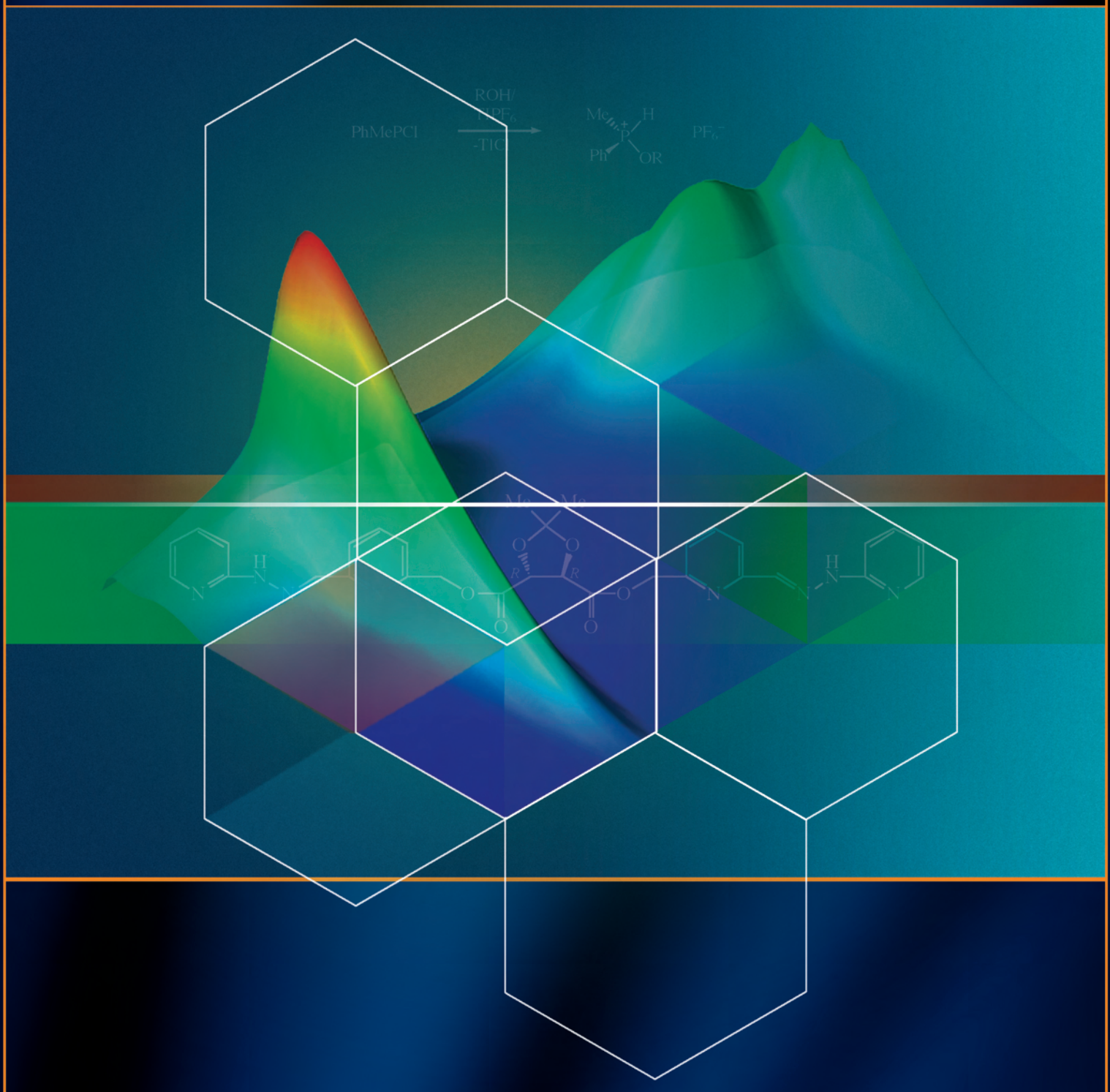
THE AUSTRALIAN NATIONAL UNIVERSITY

RESEARCH SCHOOL OF CHEMISTRY

Annual Report 2004



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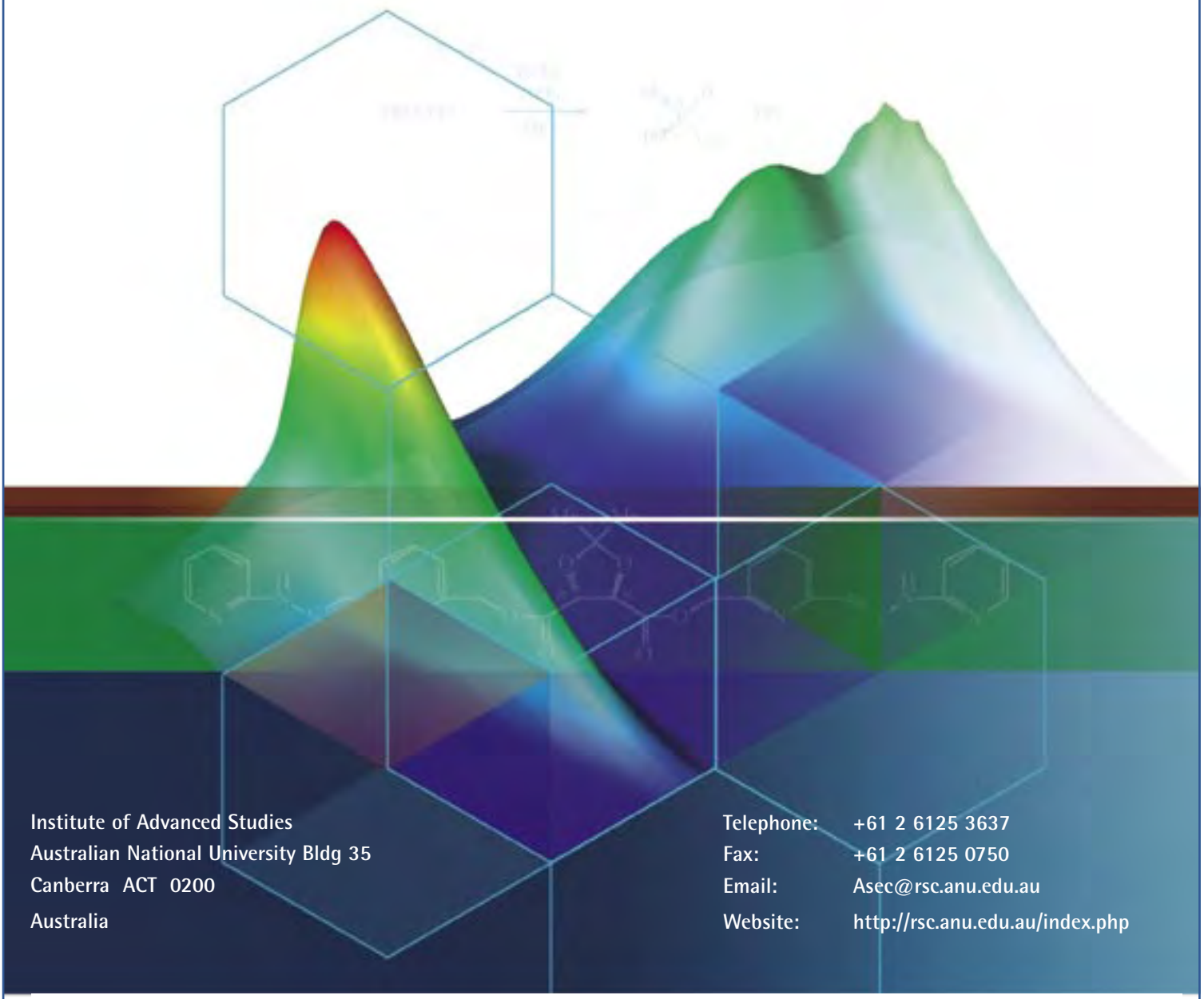

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Editorial Coordinator: Ms Michelle Baker

Front Cover: The Wigner intracule for the Li_2 molecule shows how the relative positions and momenta of the electrons are distributed — *Professor Peter Gill, Theoretical Quantum Chemistry Group*

Back Cover: The "Superbowl" molecule is capable of capturing and releasing drugs and chemicals — *Dr Mick Sherburn, Organic Synthesis, Methodology and Host-guest Chemistry Group*

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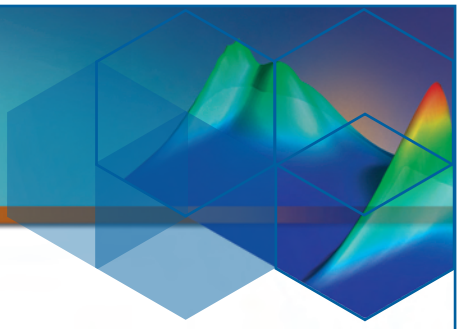


DEAN'S REPORT

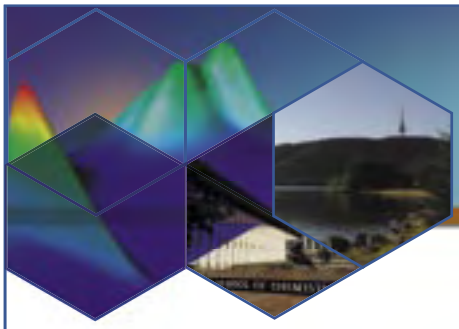
As an established 'centre of excellence', maintaining the highest international standards for over 30 years, the RSC has concentrated on areas of research of national importance and international significance. These research activities strengthen the discipline of chemistry in Australia and lead to numerous potential applications in medicine and industry, as well as maintaining a focus on fundamental research.

The Australian National University underwent a major Quality Review in 2004. The Review was conducted by a committee of twelve internationally eminent academics. The five best publications of ANU researchers were assessed by international experts in the respective research fields. The total number of international assessors involved in the ANU Review numbered over one thousand. The Executive Summary of the Review report states in part: "On the basis of all the available evidence and our own observations, we confirm the standing of ANU within the elite "Top 100" research intensive universities in the world, even among the top 50 or so." On the basis of chemistry citations, ANU chemistry already ranked in the top 100 institutions world wide. We quote from the Review's comments on chemistry research:
The research topics of the inorganic chemistry group at the Research School of Chemistry (RSC) cover a broad range of very high standard fundamental research. The School also has strengths in synthetic organic chemistry. The creative work in supramolecular chemistry and the approach to chemo-enzymatic synthesis are at the forefront of new developments internationally.

Important areas of biological and structural chemistry are being investigated, reflecting the growing importance of organic chemistry to biological problems. The ANU has some of the world's leading researchers in physical and analytical chemistry – working on colloids and interfaces, solar energy, electron diffraction and X-ray diffuse scattering. Similarly, the theoretical and computational chemistry group at RSC is regarded as one of the best in the world.

Since it was founded in 1968, the RSC has earned seven Fellowships of the Royal Society of London. Prior to 2004, the RSC had more Fellows of the Australian Academy of Science than any other chemistry department in Australia. Continuing its outstanding record of performance and recognition in this regard, Professors Christopher Easton and Martin Banwell were both elected Fellows in 2004, bringing our total membership to fifteen. Given the rules governing elections to the Academy of Science, the election of two chemists from one School or department in any one year is quite exceptional.

Other major prizes and awards won by RSC staff during 2004 include:
To Professor Banwell the Birch Medal of the RACI, the Novartis Lectureship and the Royal Society of Chemistry's Industrially Sponsored Award for Synthetic Organic Chemistry; Professor Beckwith was awarded an "Order of Australia" in the Queen's Birthday Honours List; to Professor Michael Collins the Physical Chemistry Division Medal (RACI); to Professor Chris Easton a Fellowship of the



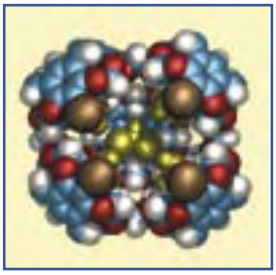
World Innovation Foundation; to Professor Denis Evans the Moyal Medal (Macquarie University) "for distinguished contributions to mathematics, physics or statistics", and our honours year student Mr Mathew Baker has been awarded the 2004 General Sir John Monash award for excellence. This scholarship will handsomely support Matthew's PhD research at Vrije Universiteit in the Netherlands.

The RSC has built on its previous ARC Grant successes with grant income for 2004 totalling approximately $4m with an additional $1m from all other sources (ref. page 111).

2004 Research Highlights

Work in the Protein Structure and Function Group, headed by Dr Nicholas Dixon, has revealed an unusual protein-DNA interaction. Copying of DNA molecules in cells that are about to divide requires that the two strands of DNA in the double helix are pulled apart. The process is stopped when a chromosome is completely copied because the two strands are held together tightly by a special protein called Tus. An intriguing problem that has occupied biochemists for twenty years is how this process can occur when the strands unzip in one direction but not the other. Experiments this year by Mark Mulcair and Patrick Schaeffer indicate that Tus works like a molecular mousetrap. The trap is set by the DNA unzipping process itself, and is sprung when a particular base in the DNA flips out of the double helix and wedges itself into a pocket in the surface of the protein. This unusual protein-DNA interaction, discovered by curiosity-driven research, should have many applications in biosensors and diagnostic devices.

