer, M A Augustin and T J Wooster **

Milk protein denaturation and stabilisation at surfaces

Australian Research Council, Linkage Project, Dairy Innovation Australia Limited and Food Science Australia, September 2007 – September 2010

Professor J W White **

4th meeting of the OECD global science forum working group on nuclear physics

Commonwealth Department of Education Science and Training, International Sciences Linkage, August 2007 – December 2007

Dr V J James, D Miller and M Read **

Solution for the controversy about the structure of hard keratin

Australian Nuclear Science & Technology Organisation, and Australian Synchrotron Research Program, March 2007 – April 2007

Dr V J James, D Miller and M Read **

Verification of the parallel arrangement of the tetrameric structure of intermediate filaments of hard alpha keratin

Australian Nuclear Science & Technology Organisation, Access to Major Research Facilities Program, March 2007 – April 2007

Dr D McGillivray, Dr P Reynolds and Professor J W White **

Packing of highly polydisperse spheres at very high volume fractions and hydration of high protein content powders

Australian Nuclear Science & Technology Organisation, Access to Major Research Facilities Program, February 2007 – March 2007

Professor S Hyde, Professor M Knackstedt and Professor J W White **

Liquid crystallography and mesoscale pores: Two-dimensional digital detection system for small-angle X-ray scattering

Australian National University, MEC Award, January 2007 – December 2007

Professor J W White and J Beattie **

Water at hydrophobic surfaces (led by U Sydney)
Australian Research Council, Discovery Project, January 2007 – December 2009

Professor J W White *

OECD global science forum working group on nuclear physics
Commonwealth Department of Education Science and Training, International Science Linkages, September 2006 – November 2006

Dr V J James *

Support to visit ChemMatCARS Advanced Photon Source USA (diagnosis of adeno lung cancer from changes in the molecular structure of hair)
Australian Nuclear Science & Technology Organisation and Australian Synchrotron Research Program, March 2006

Professor J W White and D Mather *

Access for Australian researchers to advanced neutron beam techniques (led by AINSE)
Australian Institute of Nuclear Science and Engineering, January 2006 – December 2006

Dr A J Jackson *

Protein/polysaccharide conjugate adsorption at hydrophobic surfaces
Australian Institute of Nuclear Science and Engineering, Award, January 2006 – December 2006

Professor J W White

Drying of dairy proteins
Dairy Innovation Australia Limited, Research Project, July 2005 – December 2006

Dr P Reynolds, Professor J W White, C Such and R Goodridge

Designer surfactants for creation of emulsion properties
Australian Research Council, Linkage Project, and ORICA Australia Pty Ltd, July 2004 – June 2007

Professor J W White

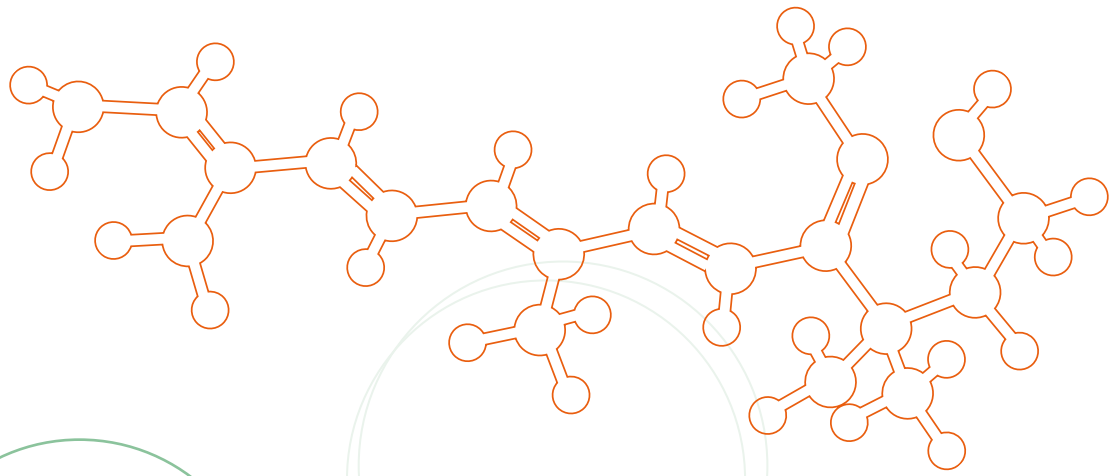
Making film-stars: Nano-composite films for solar energy capture
Commonwealth Department of Education Science and Training, Innovation Access Program, March 2004 – May 2006

Professor J W White, M A Augustin and P Clarke

Drying of dairy proteins – strategies for preserving functional properties during dehydration
Food Science Australia, January 2004 – December 2006

Professor J W White and A Perriman

Protein behaviour at interfaces
Australian Institute of Nuclear Science and Engineering, Postgraduate Research Award, July 2003 – February 2006



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

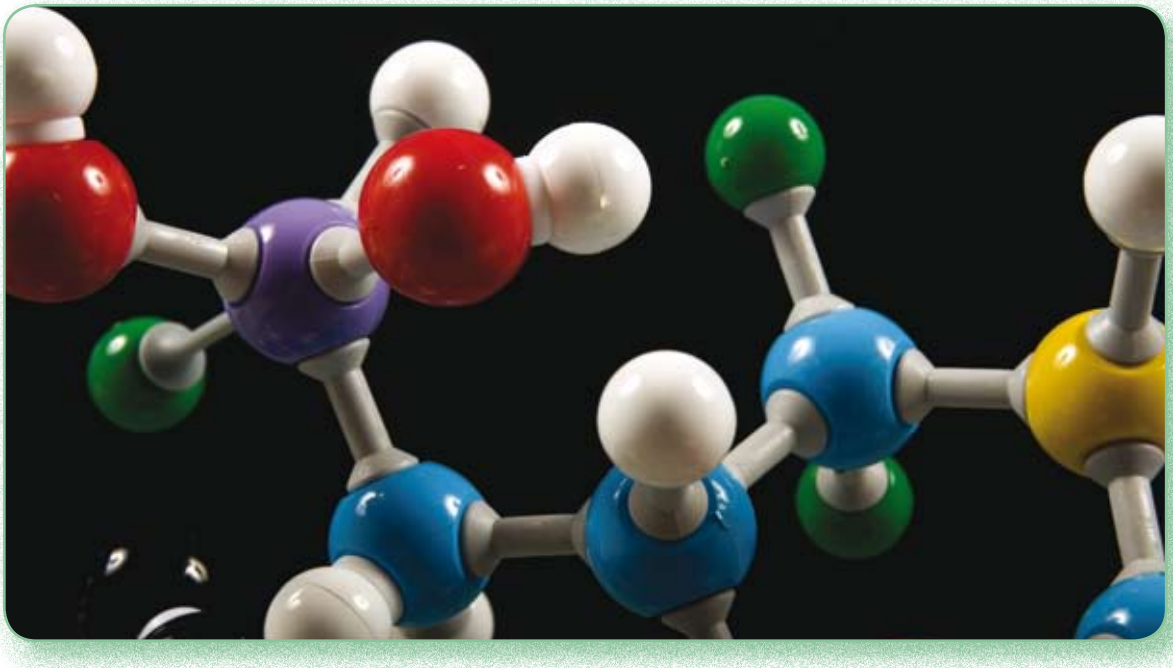
- the workshop reuses off–cuts of metal/glass/wood/plastics
- the original teak laboratory benches are redressed and reused
- precious metals (in particular platinum group metals) are recovered

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 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



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/Director on such matters as required. Dr Michelle Coote was promoted and granted tenure late in 2005, the second tenured female on the academic staff.