Dr Mick Sherburn and colleagues have developed a promising new class of nano-sized containers called "superbowl" molecules that show promise for precision drug delivery. Shaped like a miniature football stadium, the molecules are capable of delivering a wide range of drugs – ranging from painkillers to chemotherapy cocktails – to specific areas of the body, potentially resulting in improved treatment outcomes and perhaps saving lives. The molecules also show promise for a wide range of other applications, including the removal of environmental toxins and aiding in chemical purification procedures.



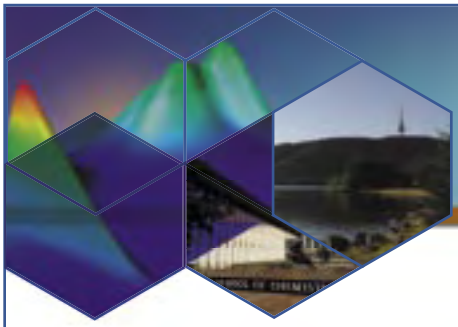
Professor Elmars Krausz, Joe Hughes, and a team of researchers at ANU, have found that the wavelength of light needed for oxygen production is much longer than previously thought. The chemical reaction which provides energy for photosynthesis, enabling plants to convert sunlight into energy and oxygen, is the most powerful process in biology. This breakthrough overturns 20 years of thinking about the photosynthesis powerplant, sending biologists, chemists and physicists back to the drawing board. These discoveries will not only have a profound impact on our understanding

and ability to control, modify and adapt natural photosynthesis, but will also extend the potential of engineered chemistry which can copy nature *via* the technique of artificial photosynthesis. Such work clearly underscores the pivotal importance of fundamental research and the need to continue to provide adequate funding for basic and enabling research in Australia.

The School is pleased to announce the formation of the new Theoretical Quantum Chemistry Group headed by Professor Peter Gill, formerly of Nottingham University, UK. Peter brings with him a postdoctoral fellow, Dr Andrew Gilbert, and three PhD scholars: Mr Darragh O'Neill, Ms Ching-Yeh Lin and Mr Siu-Hung Chien. In 1926, Erwin Schrödinger proposed that the behaviour of all matter is governed by a certain linear, second-order partial differential equation. The new group's aim is to devise and develop new methods for finding approximate solutions to this extremely difficult-to-solve equation, and to implement these within an easy-to-use software package called Q-CHEM. Such packages are helpful to other chemists, and theoretical calculations have become a valuable complement to experimental measurements.

For personal reasons, Professor Leo Radom resigned from his position as head of Computational Quantum Chemistry after 30 years. Professor Radom accepted a position in the School of Chemistry, University of Sydney, but will continue his close association with the School *via* an Adjunct Professorship.

As a result of their appointment as Fellows of the Australian Academy of Science, Chris Easton and Martin Banwell were promoted to E2 Professor. Dr David Ollis was promoted to E1 Professor, Dr Max Keniry was promoted to Senior Fellow, and Drs Yun Liu, Gloria Moyano, David Sinclair and Matthew Smith were promoted to Research Fellow. Ms Christine Sharrad received the General Staff Excellence Award for her absolutely outstanding work for the ANU Quality Review.



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: Professor Denis J Evans

Deputy Dean: Professor Christopher J Easton

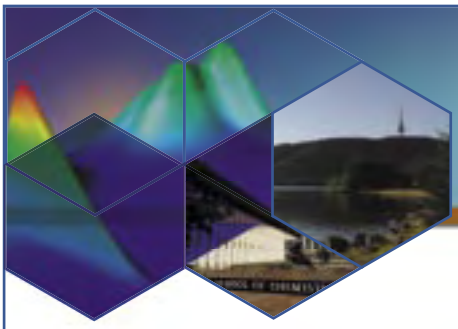
Associate Dean (Students): Professor Raymond L Withers

Group Leaders:

Professor Martin G Banwell, BSc PhD *Wellington*, FRACI, Hon FRSNZ, FAA
Professor Michael A Collins BSc PhD *Sydney*
Dr Nicholas E Dixon BSc PhD *Queensland*
Professor Christopher J Easton BSc *Flinders* PhD DSc *Adelaide*, FRACI, FAA
Dr Michelle L Coote BSc PhD *New South Wales*
Professor Denis J Evans BSc *Sydney* PhD *ANU*, FRACI, FAA
Professor Peter M W Gill MSc (Hons) *Auckland* PhD *ANU*
Dr Graham A Heath BSc PhD *Melbourne*
Professor Anthony F Hill MSc (Hons) *Auckland* DrRerNat *Bayreuth*, FRSC
Dr Max A Keniry BSc PhD *Sydney* (RSC/UNMRC)
Professor Elmars R Krausz BSc PhD *Sydney* FRACI
Professor Emeritus 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*
Professor Leo Radom (Adjunct) MSc PhD *Sydney* DSc *ANU*, FRACI, FAA
Dr Edith M Sevick BSE *Pittsburgh* PhD *Massachusetts*
Dr 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*

Laboratory Manager: Ms Lesley Harland

Academic Secretary: Ms Marilyn A Holloway



BIOLOGICAL CHEMISTRY

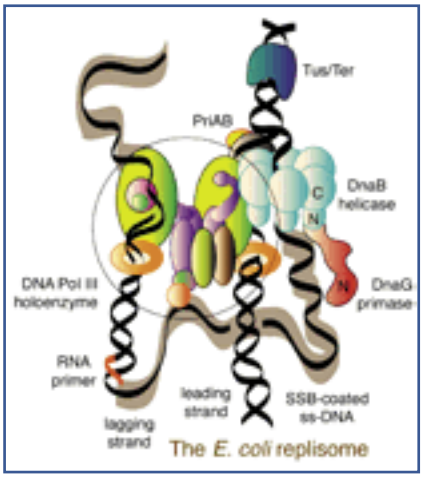
Protein Structure and Function

Dr Nicholas Dixon

Some proteins are enzymes that promote chemical reactions; others provide molecular switches that control metabolic and developmental processes through precise interactions with other proteins, nucleic acids and other ligands. In two distinct research programs, we explore the chemistry that governs the specificity and strength of interactions of proteins with substrates, inhibitors, nucleic acids, and other proteins.

The first program concerns the thirty or so different proteins that collaborate to replicate the DNA of the bacterial chromosome prior to cell division. DNA replication represents a good model system to study general aspects of protein–protein and protein–nucleic acid interactions because the proteins act together in a giant nucleoprotein assembly called the replisome, to make perfect copies of the chromosome. We use molecular genetics to engineer rich sources of the proteins and to produce mutant derivatives and segments of them, and conventional enzymology, DNA synthesis assays and protein chemistry to study protein function. Protein X-ray crystallography, ESR and high-field NMR spectroscopy, mass spectrometry, electron microscopy and computational methods are used with collaborating laboratories to further understand the structures of the individual proteins, and to relate their structures to how they work and interact with each other and with DNA. This year, we have focused our efforts on how the interaction of the replicative helicase (DnaB) with the replication terminator protein arrests progress of the replisome. We have also looked at how DnaB interacts with its loading partners, the DnaG primase, and subunits of DNA polymerase III (Pol III) holoenzyme.

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



The *E. coli* replisome

Molecular Motors in the Bacterial Replisome

The replisome contains two molecular motors that interact with each other. One is Pol III holoenzyme, the machine that actually synthesises new DNA chains during DNA replication, and the other is the ring-shaped hexameric DnaB helicase that drives the replisome and separates the two strands of DNA at the apex of the replication fork. The Pol III holoenzyme contains a catalytic core (α, ε and θ subunits), a sliding clamp (β_2), and the six subunits of the clamp loader (δ, δ', γ, τ, χ and ψ). We now have methods for the

isolation of large quantities of all ten subunits, and have isolated many sub-complexes of them for studies of their structures. Work on the structure and function of the ε proofreading exonuclease subunit is being used to model the chemical mechanism of related binuclear metallohydrolases. The structure of ε has been determined at 1.15 Å resolution, and several structures with metals other than the natural Mn(II) ions and inhibitors have been solved. Structural studies are proceeding with regions of the τ subunit that interact with the α subunit and DnaB, and methods are being devised to study these interactions in detail. In work on DnaB this year, we have focused on understanding how the helicase interacts with other proteins, including its loading partner DnaI (from *Bacillus subtilis*), the primase DnaG, and the replication terminator protein, Tus. The structures of the DnaB interaction domains of primase and DnaI have been determined using combinations of X-ray crystallographic and NMR methods. *(With B Bancia, P D Carr, S Jergic, M A Keniry, P E Lilley, K V Loscha, A J Oakley, D L Ollis, G Otting, K Ozawa, A Y Park, G Pintacuda, P Prosselkov, P M Schaeffer, X-C Su, N K Williams, and J M Carazo, Y Robledo [Centro Nacional de Biotecnología, Madrid], J M Guss [U Sydney], E Liepinsh [Karolinska Institute, Stockholm], B Hankamer, G Schenk [U Qld])*

A Molecular Mousetrap in Replication Termination

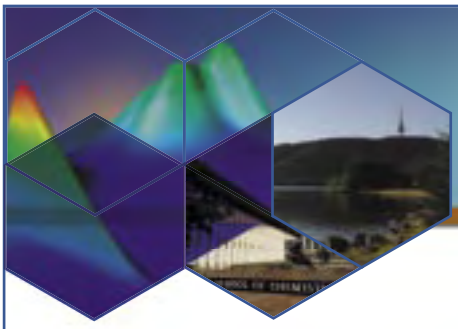
The mechanism of termination of DNA replication in *Escherichia coli* has been debated for nearly twenty years. The terminator protein Tus binds *Ter*-site DNA as a monomer, yet replication fork arrest is a polar (unidirectional) process. A replisome approaching from the 'permissive' face of the Tus-*Ter* complex can continue its progress, apparently by displacing Tus, whereas one approaching from the 'non-permissive' face is arrested. How can this be? This year we have shown that this process works like a molecular mousetrap that is set by DNA strand separation by the DnaB helicase, and sprung to create an intermediate species that is kinetically trapped by its unusually stable binding to Tus. *(With M Mulcair, A J Oakley, P M Schaeffer, and T M Hill [U North Dakota])*

New Protein Technologies

Substantial progress is being made in development of new methods for *in vitro*-directed molecular evolution of proteins with new binding specificities, for intein-mediated end-to-end cyclisation of protein domains and peptides, for preparative *in vitro* protein synthesis, for site-specific incorporation of unnatural amino acids and paramagnetic lanthanide ions into proteins, for the use of library methods for protein domain identification, and for use of mass spectrometry in studies of protein-ligand complexes. *(With M Headlam, P E Lilley, M Mulcair, G Otting, K Ozawa, A Y Park, P Prosselkov, P M Schaeffer, N K Williams, and G Coia [EvoGenix, Melbourne], R Dean [U Canberra], M Ehrenberg [U Uppsala], J L Beck, M M Sheil [U Wollongong], J M Matthews [U Sydney], D Spencer, H-X Zhou [Florida State U], K Alexandrov, A Rak [Max-Planck Institute for Molecular Physiology, Dortmund, Germany])*

Penny Lilley retired in 2004 after more than 17 years as a research assistant in the Dixon group. She was honoured for her service to the group and the School at a dinner in December, at which we presented her with a glass rose fabricated by Chris Tompkins, RSC glass blower.

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



Nuclear Magnetic Resonance — Dr Max Keniry

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

NMR Studies of the Interaction of Spermine with Oligonucleotides

Spermine, an aliphatic polycationic molecule found in all cells, plays an essential role in cell growth and differentiation. At present, there is no thorough understanding of how polyamines exert their physiological effects. Spermine is known to interact both with DNA and with proteins, yet the details of these interactions and the molecular basis of the biological function of spermine are poorly understood. There is evidence in the literature that spermine interacts with different forms of DNA in distinct and divergent modes. We have confirmed this and have characterised the complexes of spermine with duplex B-DNA and G-DNA using a specifically ^{13}C-labelled spermine and advanced NMR techniques to take advantage of the specific isotope label on spermine. The field dependence of ^{13}C T_1 and T_2 relaxation times and homonuclear and heteronuclear NOEs are used to characterise the dynamics of spermine in the presence of different forms of DNA. Spermine is bound more tightly to folded forms of G-DNA than B-DNA or linear G-DNA. Work is in progress to determine detailed dynamical models of the interaction of spermine with DNA and to expand this work to the effect of spermine on protein-DNA complexes. *(With K Clayton, J Coughlan)*

Novel Antibiotics and DNA

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

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

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

Interaction of the 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 triangular shape. 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. The basic structure of θ has not changed but two of the helices that were poorly defined in the uncomplexed θ-subunit are properly formed in the complex. We have recently mapped the binding surface of ε on θ to a hydrophobic patch on θ using advanced NMR techniques. Work is now in progress to align θ with ε using the same paramagnetic restraints that were used to refine the structure of θ. *(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])*

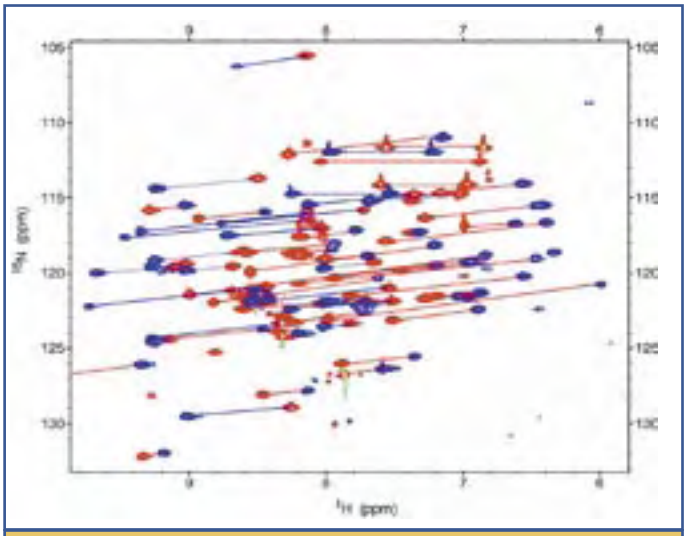
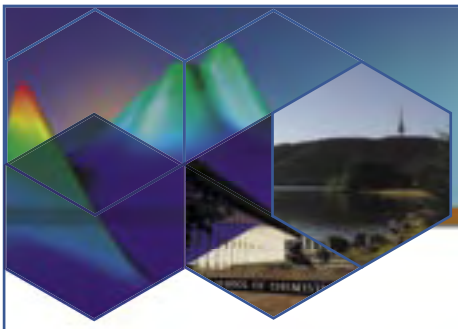


Figure: ^{15}N-HSQC NMR spectrum of ^{15}N-labelled-θ in complex with unlabelled ε showing unshifted peaks (red) and paramagnetic shifted peaks (blue) due to a lanthanide ion located at the ε active site. Red lines indicate an upfield shift and blue lines a downfield shift.

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

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

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



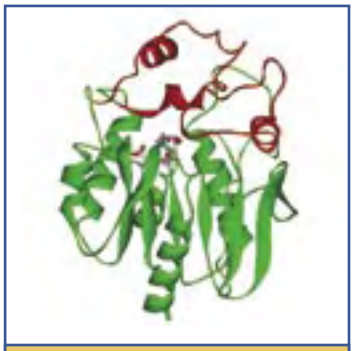
Structural Biology

Dr Aaron Oakley – ARC Fellow

Structural biology lies at the nexus between chemistry, biology, and medicine. The three-dimensional structures of biological molecules such as proteins and DNA yield a great deal of information about how they work, and can give rise to new hypotheses about their function. Understanding the structure and function of proteins is of primary importance to medicine, biochemistry and molecular genetics, since proteins drive and regulate these processes. Protein crystallography is our method of choice for structure determination efforts. We gather additional information about proteins from computational approaches such as molecular dynamics. We are investigating the structure and function of several proteins:

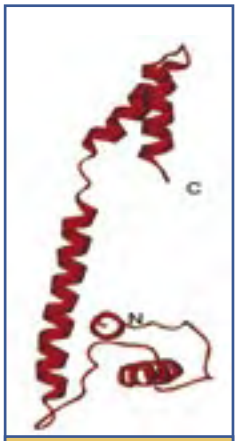
LinB

Bacteria produce enzymes that bind and degrade organic pollutants. These enzymes have potential for use in the remediation of contaminated industrial sites. We have determined the structure of a haloalkane dehalogenase called LinB at atomic resolution. This enzyme was originally isolated from a soil bacterium that was able to degrade the pesticide Lindane. It has activity against a broad range of pollutants called haloalkanes. The structure tells us how the protein might be modified in order to change its range of substrates. Our studies are complemented by *ab initio* quantum mechanical calculations that provide insight into the reaction mechanism and its energetics. *(With J Dambrosky, [Masaryk U, Brno, Czech Republic])*



Haloalkane dehalogenase LinB

DnaB and DnaG



E. coli DnaG

The molecular machine that drives the replisome and separates the two strands of DNA at the apex of the replication fork is a ring-shaped protein called DnaB. With Dr Dixon's group, we are working to determine the three-dimensional structure of this protein. Success has been achieved in determining the structure of part of another protein called DnaG. This protein binds to DnaB and synthesises the RNA primers required for DNA synthesis on the lagging strand. We recently determined the three-dimensional structure of the DnaB binding domain of DnaG. Remarkably, this protein has the same fold as the *N*-terminal domain of DnaB, suggesting an ancient evolutionary relationship between the two proteins. Models of this protein are being subjected to molecular dynamics studies to understand the role of flexibility in DnaB-binding. *(With N E Dixon, P Prosselkov, P M Schaeffer, B Bancia, K V Loscha, G Otting)*

Mannanase

endo-β-Mannanase from tomato

With researchers at University of Guelph, Canada, we recently determined the structure of a carbohydrate-degrading enzyme from tomato fruit called *endo*-β-Mannanase. The enzyme cleaves chains of mannan sugars, which are found in plant cell walls. This enzyme appears to be involved in fruit softening during ripening. We are now using modelling and molecular dynamics to understand how the substrate mannan, binds to the enzyme prior to cleavage. This will enable us to understand how Mannanase and similar enzymes recognise their substrates. The long-term goal is to be able to tailor-make carbohydrate cleaving enzymes for industrial processes and research. *(With J D Bewley, R Bourgault, [U Guelph, Canada])*

Glutathione S-transferases from Mosquitos

A glutathione S-transferase from *Anopheles dirus*

In collaboration with workers at Mahidol University, Thailand, we are investigating the structure and function of glutathione S-transferases (GST) from the mosquito *Anopheles dirus* species B, an important malaria vector in South-East Asia. These enzymes are important, because they can break down pesticides used to control mosquitos. We have so far determined the structure of two isozymes from an unusual gene that gives variants through alternate splicing. In the long term, we aim to understand how the enzymes bind and detoxify pesticides and how this might be ameliorated. *(With A Ketterman [Mahidol U, Thailand])*

Co-factor-free Oxygenases

Renilla reniformis

Reactions involving oxygen are normally "spin forbidden" and many of the enzymes that use it as a reactant employ special cofactors such as copper or iron that help oxygen to become reactive. A group of enzymes known collectively as co-factor-free oxygenases are capable of catalysing reactions involving oxygen without the aid of such co-factors. We aim to unlock the secret of how nature "tricks" oxygen into performing normally-forbidden reactions. In particular, we are examining the luciferase from the sea pansy *Renilla reniformis* and a hydroxy-4-oxoquinoline 2,4-dioxygenase from a soil bacterium. Both enzymes are members of the same structural family but appear to have evolved independently. *(With R Qi, and S Fetzner [U Oldenburg, Germany])*

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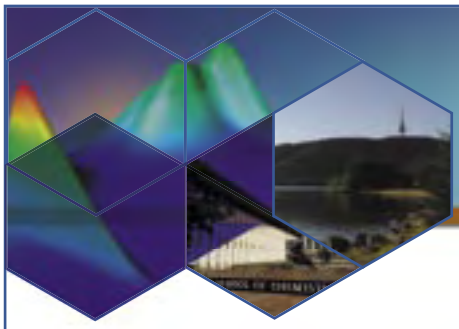

Protein Crystallography and Engineering Professor David Ollis

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

In the past year, we have published a paper that describes the importance of enzyme inhibitors in the evolution of new enzymes. We have also developed methods to allow *Escherichia coli* to grow by using common pesticides, like Paraoxon, as the sole source of phosphorous. This latter discovery greatly facilitates the directed evolution of pesticide degrading enzymes. We have also solved the structure of the *N*-terminal domain of *E. coli* glutamine synthetase adenylyl transferase.

Structure of a Regulatory Protein Involved in Nitrogen Uptake by Bacteria

Over the last year the structure of the *N*-terminal domain of *E. coli* glutamine synthetase adenyl transferase (AT-N) was determined. This was a collaborative effort with a group in the James Cook University, Townsville. *(With P D Carr, Y Xu, and S Vasudevan [James Cook U])*

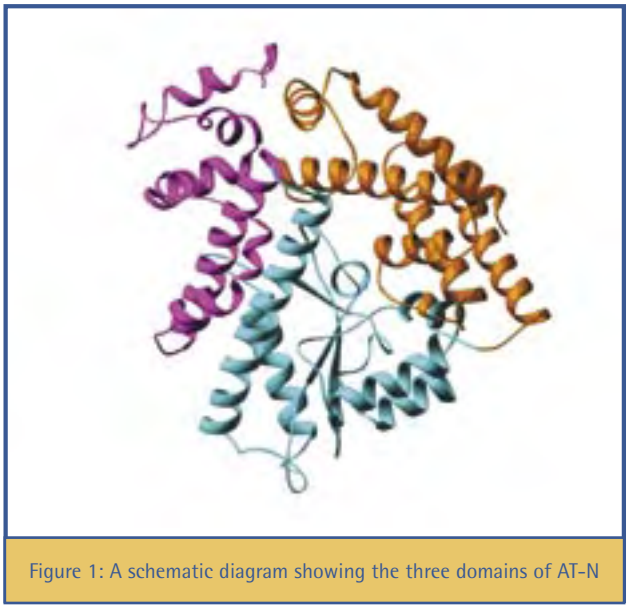

Figure 1: A schematic diagram showing the three domains of AT-N

Enzyme Engineering with an Organophosphate Degrading Enzyme

We have cloned and expressed an enzyme from *Enterobacter aerogenes* (GpdQ) that is capable of rapidly degrading phosphate diesters such as dimethyl phosphate. When this enzyme is co-expressed in *E. coli* with the organophosphate degrading enzyme from *Agrobacterium radiobacter* (OPDA), *E. coli* can use organophosphate pesticides as the sole form of phosphate for its growth. This has facilitated the directed evolution of OPDA and enabled us to improve the catalytic activity of OPDA towards a number of substrates. *(With P D Carr, J-W Liu, S Yu-McLoughlin)*

The β-subunit of the IL-5 Receptor – Identifying the Interaction Site

IL-5 is a regulator of growth, differentiation and activation of the white blood cell eosinophils. These cells are of major importance in the body's response to invasion by parasites and asthma inducing aeroallergens. Structure based site-directed mutagenesis of the β-common receptor successfully identified amino acid residues that are crucial for binding the cytokines IL-3, IL-5 and GM-CSF. *(With P D Carr, J Murphy, and I G Young [JCSMR, ANU])*

The Structure of an Intein

We have obtained the structure of the protein splicing intein from the DnaB gene of *Synechocystis sp.* PCC6803. *(With P D Carr, N E Dixon, and K Alexandrov, A Rak [Max-Planck Institute for Molecular Physiology, Dortmund, Germany])*

Figure 2: Schematic diagram of the DnaB intein.

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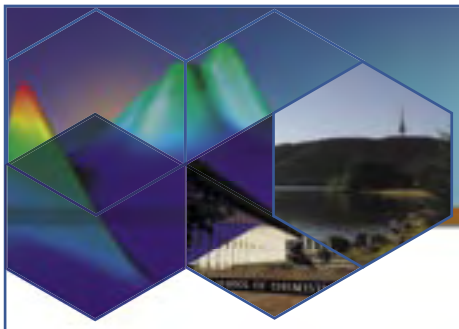


Biomolecular NMR

Professor Gottfried Otting

The group develops novel tools for biomolecular applications of NMR spectroscopy. Emphasis is placed on extending the range of protein targets that can be investigated by NMR in pharmaceutical drug development. Thus, methods are developed for rapid identification and characterisation of ligand binding sites, including protein-protein and protein-DNA interactions. In addition, NMR is used to determine the three-dimensional (3D) structures of proteins and protein domains. This research is supported by a new 800 MHz NMR spectrometer installed in April 2004.

We discovered that binding of a paramagnetic lanthanide ion at a specific protein site provides a novel route to assign the NMR signals of the protein to its specific amino acids with unprecedented ease and speed.