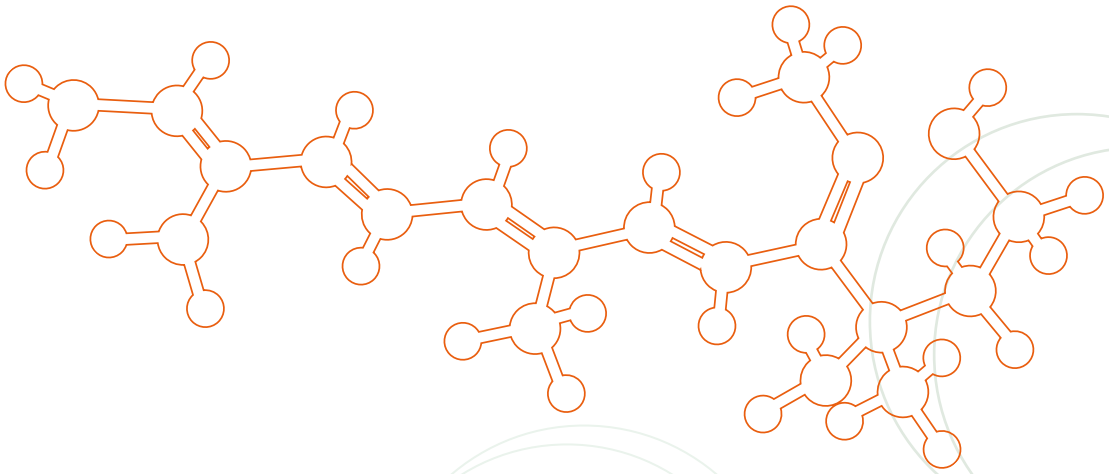
Scholar and Academic Staff Recruitment Profiles

In the PhD annual recruitment program the percentage of successful females has steadily risen from 24% in 1994 to 61.5% in 2007. In the Summer Scholar program the percentage of successful female applicants was 53% in 2007.

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 1998.

Academic	1998*	1999	2000	2001	2002	2003*	2004	2005	2006	2007
Positions advertised	17	7	13	10	3	16	5	5	9	5
No. appointments w/out advertisement					2	4	15	16	18	11
Total appointments	12	6	15	12	8	25	19	21	27	16
Total of women appointed as a %	42	16	47	33	50	12	32	23	44	25
Female PhD scholars recruited as a %	30	25	21	27	33	37	39	44	41	62

* = Rita Cornforth Fellow recruitment years (this Fellowship is for early-career female researchers only)



STAFF LIST

Academic Staff

* departed during 2006
ˆ started during 2007
departed during 2007

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(Hons) *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*

Wild, S Bruce BSc *NSW* PhD *Manchester* FRACI, FRSC, FAA

Withers, Raymond L BSc PhD *Melbourne*

White, John W CMG MSc *Sydney* MA DPhil *Oxford* FRSC, FRACI, FAPS, FAA, FRS

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)

McLeod, Mal BSc(Hons) *Monash* PhD *Cambridge* ˆ

Fellow

Oakley, Aaron J BSc *Tasmania* PhD *St Vincent's IMR Melbourne* #

Rita Cornforth Fellow – 2006

Coote, Michelle L BSc PhD *NSW*

Research Fellows

+ denotes ARC grant funded

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* +#

Prosselkov, Pavel MSc PhD *Woronezh* *

Robinson, J Kenneth BA PhD *Oxford* *

Sinclair, David J BSc PhD NSW * (RSC/Dept Chem)