To follow up on this discovery, we are working on widely applicable methods to attach lanthanide ions to proteins that don't have a natural ion binding site. One such strategy involves the synthesis of chemical compounds which on one side specifically attach to cysteines in proteins and on the other side carry a paramagnetic lanthanide ion. The work includes the production of proteins containing

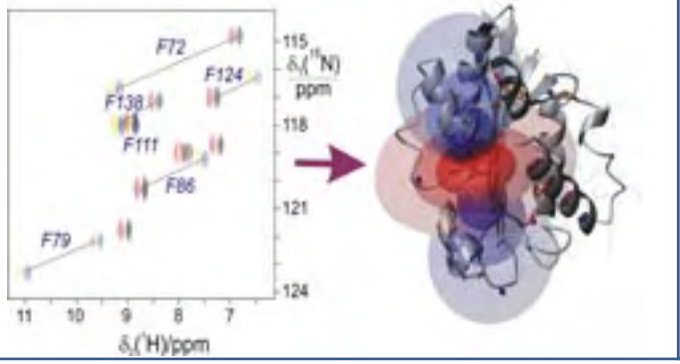
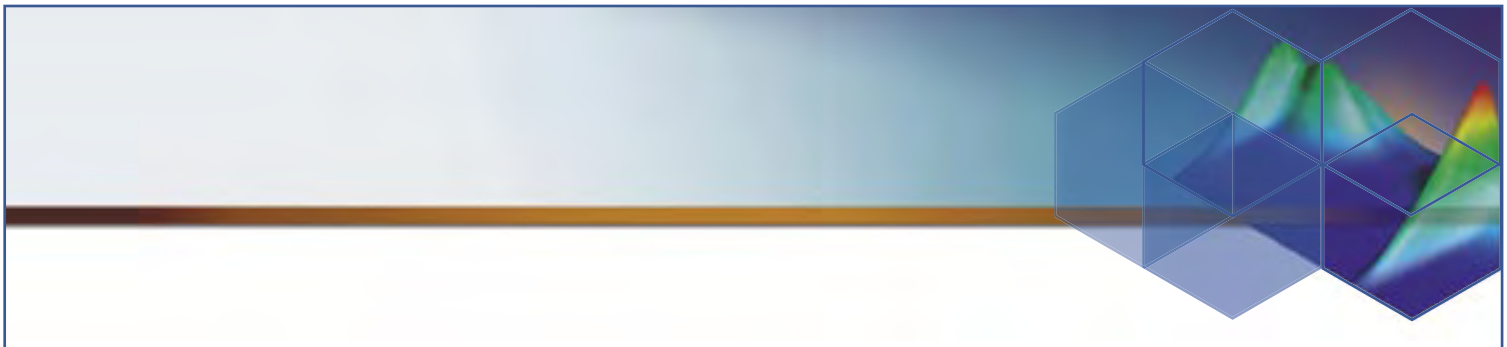


Figure: From NMR spectra to resonance assignment, structure determination and interaction studies of proteins. A wealth of structural information is gained by tagging with a paramagnetic ion. Isosurfaces of the anisotropic magnetic susceptibility (blue and red) are superimposed on the structure of the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

single cysteines at specific sites and the application of high-yield *in vitro* protein expression techniques which are being developed in collaboration with Dr Nicholas Dixon to allow inexpensive residue-selective ^{15}N-labelling of proteins.

Labelling proteins with lanthanide tags opens up a wide range of applications which were hitherto difficult or impossible to address by NMR or other methods. For example, they will provide a tool for 3D structure determination of small regions in large proteins, *i.e.* to "zoom" in on a region of a protein and study its structure without having to analyse the rest of the protein. It has long been known that lanthanides provide structural information to NMR spectroscopists. The lanthanide tagging approach promises to broaden these applications considerably. For example, it will provide information about the orientation of small chemicals (drug candidates) as they bind to protein targets. Finally, lanthanide labelling will allow the characterisation of large amplitude motions of proteins with unprecedented accuracy.

The highlight of the year was the installation of the 800 MHz NMR facility in the RSC. The system presents the highest magnetic field available for NMR in Australia and will be equipped with a cryoprobe for maximum sensitivity early in 2005. Purchased with support from the Australian Research Council, ANU, U Sydney, UNSW, U Wollongong, U Newcastle and UNSW College at ADFA, the spectrometer is set up for remote operation so that it can be operated by interstate users from their desktop computers *via* the internet.



Continuing major collaborators are Dr Nicholas Dixon and Dr Max Keniry, Dr Thomas Huber (Queensland U), Drs Edvards Liepinsh, Anatoly Sharipo (Latvian U) and Dr Laszlo Patthy (Hungarian Academy of Sciences).

Fast Algorithm for the Assignment of NMR Spectra

The assignment of NMR resonances to specific protons of a protein is a time-consuming task which can be very much shortened by the use of a novel strategy, if the 3D structure of the protein is known and a lanthanide ion can be bound to the protein at a specific site. The strategy has been verified for a 30 kDa ^{15}N-labelled complex formed between the *E. coli* proteins epsilon and theta. *(With N E Dixon, M A Keniry, A Y Park, and T Huber [U Qld], G Pintacuda [Karolinska Institute, Stockholm])*

In vitro *Expression of Residue-selectively Isotope Labelled Samples*

The cell-free expression system available in Dr Nicholas Dixon's laboratory was used to express samples of selectively ^{15}N-labelled human cyclophilin. The yields were sufficiently high that NMR spectra (^{15}N-HSQC spectra) could be recorded straight from the reaction medium without any protein purification or concentration step. The spectra were analysed for metabolic side reactions of the labelled amino acids that might be catalysed by enzymes present in the reaction medium. The data provide a catalogue of spurious signals which can be encountered in NMR spectra of *in vitro* synthesised and unpurified protein samples. *(With N E Dixon, K Ozawa, M J Headlam)*

Structure Dependent ^{1}H NMR Relaxation Due to Curie-spin/CSA Cross-correlation

^{1}H magnetisation relaxes more quickly if a paramagnetic ion is present in the same molecule. We discovered that this long-held belief can be quite wrong under certain circumstances. In fact, the ^{1}H spins may even relax more slowly in the presence of display enhanced relaxation! This effect is due to cross-correlated relaxation between the chemical shift anisotropy (CSA) of amide protons and the Curie-spin relaxation caused by the presence of paramagnetic ions with rapidly relaxing electron spins. A theoretical study showed that the effect can be experimentally relevant. *(With G Pintacuda, and A Kaikkonen [Karolinska Institute, Stockholm])*

Protein Solvation by NMR and MRD

The residence time of hydration water molecules on the surface of proteins and peptides was investigated by a high-resolution NMR spectroscopy and magnetic resonance dispersion (MRD). A new relaxation model assuming different diffusion coefficients of hydration and bulk water provides a consistent theory which explains the data obtained with both techniques. The result shows that solvent-exposed hydration water molecules have residence times in the picosecond time range even at temperatures near the freezing point of water. *(With B Halle, K Modig [Lund U Sweden], E Liepinsh [Karolinska Institute, Stockholm])*

Protein Structure Determinations

The 3D structure of human CLP was published. The protein binds to 5-lipoxygenase which is an important drug target for the suppression of inflammation. *(With E Liepinsh, O Rådmark [Karolinska Institute, Stockholm])*

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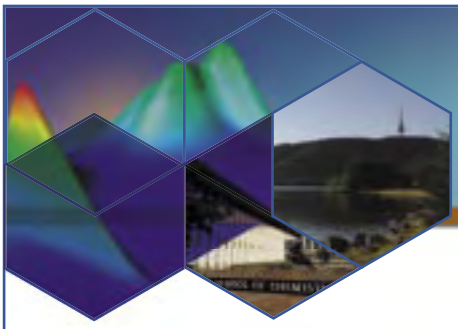
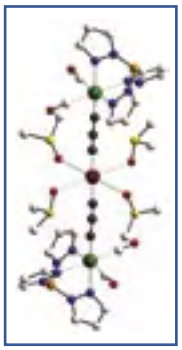


INORGANIC CHEMISTRY

Synthetic Organometallic and Coordination Chemistry
Professor Anthony Hill

Our work covers a wide range of topics 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 and 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 directly take part in ligand transformations but may moderate these indirectly . This work is currently centred on two classes of ligands; polythiamacrocycles and poly(methimazolyl)chelates.

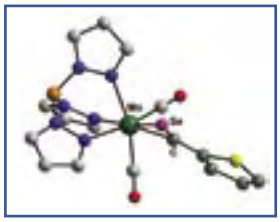
Dimetallapolycarbyls: Tri-, Tetra-, Hexa- and Octa-carbido Molecular Wires: $L_nMC_xML_n$ (x = 3, 4, 6, 8)



The vast majority of compounds in which two metal centres are linked by a linear chain of carbon ('molecular wires') are based on an even number of carbon atoms. This is simply because the majority of routes to such compounds involve alkyne, diyne and poly-yne modifications, *i.e.*, the carbon is introduced in packets of two, -C≡C-. Furthermore, such chains are typically bound to metal centres *via* a simple metal-carbon single bond. This has resulted in a number of gaps in what is otherwise an intensely studied field. We have, therefore, targeted the development of synthetic routes that will afford access to (i) bimetallics with *odd* numbered carbon chains and (ii) carbon chains that are bound to the metal centres *via M–C multiple bonding*. Highlights this year have included the syntheses of the first bis(tricarbido) trimetallics centred on ruthenium, iridium and mercury (see right); the first example of the catalytic demercuration of bis(metallapolycarbyl)mercurials; and the first bimetallic hexacarbido complex with a hexa-2,4-diynyl-1,6-diylidyne bonding pattern (see left). These results provide the basis for the award of ARC Grant DP0556236 to commence in 2005. *(With R Dewhurst, A C Willis)*

Metal butadiynyls L_nMC_4H are also key building blocks for the construction of bimetallics spanned by the tetracarbido linkage $L_nMC_4ML_n$. Whilst numerous examples now exist, surprisingly little subsequent functionalisation of the C_4 unit has been reported. In addressing this, we have succeeded in obtaining the first transition metal examples of bimetallics spanned by CCCHC, CCCCCHC and CCCHCH linkages, the latter *via* the hydrometallation of a terminal σ-butadiynyl complex. *(With M J Bartlett, M K Smith)*

Organometallic Chemistry of Unsaturated Organoselenium Compounds

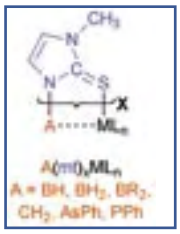


Last year we reported the remarkable fragility of C–Se bonds in isoselenocyanates and alkynyl selenoethers when presented with various organotransition metal complexes. Rather than viewing this as a problem, we have taken a different approach and exploited this reactivity. Effective single-atom selenium transfer reagents are rare, however, we have been able to show that isoselenocyanates are able to serve this purpose. This has been demonstrated in the reactions of RNCSe (R = $C_6H_2Me_3$-2,4,6) with a range of alkylidynes which provide the first examples of group 6 selenoaroyl complexes, including both

mononuclear (see above left) and binuclear examples. The side product in these reactions is the free isonitrile RNC and it could be shown that isonitriles can thereby serve to catalytically activate elemental selenium. *(With L M Caldwell, A C Willis)*

Methimazolyl Chelate Complexes

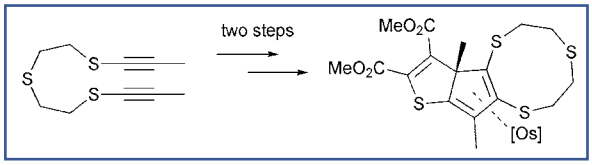
Previous annual reports have described a range of 'scorpionate' ligands in which a bridgehead group ('A') bound to two or three ('x') methimazolyl heterocycles ('mt') acts as a chelate to a metal centre ('ML_n') [ARC Grant DP034270]. The majority of recent work has involved boron derivatives with which the metal associates *via* a transannular dative M→B bond within a cage structure (metallaboratranes). These were previously limited to our own studies of examples involving zerovalent metals from group 8, wherein the M→B bond was bridged by three *mt* buttresses. Thus, questions arose as to (i) their generality and (ii) the need for three *mt* bridges. Both questions have been partially addressed. Firstly, the metallaboratrane class of compounds has now been successfully extended to included metals from group 9 (Ir, Rh) and 10 (Pt), 0, +1 and +2 metal oxidations states, d^8 and d^{10} electronic configurations and geometries involving 5 or 6 coordinate metals. Thus the metallaboratrane motif appears to be generally accessible for late transition metals with high d-occupancies. Furthermore, the isolation of a di-buttressed iridaboratrane, devoid of the geometric constraints of the previous tri-buttressed examples, substantiates the claim that there is a genuine electronic basis for invoking M→B bonding and that it is not simply a ramification of a constrained cage geometry.



The second thrust of this research involves the study of methimazolylborate coordination to early transition metals with low d-configurations and high oxidation states. This might appear to represent a mismatch of metal and donors within the hard and soft acid and base conceptual framework. We have, however, shown that a range of derivatives based on metals from groups 4 (Ti, Zr), 5 (Nb, Ta) and 6 (Mo, W) are indeed accessible, although as might be expected, they are highly reactive. A variety of organometallic $H_2B(mt)_2$ and $HB(mt)_3$ complexes have thus been obtained bearing carbonyl, stannyl, alkyne, cyclopentadienyl, allyl, imido or phosphine ligands. *(With R J Abernethy, I R Crossley, E R Humphrey, A D Rae, M K Smith, N Tshabang, A C Willis)*

Polythioether Macrocycles

The cyclisation of α, ω-dialkynyl polythioethers provides a potential route to macrocyclic thioethers. We have now applied this approach to systems that also incorporate CO or CS within the alkyne coupled ring to provide cyclopentadien-one and cyclopentadien-thione complexes. In the latter case, the sulfur group is particularly nucleophilic and we have observed a novel [3+2] cycloaddition reaction with an activated alkyne to regioselectively provide an unusual tricyclic tetrathia-macocycle. *(With A D Rae, M Schultz, A C Willis)*



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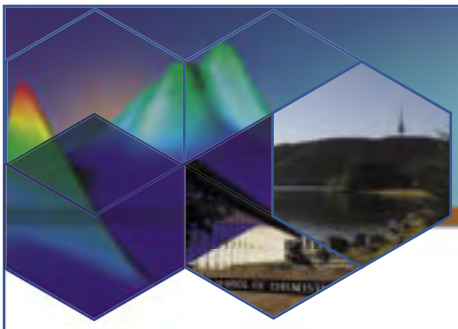
Members of the research group



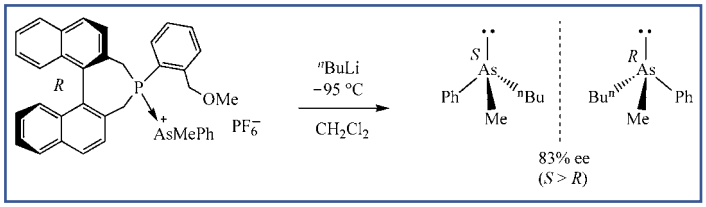
Inorganic Stereochemistry and Asymmetric Synthesis
Professor Bruce Wild

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

Elizabeth Krenske received a grant from the Australian–German Joint Research Cooperation Scheme to work as an exchange student in the University of Leipzig for one month (September). Elizabeth also visited the National University of Singapore, where she presented a lecture on her work.

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

Our work on phosphine-stabilised arsenium salts has continued, with a fuller investigation of reactivity at the arsenium centre. We have carried out a detailed study of nucleophilic substitution reactions with organometallic nucleophiles, including organolithium, Grignard, and organozinc reagents. The synthetic route to the phosphine auxiliary has been improved, and it has enabled the preparation a range of optically active tertiary arsines in stereoselectivities ranging from 25% to 83%. For example, the reaction of the methylphenylarsenium adduct of the phosphine with ^{n}BuLi at –95 °C in dichloromethane leads to (*S*)-(*n*-butyl)methylphenylarsine in 83% enantiomeric excess. This work has been complemented by theoretical calculations for the stereochemical analysis of model adducts. *(With M L Coote, E H Krenske, K A Porter, A C Willis)*

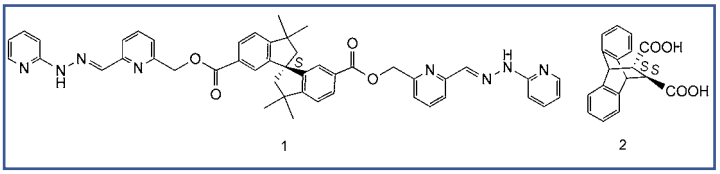


Macrocyclic Diphosphine-stabilised Diarsenium Salts

The bis(tertiary phosphine) $Ph_2PCH_2CH_2CH_2PPh_2$ (dppp) reacts with bis(iodophenylarsino)-1,2-ethane in dichloromethane in the presence of aq. NH_4PF_6 to give an 18-membered phosphine-stabilised tetra-arsenium salt, which has been characterised by X-ray crystallography. Treatment of the salt, which contains four chiral arsenium groups, with MeLi in –78 °C furnished (*R*,R**)-(±)/(*R*,S**)-$MePhAsCH_2CH_2AsMePh$ with liberation of the dppp. The diastereoselectivity of the reaction is negligible, but if the dppp is replaced by the enantiomerically pure diphosphine (*S,S*)-skewphos, the corresponding diphosphine-diarsenium complex affords, upon treatment with MeLi at –78 °C, the diarsine with the following stereoselectivities: (*R*,R**)-(±)/(*R*,S**) = 60:40 and (*R,R*):(*S,S*) = 60:40. The identities of the products and stereoselectivities of the reactions have been determined by complexation of the diarsine with enantiomerically pure (*S,S*)-$[Pt(OTf)_2\{1,2\text{-}C_6H_4(PMePh)_2\}]$ and analysis of the ^{31}P NMR spectrum of the resulting mixture of complexes. *(With A C Willis, X Zhou)*

Stereoselective Synthesis of Two-bladed Propeller Octahedral Metal Complexes

We have embarked on a project aimed at demonstrating that chiral metal complexes can be prepared by inorganic asymmetric synthesis. The approach being adopted is to transfer chiral information to a metal centre by means of an enantiomerically pure chiral auxiliary attached to appropriate chelating agents, as in 1, with the auxiliary group subsequently being removed to leave the configurationally pure metal complex. Ligand 1 has been shown to diastereoselectively complex zinc(II) and iron(II) to produce dinuclear metal double α-helix helicates; the *S*-enantiomer of the ligand generating two metal centres of Δ-configuration. This is in contrast to the corresponding ligand containing the chiral auxiliary 2, which complexes iron(II) to produce a side-by-side helix helicate, the *S,S*-enantiomer of the ligand generating two metal centres of opposite configuration. *(With R J Warr, A C Willis, A D Rae)*



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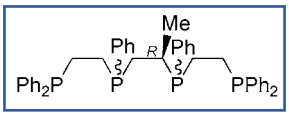
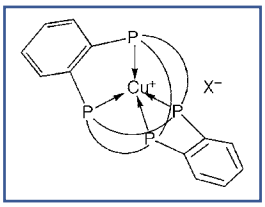
Stabilisation of Parallel and Double α-helix Conformers of Dinuclear Metal Helicates Containing Tetra(tertiary Phosphines)

The ligand (R_C)-Me-tetraphos has been synthesised from (*R*)-propane-1,2-ditriflate and appropriate phosphide reagents. The tetraphosphine has been isolated initially as a mixture of the borane adducts of the four possible diastereomers, chiral at carbon (*R*) and the two configurationally stable phosphorus stereocentres. One diastereomer of the mixture has been isolated by fractional crystallisation. A highly stereoselective synthesis of this diastereomer has also been achieved by stereospecific displacement of the triflate groups from (*R*)-propane-1,2-ditriflate with an enantiomerically enriched phosphide–borane reagent. Molecular modelling of the structures of the cations of the complexes $[M_2\{(R)\text{-Me-tetraphos}\}_2](PF_6)_2$ containing the various diastereomers of the tetraphosphine indicates that the ligand containing two inner-phosphorus stereocentres of *R*-configuration will stabilise the double α-helix conformer of a double-stranded dimetal helicate with univalent Group 11 ions. *(With H Kitto, A D Rae, A C Willis)*



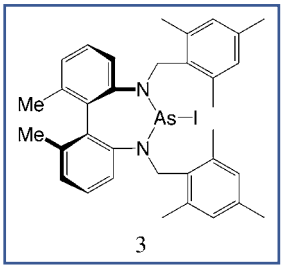
Tetrahedral Phosphine Cage Ligands and Complexes



Molecular modelling has indicated that it should be possible to synthesise a tetrahedral phosphine cage complex by the reaction of the appropriate 1,2-phenylenebis(alkenylphosphine)copper(I) complex with the analogous 1,2-phenylenebis(phosphine) complex under basic conditions. Current work is concerned with the synthesis and purification of the key starting materials 1,2-phenylenebis(dichlorophosphine) and 1,2-phenylenebis(phosphine) and their copper(I) complexes. *(With K Wells)*

Deracemisation of Chiral Arsines and Phosphines

Synthetic techniques for the production of chiral phosphines and arsines are presently limited by the necessity of resolution. Previous work within the group has identified the inversion of chiral phosphines in the presence of iodoarsines resulting in racemisation at equilibrium. Current research is focused on the synthesis of chiral iodoarsines to facilitate the deracemisation of phosphines of type 3. These will hopefully provide enantioenriched phosphines without the need for traditional resolution. *(With N L Kilah)*



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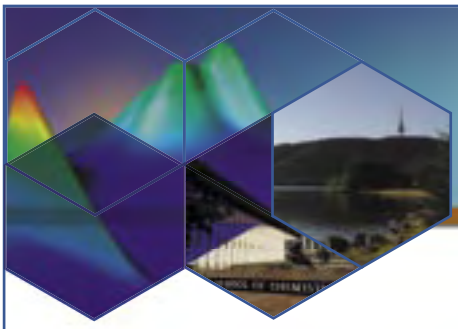
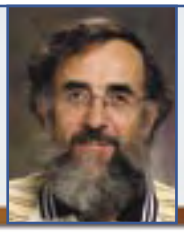




Solid State Inorganic Chemistry — Professor Ray Withers

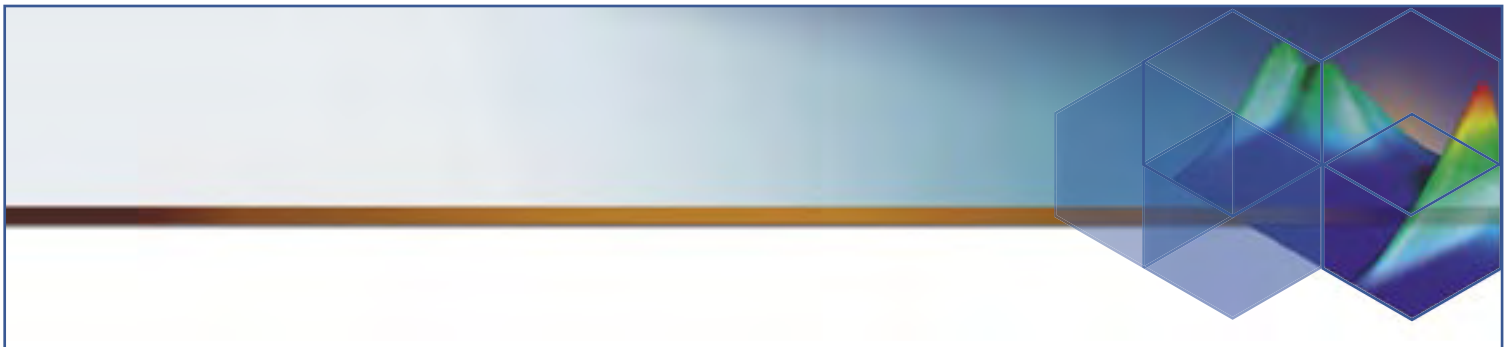
We aim to understand and exploit the factors (strain, composition, band structure etc.) that determine structure and function in the crystalline solid state. Our interest is in the balance between local crystal chemistry, strain and longer range order in a wide range of compositionally and/or displacively flexible crystalline solids. The principal experimental research tools used are solid state synthesis, transmission and scanning electron microscopy in combination with powder and single crystal diffraction. On the theoretical side, group theory, lattice dynamical calculations and bond valence sum analysis are the principal techniques employed. Crystalline systems investigated include wide range non-stoichiometric solid solutions, displacively flexible framework structures, ferroic phases and phase transitions, solid electrolytes, dielectric materials and incommensurately modulated structures. Achievements over recent years include the first coherent view of the crystal chemistry underlying the phenomenon of ferroelectricity within the Aurivillius family of displacive ferroelectrics, the use of compositely modulated structure formalism to understand "infinitely adaptive", non-stoichiometric solid solutions, and the discovery and subsequent modelling of displacive flexibility and its consequences in the silica polymorphs and various zeotypic microporous molecular sieve materials.

A Combined Diffraction and Hard-mode Infrared Spectroscopy Study of Composition-induced Structural Phase Transitions in the $(Ba_{1-x}La_x)_2In_2O_{5+x}$ ($0 \leq x \leq 0.6$) System

As part of an ongoing ARC-funded project into the effects of substitutional strain on local crystal chemistry, a combined diffraction and hard-mode infrared (IR) powder absorption spectroscopy study of composition-induced structural phase transitions in the $(Ba_{1-x}Lax)_2In_2O_{5+x}$ ($0 \leq x \leq 0.6$) system has been carried out. This system is of interest as a high-temperature fast oxide ion conductor for use in a wide range of electrochemical devices including oxygen sensors, solid oxide fuel cells and oxygen separation membranes. A recently introduced autocorrelation analysis method has been used to quantify composition-induced structural phase changes *via* a careful analysis of peak positions and line broadening in IR spectra as a function of composition. An orthorhombic brownmillerite to three-dimensionally disordered cubic perovskite phase transition in this system is signalled by a drastic change in slope of both wave–number and average linewidth as a function of composition. Some evidence is found for the existence of an intermediate tetragonal phase (previously reported to exist from electron diffraction data) around x ~0.2. The new spectroscopic data have been used to compare microscopic and macroscopic strain parameters arising from variation in composition. *(With Y Liu, L Norén, T R Welberry, and S Moussa, A Pring, C Tenailleau [South Australian Museum], M Carpenter, S Tarantino, M Zhang [U Cambridge, UK])*

A Structure, Conductivity and Dielectric Properties Investigation of $A_3CoNb_2O_9$ ($A = Ca^{2+}, Sr^{2+}, Ba^{2+}$) Triple Perovskites

There has recently been considerable interest in the structures and associated physical properties of $A_3Co^{2+}Nb^{5+}{}_2O_9$ (A = Ca, Sr and Ba) complex 1:2 perovskites, mainly as a result of their potential photocatalytic and microwave dielectric applications. A careful investigation has therefore been carried out into their room temperature structures as well as their temperature-dependent conductivity and dielectric properties. A constrained modulation wave approach to Rietveld structure refinement is used to determine their room temperature crystal structures. Correlations between these crystal structures and their physical properties are found. All three compounds undergo insulator to semiconductor phase transitions as a function of increasing temperature. The hexagonal $Ba_3CoNb_2O_9$ compound acts as an insulator at room temperature, while the monoclinic $Ca_3CoNb_2O_9$ compound is already a semiconductor at room temperature. *(With D J Goossens, Y Liu, L Norén, V Ting, and C Ferraris, S Madhavi, T J White, [School of Materials Engineering, Nanyang Technological U, Singapore], M James [Bragg Institute, Australian Nuclear Science and Technology Organisation])*



The Pyrochlore to 'Defect Fluorite' Transition in the $Y_2(Zr_yTi_{1-y})_2O_7$ System and its Underlying Crystal Chemistry