Zank, Johann DiplChem DrRerNat *Tech Munich* *+

Postdoctoral Fellows

+ denotes ARC grant funded

Addicoat, Matthew BSc(Hons) PhD *Adelaide* ˆ

Apponyi, Margit BSc(Hons) PhD *Adelaide* *

Augustine, Anu MSc PhD *India* ˆ

Axford, Lorraine MChem *Wales* PhD *Bristol* +*

Backes, Michael DiplChem DrRerNat *RWTH* Aachen +*

Barr, Lorna BSc *Strathclyde* PhD *ANU* +*

Biju, Akkattu BSc MSc *Mahatma Ghandi U* PhD *Kerala* #

Bluechel, Christian Dip Chem *Regensburg* PhD *ETH Zurich* #

Cade, Ian MSc PhD *Imperial College* ˆ

Carberry, David M BSc BEng Hons PhD *ANU* *

Chan, Eric BSc(Hons) PhD *UWA* ˆ

Chand, Satish BSc *Fiji* MSc *Macquarie* PhD *ANU*

Cieslinski, Marta M BSc *Adelaide* PhD *ANU* *

Cordiner, Richard MSc PhD *Durham*

Crittenden, Deborah BSc PhD *Sydney*

Crossley, Ian R MChem PhD *UMIST* *

Dauge, Delphine M DEA *Orsay* PhD *École Polytechnique*, Palaiseau +*

Dawson, Ryan BSc *Adelaide* PhD *ANU* ^

Dumont, Elise BSc MSc *ENS Paris* PhD *Paris VI* #

Evenhuis, Christian R BSc *Hobart* PhD *ANU*

Foot, Jonathan S MSc *Edinburgh* PhD *York* +*

Gamble, Allan B BMedChem(Adv) GCertBus PhD *UOW* ^

Gebert, Antje Dip MSc PhD *Albert-Ludwig* +^

Godsi, Oded BA MA *Tel-Aviv* PhD *Technion Israel* +#

Gresser, Mary BSc(Hons) PhD *Wollongong* ^

Headlam, Madeleine J BSc PhD *WA* +*

Högermeier, Jens DiplChem *Hannover* DrRerNat *FU Berlin* +^

Hughes, Joseph BSc(Hons) PhD *ANU* #

Izgorodina, Ekaterina I BSc MSc *Ivanova State U Chem/Tech*, Russia DrRerNat *Münster* *

Jackson, Andrew J MChem DPhil *Oxford* +*

Kim, Hye-Kyung BSc MSc *Yeungnam* Korea PhD *Chalmers* +

Knoke, Mario Diplom PhD *Göttingen* +*

Krenske, Elizabeth H BSc *Qld* PhD *ANU* +#

Larsson, Ann-Kristin MSc PhD *Lund*

Liang, Haobo BSc *Peking* PhD *Vanderbilt* +^

Lin, Ching Yeh (Leaf) BSc *Chiao-Tung* PhD *ANU*

Lin, Jack BSc MSc PhD *Tsing Hua* ^

Longshaw, Alistair MSc *Durham* PhD *Manchester*

Loscha, Karin Dip *Goettingen* PhD *ANU* +^

Louis, Ignace BSc(Hons) *Sydney* PhD *UNSW*

Martin, Stephen A BSc PhD *RMIT* +#

Mata, Jitendra BSc MSc PhD *V.N.S.G.*

Maulana, Ilham MSc *Syiah Kuala* PhD *Leipzig*

McAteer, Stephen M MChem *Southampton* PhD *Leeds* +*

McGillivray, Duncan BA/BSc *Auckland* BSc(Hons) *ANU* DPhil *Oxford* #

Menon, Rajeev BSc MSc *Calicut* PhD *Kerala* ^

Mulcair, Mark D BSc *Monash* PhD *ANU* +*

Namazian, Mansoor BChem *Isfahan* MSc *Tarbiat Modarres* PhD *UQ*

Offermann, Daniel A BSc PhD *Monash* +#

Onagi, Hideki BAppSc *Western Sydney* BScHons PhD *ANU* +

Park, Ah Young BSc *Victoria U* Hons PhD *ANU* #

Payne, Alan D BSc PhD *WA* +

Pearson, Emma BSc(Hons) *UWA* PhD *ANU* ^

Pearson, Jason BSc(Hons) *Cape Bretton* PhD *Dalhousie* ^

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 *Qld* +*

Steffen, Ronald Dipl PhD *Tech U Berlin*

Steinbach, Joerg Dipl DrRerNat *Kaiserslautern* +*

Su, Xun-Cheng MSc PhD *Nankai* China +

Varganov, Sergey MSc *Siberian State Aerospace U* CSc *Russian Academy of Science* PhD *Iowa*

Viswanathan, Bala BSc MSc *McGill* PhD *Dalhousie* +*

Wagler, Jörg Dip Chem DrRerNat *TU Bergakademie* #

Watts, Zachary BAppSci(Hons) *RMIT* PhD *ANU* ^

White, Richard MChem PhD *Leicester* +^

Williams, Stephen R B AppSci PhD *RMIT* +

Zhang, Yi-Jun BSc *Sun Yat-Sen* PhD *SIOC Chinese Academy of Sciences* +^

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 *LaTrobe* *

ARC Linkage Australian Postdoctoral Fellow (CSIRO)