As a result of its high oxide ion conductivity at moderate to high temperature as well as its low activation energy for such oxide ion conduction, 'defect fluorite' type yttrium-stabilized zirconia is currently widely used as the solid electrolyte of choice in solid oxide fuel cells (SOFCs) as well as in sensors measuring oxygen partial pressure in car exhaust systems. Such properties, however, are not the only desirable characteristics required for use in SOFCs. Another very important physical requirement is chemical stability and compatibility with adjoining electrode materials. There has been much recent interest in a monolithic fuel cell design in which cathode, electrolyte and anode are inherently compatible as a result of being made up of essentially the same $A_2(B'_yB_{1-y})_2O_7$ (A = Y^{3+}, Gd^{3+}; B = Ti^{4+}; B' = Zr^{4+}, Sn^{4+}) 'pyrochlore'-type (mixed oxide ion as well as electronically conducting) materials. Particular interest has focussed on the $Y_2(Zr_yTi_{1-y})_2O_7$ system as a result of the electronic conductivity introduced by the presence of the Ti ions as well as the ".... remarkable increase in (oxide ion) conductivity of three orders of magnitude as the Ti cation is replaced by the larger Zr cation ....". A careful diffraction and dielectric properties investigation of the previously reported single phase, pyrochlore structure type $Y_2(Zr_yTi_{1-y})_2O_7$, $0 \leq y \leq 0.9$, (YZT) solid solution has therefore been carried out. *(With Y Liu, L Norén)*

The Systematics of Problem Pseudo Symmetric Crystal Structures

Many structures cause problems for structure determination and refinement using X-ray diffraction techniques. Often an idealised 1:1 disordered parent structure can be found that corresponds to the Fourier transform of a strongly diffracting subset of reflections. The apparent Laue symmetry of this idealised structure must be lowered to account for the extra (satellite) reflections. To a first approximation this is achieved by ordering the disorder to create intensity for the satellite reflections without altering the intensities of the parent reflections. Often this ordering is not perfect. As a consequence, stacking faults and twinning result, necessitating the use of constraints and restraints to control the refinement and obtain a respectable looking answer. Often possible structures are associated with alternative orientations or origins for the stacking of ordered columns or layers. This allows the use of structure factor algebra to combine such layers or columns in a generalised twin-disorder model using appropriate parameters. This sometimes results in alternative space groups or alternative orientations for a structure. Sometimes observed intensities cannot be described using the twinning of a simple average structure and account must be taken of the consequences of having different regions of a crystal with different twin-disorder parameters. Final refinement requires lowering the symmetry of the layers or columns because of the packing. It is often useful to maintain the twin disorder parameters previously obtained as a sensible constraint on refinement, especially a stacking fault that simply changes the scale of certain reflections. *(A D Rae)*

The Identification of Twin Planes in Monoclinic and Triclinic Crystals

Currently the X-ray diffraction unit is identifying and refining several twinned crystals each year. Being unaware of the twinning usually does not preclude an initial structure solution. However, satisfactory refinement is only obtained by correctly identifying the twin rule so that the indices and relative positions of partially overlapping reflections is correctly determined. We have found that for packing of molecules the correct twin plane usually has the smallest repeating area. Often twinning is associated with the packing of approximately symmetric layers in such a way as to lower this layer symmetry. The layer symmetry then provides a mechanism for twinning and for the creation of possible polymorphs. *(A D Rae)*

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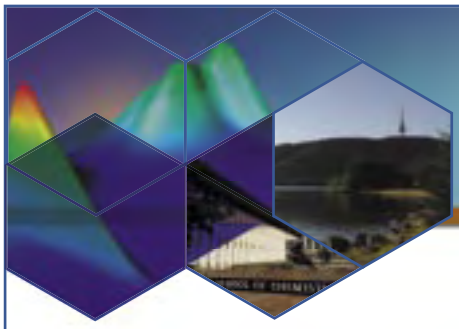

ORGANIC CHEMISTRY

Synthesis and Mechanism — Professor Martin Banwell

The group's activities remain focused on the development of new synthetic strategies and methodologies as well as the application of these in the total synthesis of biologically active natural products and certain analogues. The whole-cell biotransformation, in collaboration with Dr Gregg Whited of Genencor International (Palo Alto, CA), of various poly-substituted aromatics into metabolites suitable for construction of key parts of various structurally complex and clinically significant compounds is another important area of activity. The metabolites resulting from such processes are not only enantiomerically pure but also sufficiently rich in functionality that they can serve as important new starting materials in our synthesis program. Two key targets of particular interest at the present time are vinblastine (a binary indole-indoline alkaloid used in the treatment of early childhood leukaemia and bladder cancer, see figure 1) and galanthamine (a plant-derived alkaloid used in the treatment of Alzheimer's disease). Australian companies have funded a significant portion of our work. For example, Progen Industries, a Brisbane-based biotech company, is continuing to support two postdoctorals who have been working on a very enjoyable collaborative project focused on novel carbohydrate and related chemistries. An APA(I)-funded PhD scholar has recently started work on a collaborative project with Biota Holdings and another similarly funded scholar is working with Starpharma Pty Ltd on the development of new drug delivery systems. Collaborations with the Melbourne-based company Cytopia and our colleague Professor Chris Parish (JCSMR) continue and have resulted in the identification of novel analogues of certain alkaloids that display potent anti-angiogenic activity but show none of the toxic effects of the natural products themselves. The Alexander von Humboldt Foundation is providing Feodor Lynen Fellowships to two German postdoctorals working in the group, one of whom is focusing on developing, in collaboration with A/Professor Mary Garson of the University of Queensland, a total synthesis of the marine alkaloid haliclonacyclamine A. The bis-piperidinyl core of this target molecule has recently been obtained and efforts are now underway to construct, using ring-closing alkyne metathesis techniques, the two remaining ring systems associated with this ecologically important compound. In a joint venture involving Dr Paul Savage of CSIRO Molecular Science we have recently completed total syntheses of both enantiomeric forms of the stilbenolignan aiphanol and thereby determined the absolute stereochemistry of this natural product.

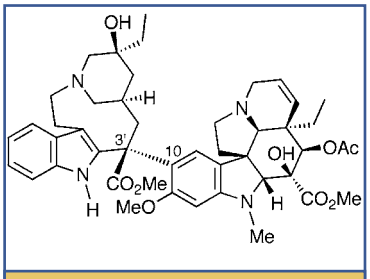

Figure 1: Vinblastine, a binary indole-indoline alkaloid used for the clinical treatment of certain types of cancer.

Other research highlights include:

(i) the completion of a total synthesis of aspidospermidine, an alkaloid embodying certain key structural components associated with the clinically significant natural product vinblastine;

(ii) the identification of techniques for constructing the pivotal C10-C3' linkage between the northern and southern hemispheres of vinblastine;

(iii) the enantiodivergent construction of the pivotal quaternary carbon centre associated with both the natural and non-natural enantiomeric forms of the alkaloid galanthamine;

(iv) the development of the first enantioselective total synthesis of the macrolide (–)-cladospolide B (Figure 2) and the subsequent revision of the absolute stereochemistry of the natural product;

(v) the exploitation of novel cyclopropane ring-cleavage reactions in the construction of certain unusual terpenoid and alkaloid frameworks.

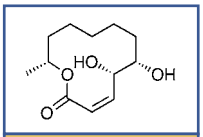

Figure 2: Cladospolide B, a fungal metabolite possessing novel plant growth regulating properties.

In the methodological area, extensions of our studies on palladium[0]-catalysed Ullmann cross-coupling chemistry have continued and a range of new heterocyclic systems are now available as a result. Several patents relating to this work have been filed.

Exploitation of cis*-1,2-Dihydrocatechols and Quinic Acid 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 Diels–Alder chemistry continues to be a major area of activity and the adducts derived from such processes have been converted, using photochemical processes, into the polycyclic skeleta associated with a diverse range of terpenoid natural products. Other natural products being targeted include the alkaloids galanthamine (a clinically useful agent for the treatment of Alzheimer's disease), brunsvigine and vindoline (a clinically important anti-cancer agent) as well as the macrolide tricholomenyn B (a potent anti-mitotic agent), the fungal metabolite diversonol and the plant-growth regulating substance cladospolide C. The preparation of various sugar mimetics has been another activity in this area and one that has been carried out with commercial partners. *(With K Austin, M Bonnet, L Fearnside, M Friend, G J Harfoot, J Jury, O P Karunaratne, D T J Loong, D W Lupton, X H Ma, J Renner, and R H Don, V Ferro [Progen Industries Ltd, Brisbane], J N Lambert [Biota Pty Ltd, Melbourne], G Krippner, T McCarthy [Starpharma Pty Ltd, Melbourne], G M 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 various contexts, with one especially notable activity being focused on the construction of the spirocyclic framework associated with the erythrina alkaloids. The exploitation of pyrroles as nucleophilic scaffolds for the construction of various heterocyclic compounds also continues to be a major activity within the group. Novel modes of reactivity involving this ring system have been developed recently and these have been or are currently being exploited in the construction of various biologically active systems including showdomycin analogues. Other work has focused on the development of chemoenzymatic routes to the spinosyin class of insecticides and the carbotricyclic core of these natural products has now been obtained but more efficient routes to this important substructure will need to be developed before total syntheses can be completed. *endo*-Selective Diels–Alder cycloaddition reactions are being developed with this objective in mind. Novel aldol chemistries have been exploited as a means for construction of the bis-piperidinyl core associated with the Australian marine natural product haliclonacyclamine A. Significantly, ecological and other evaluations of this core molecule, as carried out by our collaborators including A/Professor Mary Garson, reveal that the compound retains much of the potency of the structurally much more complex parent (natural) compound. *(With D A S Beck, S Chand, J Crossman, S Gross, M J Harvey, O J Kokas, S Lampe, D Pinkerton, J Renner, P Stanislawski, M O Sydnes, R Taylor, and C Burns [Cytopia, Melbourne], R H Don, V Ferro [Progen Industries Ltd, Brisbane], M J Garson [U Qld], C R Parish [JCSMR, ANU], G P Savage (CSIRO Molecular Science, Melbourne])*

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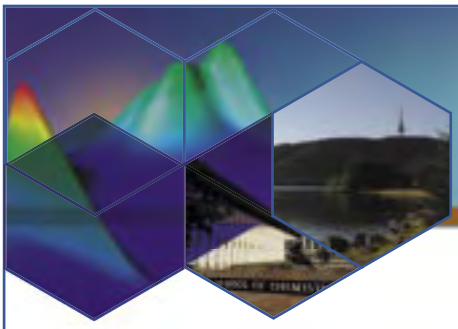


Biochemical Reactions and Molecular Recognition
Professor Chris Easton

One theme of our research involves the analysis of chemical reactions, particularly those occurring in biological systems. Our objectives in this area are: i) to develop methods to regulate biochemical processes associated with disease states, ii) to produce physiologically active compounds with potential as pharmaceuticals, and iii) to develop biomimetic synthetic methods and catalysts. The other main field of research is in the area of supramolecular chemistry and molecular recognition, and involves the design, synthesis and evaluation of molecular hosts. Applications of this chemistry in the development of catalysts, molecular reactors and devices, and photochemical and thermal switches are being pursued.

Highlights of our recent results include the development of:

(i) enzyme inhibitors to down-regulate, and prohormones to up-regulate, the biosynthesis of peptide hormones;

(ii) models to predict the susceptibility of amino acids and peptides towards free radical processes associated with disorders such as Alzheimer's and cardiovascular disease;

(iii) molecular ratchets, sensors, shuttles, tweezers and switches;

(iv) molecular reactors to catalyse and control the regioselectivity of carbon-carbon bond forming reactions;

(v) novel spectroscopic techniques to analyse melamine-urea-formaldehyde and related resins, and improve the manufacture there of, and

(vi) compounds to inhibit and stimulate ion-flux through calcium ion channels.

Personnel highlights included the graduation of PhD students L Barr and M Gebara-Coghlan and MPhil student P G Dumanski. Dr H Onagi, who graduated in 2003, was awarded the 2004 J G Crawford Prize of the University for his PhD thesis, and the 2004 RSC Dean's Prize for best thesis. R Dawson received a prize for his presentation at the 20th Royal Australian Chemical Institute Conference in Cairns. A Philbrook received sponsorship from Orica (Australia) Pty Ltd to travel to Washington, USA, where she presented the opening lecture at the 38th International Wood Composites Symposium. Z Watts received an award from the National Institute of Biosciences to participate in the 9th International Symposium on Free Radicals in Corsica. Dr John Storey of the University of Aberdeen and Professor Keith Jones of Kingston University each visited for several months.

Free Radical Reactions of Amino Acids, Peptides and Proteins

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

have been designed and synthesised. We have produced enzyme inhibitors to down-regulate, and prohormones to up-regulate, the biosynthesis of peptide hormones. We are currently evaluating the potential of these compounds as pharmaceutical agents for treating human and animal disease states associated with hormone imbalances. *(With B J W Barratt, A Buchan, L Y F Chow, A J Herlt, I Li, A J Mortimer, L Radom, J S Simpson, Y-C Tsai, Z I Watts, A Wright)*

Supramolecular Chemistry and Molecular Recognition

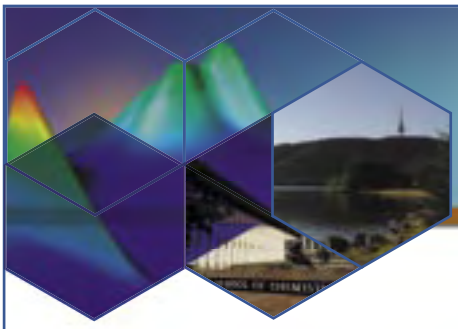
This work exploits cyclodextrins as molecular hosts. Our early work in this area resulted in pharmaceutical formulations that are in everyday clinical use worldwide. In more recent studies modified cyclodextrins are being developed and exploited as molecular scaffolds for the construction of catalysts,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

Other Collaborative Research

Other research involves studies of the structure of melamine-urea-formaldehyde resins, and the search for alternative reagents and improved manufacturing processes. Biochemical molecular recognition processes are also being studied, including the design and development of compounds to inhibit and stimulate ion-flux through calcium ion channels. *(With A Philbrook, J K Robinson, and A Dulhunty, M Casarotto [JCSMR, ANU], N Dunlop [Orica (Australia) Pty Ltd and the UnIChe program], A Ferrante, A Poulos [Adelaide Medical Centre for Women and Children])*

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

The research group summit Mt Kosciusko in March

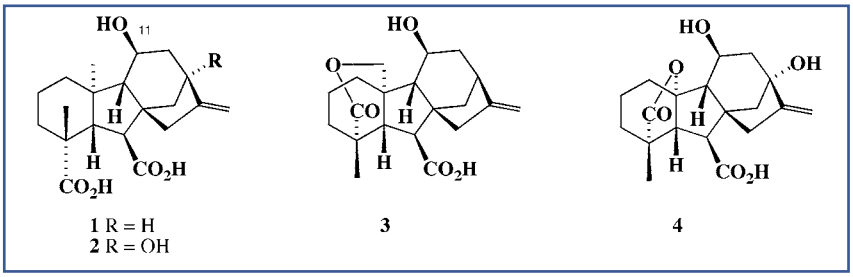


Organic Synthesis — Professor Lew Mander

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

Structural and Synthetic Studies on New Gibberellins

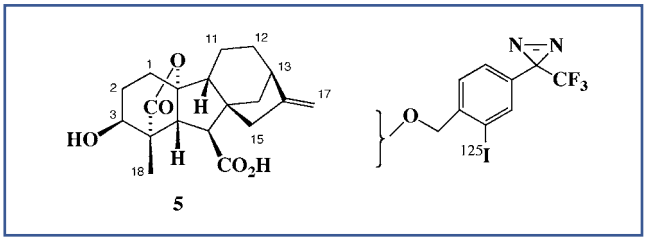
As part of a continuing program directed at the identification of new naturally occurring gibberellins, we have found four new 11β-hydroxy variants in the immature seeds of loquat fruit, namely compounds **1–4**. Their structures were confirmed by synthesis of the methyl esters from gibberellic acid. *(With T V Hau, T P Le, B Twitchin)*



See also: http://www.plant-hormones.info/gibberellins.htm

Preparation of Photo-affinity Probes for Labelling of Gibberellin Receptors

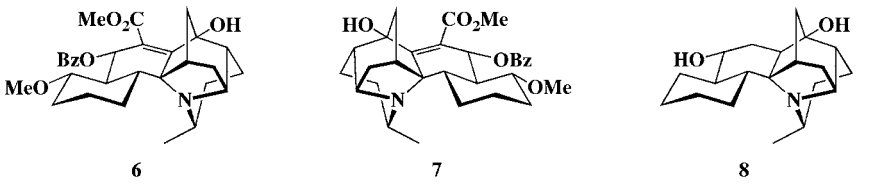
In order to understand more fully the molecular basis of gibberellin bioactivity, we are presently undertaking the synthesis of gibberellins with attached groups designed to crosslink to binding sites in receptors and other gibberellin ("GA")-binding proteins. Trifluoromethyl aryl diazirines have been



shown to be some of the most effective auxiliaries for photo-affinity labelling, but their steric bulk may interfere with binding. Before attempting to prepare a fully elaborated probe, we have made and tested a series of benzyloxy substituted GAs and evaluated their bioactivity. Substituents at C–1, C–2, C–11, C–12, C–13, C–15, C–17 and C–18 (see structure **5** for numbering) have been screened in leaf-growth and the barley endosperm bioassays with those substituted at C–2α, C–11 and C–12 shown to retain acceptable levels of bioactivity. Current efforts are being directed at the elaboration of the "fully equipped" probes which will then be tested for bioactivity. *(With J R Crow, M J McDonough)*

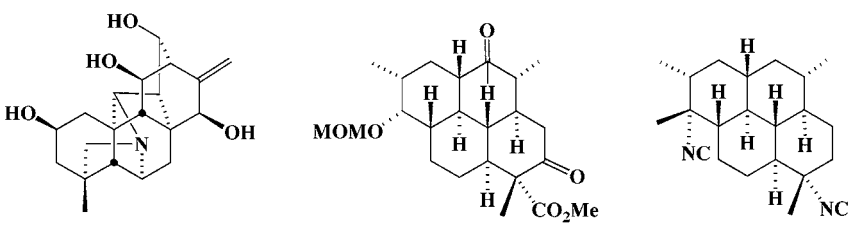
Total Synthesis of Natural Products

Synthetic studies are being directed towards the assembly of several highly caged natural products. They include members of a group of 28 novel alkaloids isolated from the Northern Australian rain forest species, *Galbulimima belgraveana*. Recent X-ray crystallographic studies have revealed the absolute configuration of the more complex alkaloids to be antipodal to the structures that were originally assigned in the mid-60's. For example, himandrine possesses structure **6**, not **7**. Recent studies have culminated in the assembly of the hexacyclic skeleton **8** while current efforts based on elaboration of the original approach are expected to afford the complete structure **6**.



6 **7** **8**

Preliminary studies on the construction of the heptacyclic family of diterpenoid alkaloids typified by hetisine **9** have been undertaken. A number of promising leads have been developed, culminating in a tetracyclic intermediate, while the advanced tetracyclic diester **10** has been prepared *en route* to the total synthesis of the anti-malarial diterpenoid, diisocyanoadociane **11**. *(With G Del Signore, O E Hutt, K A Fairweather, P D O'Connor, A C Willis)*



9 **10** **11**

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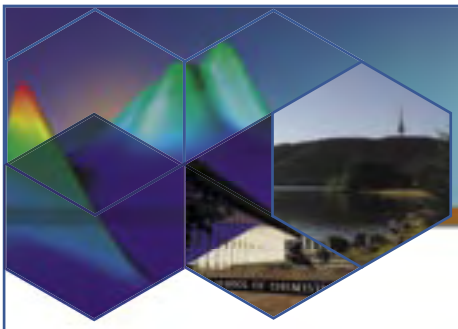
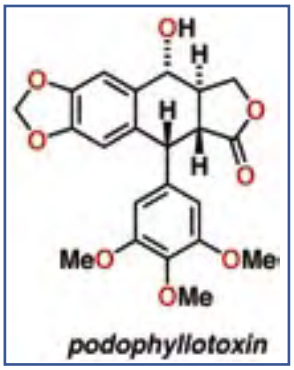


Organic Synthesis, Methodology and Host-guest Chemistry
Dr Mick Sherburn

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

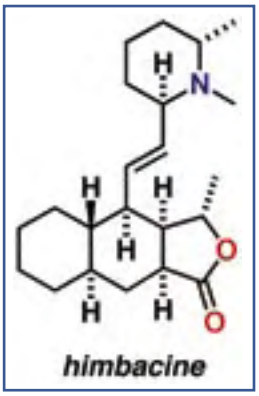
Efficient Total Synthesis: Anti-tumour and Anti-Alzheimer's Natural Products

Lignans like podophyllotoxin have cancer-fighting properties and are used in chemotherapy. An efficient and highly modular approach for the synthesis of these compounds has been developed, culminating in several total syntheses including that of podophyllotoxin. This strategy has several advantages over previous syntheses, the most significant being that it allows a high level of convergency at the end of the synthetic route. Biological evaluations of many of our anti-cancer compounds are presently being carried out in Australia and the USA.



podophyllotoxin

Himbacine is a natural product isolated from *Galbulimima baccata*, a species of tree found in Northern Australia and Papua New Guinea. Himbacine was found to exhibit strong, selective binding to muscarinic receptors of the M2-subtype. Speculation that selective presynaptic muscarinic receptor antagonists might find application in the treatment of neurodegenerative disorders such as Alzheimer's disease provoked our interest in Galbulimima alkaloids. A modular total synthesis of himbacine was completed this year. The synthesis draws upon new chemistry developed in other projects currently underway in the group. A dozen new structural variants of himbacine are currently undergoing biological testing with collaborators at the University of Melbourne. *(With A J Scott, L A Sharp, L S-M Wong, and F J Mitchelson [U Melbourne], J Fischer, A J Reynolds [U Sydney])*



himbacine

A Deeper Understanding of the Most Important Organic Reaction

The Diels–Alder reaction is one of the most powerful and most commonly used reactions in synthetic organic chemistry. Predicting, controlling and explaining the stereochemical outcome of its intramolecular variant 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 (**Figure 1**). This deeper understanding is driving the development of new methodology. We have developed

a novel, efficient and very general way to produce complex polycyclic molecules with useful biological properties from simple, unsaturated, acyclic precursors using sequences of Diels–Alder reactions. *(With T N Cayzer, L C H Kwan, N A Miller, A D Payne, E Pearson, R Tripoli, C I Turner, and M N Paddon-Row [U NSW])*

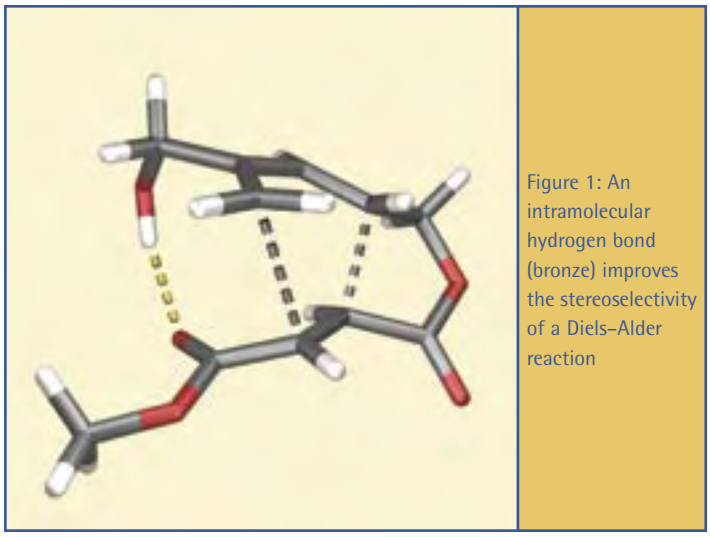


Figure 1: An intramolecular hydrogen bond (bronze) improves the stereoselectivity of a Diels–Alder reaction

Host-guest Chemistry

Research in this area is concerned with the design and synthesis of host molecules based upon cavitands (rigid, bowl-shaped molecules, **Figure 2**) for molecular recognition, complexation and catalysis. Investigations into potential uses of these intriguing hosts as molecule-sized devices is under way. *(With E S Barrett, A J Edwards, N Kanizaj, D J Sinclair)*

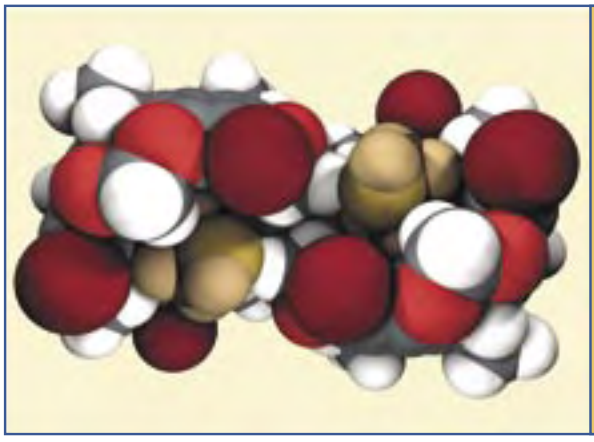
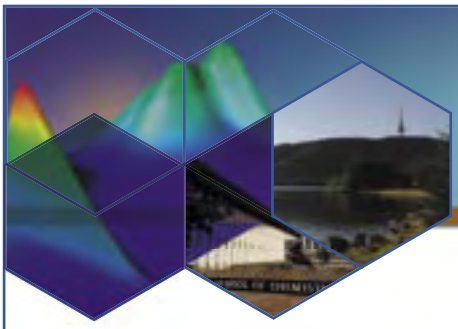


Figure 2: A crystal structure of one of our double-cavity hosts binding two ethanol molecules (bronzed)

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



PHYSICAL AND THEORETICAL CHEMISTRY

Theoretical Chemical Physics — Professor Michael Collins

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

Ab initio quantum chemistry provides accurate information about the energetics of chemical reactions. The potential energy surfaces (PESs) are constructed as an interpolation of this *ab initio* data evaluated at a relatively small number of relevant molecular geometries. Significant progress has now been achieved for moderate sized molecules, so that many different chemical reactions have been investigated. Most of these reactions involve competing mechanisms or reaction pathways and could not be treated using simpler approximate methods. The end result of this work should be a much clearer understanding of the mechanisms of reaction at the molecular level. We are currently pursuing a number of objectives, including further development of the methodology, PES for larger molecular systems, highly accurate PES for quantum reaction dynamics studies of four and five atom systems, many-body expansions for the weak interactions involved in molecular clusters, and coupled surfaces for nonadiabatic reactions.