Ozawa, Kiyoshi BEng *Yokohama*, MSc PhD *Tokyo*

Progen Industries Fellows

Bonnet, Muriel Dipl *Bordeaux* PhD *ETH* Zurich *

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 *

Honorary 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 2006
^ left during 2007
+ started in 2007

Business Office

Harland, Lesley BSc MSc *E Anglia* *
Laboratory Manager

Scarr, Lorraine *
Business Officer

Holloway, Marilyn *
Academic Secretary

Bayley, Neil BInfTech *ANU*
Purchasing Officer

Meharg, Seona ^
Student & Marketing Officer

Neulinger, Stephanie +
A/g Student & Marketing Officer

Slocum, Maureen
Academic Staff Administrator *

Monaghan, Lorna M *
Administrative Assistant

O'Brien, Brendan J
Administrative Assistant

O'Toole, Elouise E *
Administrative Assistant

Russell, Kurt
Requisitioning Clerk

Davies, Christine ~*
Receptionist

Rawlings, Kim C ~^
Receptionist

Murray, Valerie J ~
Student Administrative Assistant

Departmental Administrative Assistants

Arnold, Julie ~*
Biological

Slocum, Maureen +
Biological & Organic Chemistry

Perri, Gavin ~
Inorganic Chemistry

Neulinger, Stephanie ~^
Physical & Theoretical Chemistry

Riches, Susan
Centre of Excellence

Britton, Lena ~ BSc (Bus Admin) *Goteborg*
UnlChe/ Oxford Australia Scholarship Fund

The Dean/Director'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*

Clarke, Ian J

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* ~

Koehne, Russell T AssocDipEng *CIT*

Lee, Stephen B

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, Ruhu BSc *Lanzhou* China

Sharp, Phillip Patrick BSc(Hons) *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* ~

Programmers

Blake, Christopher J BSc(Appl) *Canberra CAE* GradDip (Comp) *Canberra*

Cohen, Pam BA *ANU* GradDip(CompSci) *Canberra CAE* ~

Delfs, Christopher D BSc PhD *WA*

Lindsell, Graeme A BSc *NSW* PhD *ANU*

Chemistry Librarian (ANU Staff)

Smith, Joan E

Stores Staff

Galarza, Marcelo

Scarr, Barry

Security Officers

McGlinchey, Hugh

Jamieson, Stephen

Smith, Don M

Stuart, Ian

Tea Assistant

Van Kampen, Lena*

STATISTICS

Total academic staff at 31 March 2005			82.5	(17)
Standard appointments	17.5	(1)		
Fixed term appointments (excluding PDFs)	17	(3)		
School funded	4.5	(1.5)		
ARC grant funded)	9.5	(1.5)		
UnIChe grant funded	1	(0)		
ARC Federation Fellow	1	(0)		
ARC QEII Fellow	1	(0)		
Total Postdoctoral Fellows	48	(13)		
ARC PDFs	.5	(.5)		
School funded PDFs	4.5	(3)		
ARC grant funded PDFs	37.5	(7.5)		
Progen funded PDFs	1.5	(1)		
ARC/CSIRO Linkage funded PDF	1	(0)		
National Science Foundation Fellowship	1	(1)		
Feodor Lynen funded PDFs	2	(0)		
Visiting Fellows during 2005 (including Post-retired)			33	(3)
Postgraduate students at 31 March 2005 (excluding 5 students on program extension)			55	(31)
PhD degrees awarded			13	(4)
MPhil degrees awarded			1	(0)
General staff at 31 March 2005 (FTE)			69.11	24.11
Technical/Research	37.58	(7.08)		
Administrative/Computing	20.68	(13.18)		
Other	10.85	(3.85)		

ANU College of Science
Research School of Chemistry

The Australian National University
Building 35
Science Road
Canberra ACT 0200
Australia

T: +61 2 6125 3637
F: +61 2 6125 0755
W: http://rsc.anu.edu.au/index.php
E: directoradm@rsc.anu.edu.au

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