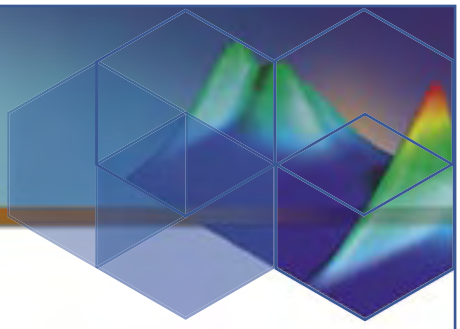
The group's work has been enhanced through collaborations with overseas scientists including the dynamics group of Professor Aoiz and Dr Jesus F. Castillo, Universidad Complutense de Madrid, Associate Professor Dong Hui Zhang at the National University of Singapore, Professor David Yarkony, Johns Hopkins University (nonadiabatic dynamics), Dr Cedric Crespos and Professor Geert-Jan Kroes, University of Leiden (reaction at surfaces), and Professor Mark Gordon, Iowa State University.

Classical Reaction Dynamics for $H+N_2O \leftrightarrow OH+N_2$

We have completed an accurate study of this reaction using classical dynamics on a PES constructed with a high level treatment of electron correlation. The theoretical dynamics confirm the presence of two competing reaction mechanisms and show good agreement with the experimental observations by the Brouard group at Oxford. *(With J Castillo and colleagues [U Complutense de Madrid])*

Hydrogen Abstraction in $H\bullet + CH_4$

The abstraction reactions, $H\bullet + RH \rightarrow H_2 + R\bullet$, have been observed to yield an unusual distribution of rotation–vibration states in the H_2 product. To investigate the mechanism of this class of important combustion reactions, we have continued to pursue accurate PESs for the simplest example, $H\bullet + CH_4$. To facilitate very high dimensional quantum scattering calculations of this reaction, new algorithms for evaluating the PES at billions of molecular configurations have been developed. *(With D H Zhang [National U Singapore])*



Nonadiabatic Chemical Reactions

Many reactions, particularly in combustion and atmospheric chemistry, take place in more than one electronic state. The PES for these electronic states can intersect, and new methods have been developed to describe all the energy surfaces involved and their "interactions".

The code development for this very difficult and important project has been accomplished for the case of two electronic states. Calculations on a model system have verified that it is possible to construct, by interpolation, the potential energy matrix which governs a nonadiabatic reaction. We have now completed the quantum scattering calculations for a simple three atom system to demonstrate the accuracy of the method. *(With C Evenhuis, D H Zhang [National U Singapore], D Yarkony [Johns Hopkins U, USA])*

Deuterium Exchange

Deuterium takes an active part in interstellar chemistry, leading to an enhancement of the abundances of deuterated molecules. In interstellar clouds, such processes are known as deuterium fractionation. The most relevant of them are thought to be gas phase ion-molecule reactions; specifically the reactions $H_3^+ + HD \rightarrow H_2D^+ + H_2$ and $H_3^+ + D \rightarrow H_2D^+ + H$. Accurate molecular potential energy surfaces for both systems has now been evaluated, so that accurate theoretical rate coefficients can be evaluated for these reactions and isotopic analogues. *(With G Moyano)*

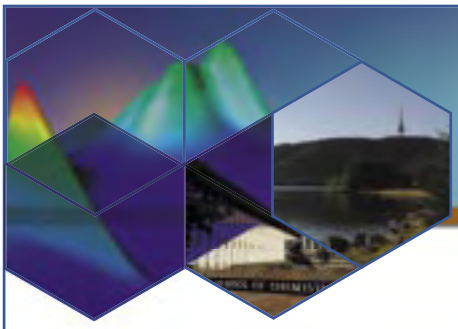
Improved PES Construction

The construction of PESs from *ab initio* quantum chemistry calculations is computationally expensive. We have investigated how to improve the efficiency of this procedure through more optimal selection of the data points used in the interpolation procedure. Two new methods have been developed and shown to produce accurate surfaces for a reduced number of *ab initio* calculations. *(With G Moyano)*

Approximate Ab Initio *Quantum Chemistry*

Ab initio electronic structure theory provides the practical means to calculate the total electronic energy of moderate-sized molecules. From their data one can calculate thermochemical properties and, in principle, the complete potential energy surface which governs the motion of the atomic nuclei. Hence, chemical reaction dynamics, rate coefficients, and other observables may be evaluated. However, the computational time required to calculate the total electronic energy increases rapidly with the number of electrons in the molecule, and with the level of *ab initio* theory employed. We have developed a systematic series or 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. *(With V Deev)*

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



Computational Quantum Chemistry, Polymer Chemistry
Dr Michelle Coote – ARC Fellow, Rita Cornforth Fellow Elect

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 structures of molecules, their vibrational frequencies and their energies. This provides detailed information on the mechanisms of reactions, as well as calculations of their kinetics and thermodynamics. Much of this information is very difficult to obtain experimentally, particularly for very reactive or hazardous compounds. Quantum chemistry provides a viable alternative approach for studying these compounds, and is thus an important complement to experimental procedures.

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

During 2004, our main focus has been the RAFT polymerisation process —an important CSIRO-invented technique for controlling free radical polymerisation. Our work on this process has helped to clarify the reaction mechanism and to develop guidelines for optimising the process. Our first computer-designed RAFT agents are now being tested experimentally, in collaboration with the Centre for Advanced Macromolecular Design, University of New South Wales. We have also enjoyed a stimulating theoretical-experimental collaboration with the group of Professor Arend Schouten, University of Groningen, with whom we are working to design degradation resistant PVC. We look forward to working with Professor Bruce Wild in 2005 on a new ARC-funded project to design stereoregular polyphosphines.

Accurate Computational Methods

Applying quantum-chemical methods to polymeric systems poses a major challenge. Not only do accurate methods require significant computer power, the computational cost of a method scales exponentially with the size of the molecule. In order to adapt quantum chemistry to the study of polymerisation processes we have been evaluating the accuracy of computational methods and identifying reliable low-cost procedures. We have also been designing small model reactions that effectively mimic the behaviour of real polymer systems. We have recently published guidelines on the application of quantum chemistry to free-radical polymerisation in the new edition of the *Encyclopedia of Polymer Science and Technology* (Wiley, 2004). We are designing an *ab initio* polymerisation reactor in which quantum-chemical calculations are combined with kinetic modelling, so as to predict the macroscopic outcome of a polymerisation process. *(With L Radom, R Gomez-Balderas, D J Henry)*

Fundamental Aspects of Radical Reactions

In order to understand the mechanism of complicated radical-based processes (like polymerisation) it is important to study the prototypical systems first. During the last year we have examined reactivity and selectivity preferences in radical addition to double bonds, and have explained unusual substituent effects in alkyl-oxygen bond dissociation energies. We have used this information as a foundation for interpreting substituent effects in the RAFT polymerisation process. We have also identified the factors influencing barrier heights in hydrogen abstraction reactions involving thiols, and highlighted the important role of polar interactions in these systems. This work will assist in the design of improved chain-transfer agents in free radical polymerisation, and will also be significant for the study of these reactions in biological systems. *(With K A Beare, L Radom, R Gomez-Balderas, D J Henry, and A Pross [Ben Gurion U, Israel])*

Controlled Radical Polymerisation

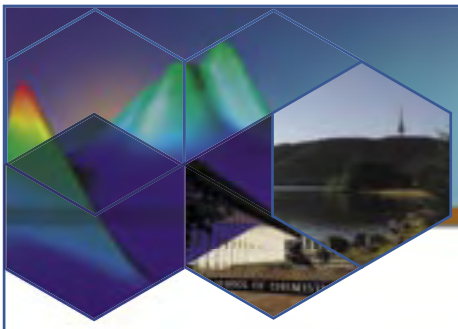
The Australian-invented RAFT process was developed to control the molecular weight and architecture of polymers resulting from free radical polymerisation. We have been using quantum chemistry to build a detailed mechanistic picture of this important process with a view to designing improved RAFT agents for 'difficult' monomers, such as acrylonitrile. During the last year, we have provided explanations for why certain RAFT polymerisations are inhibited or retarded, and provided evidence for long-lived intermediate radicals in certain systems. We have also completed a major study of the effects of substituents on both the kinetics and the thermodynamics of the RAFT process. Building on these studies, we have now moved to the practical problem of RAFT agent design and our first computer-designed RAFT agent is currently being tested experimentally at the University of New South Wales. We have also been exploring the possibility of controlling free radical polymerisation using phosphorus-based RAFT agents, or *via* a new "Controlled Radical Addition Polymerisation" process that we are developing in collaboration with the University of New South Wales *(With K Green, J Hodgson, D J Henry, C Barner-Kowollik, T P Davis, M H Stenzel, A Feldermann, H Chaffey-Millar [UNSW])*

Degradation-resistant PVC

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

Members of the Research Group

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



Liquid State Chemical Physics — Professor Denis Evans

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

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

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

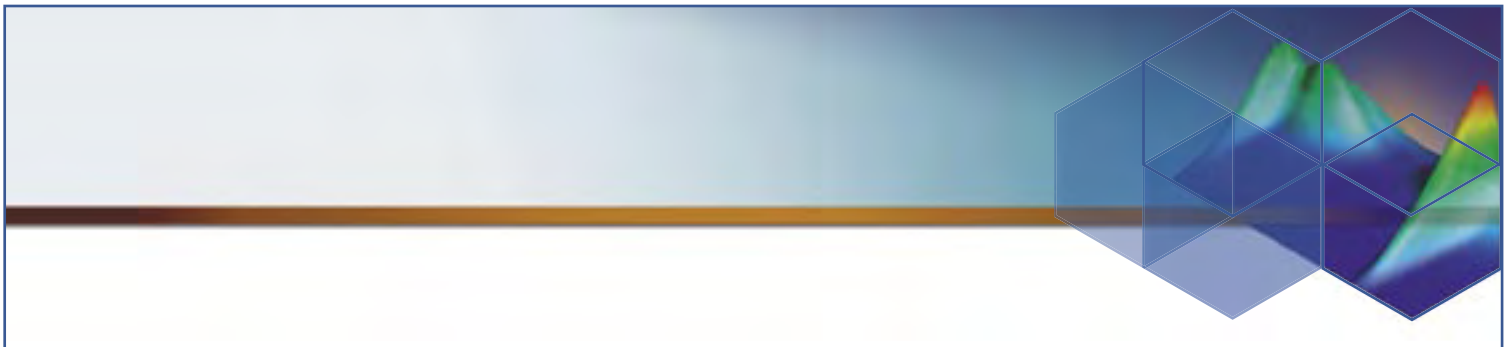
Fluctuation Theorem (FT)

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

Deterministic Thermostats

We have demonstrated how the FT remains independent of thermostatting details for an infinite class of fictitious time-reversible deterministic thermostats. We have shown this theoretically and provided an explicit numerical demonstration firmly establishing how the fictitious thermostat is a convenient but ultimately irrelevant mathematical device. This is important because the derivation of the FT uses fictitious thermostats. Until now, thought (gedanken) experiments have been used to argue that the theory is also directly relevant to laboratory experiments, where the temperature is controlled by a large heat reservoir.

In other work we have discovered that the class of thermostats that Hoover and Evans invented in 1982, is unique. These thermostats which can be derived from Gauss' Principle of Least Constraint applied to fix the kinetic energy of the system, are the only thermostats which permit an equilibrium state. In finite sized systems, if we use non-Gaussian methods to constraint the kinetic energy or we use Gauss' Principle to constrain other moments of the kinetic energy, then the thermostats so derived cannot support an equilibrium state. They are auto-dissipative. This discovery was quite surprising. When the number of degrees of freedom employed in the thermostat becomes infinite, this auto-dissipative aspect of non-Gaussian thermostats can vanish. *(With D J Searles [Griffith U])*



Deterministic Fluctuation Theorem (FT) Applied to Glassy Systems

Work has begun on the application of the FT to glassy systems. Nonequilibrium molecular dynamics simulations are used to provide a realistic model glassy system. The FT provides theoretical expressions, which may be used to probe the distribution function of a glassy system in the absence of an external field. Applying the theory to glassy systems, which dominantly exhibit elastic storage on the simulation time scale, can give very different results to equilibrium fluids, which predominantly exhibit viscous dissipation on the simulation time scale.

Kawasaki Identity

We showed that the Kawasaki Identity can be proved in three lines of simple algebra from the Evans-Searles FT. We have conducted the first experimental tests of the so-called Kawasaki Identity. This identity is a useful diagnostic check on optical tweezers apparatus. *(With E M Sevick)*

Second Law Inequality

We have derived an inequality for the dissipation function that appears in the Evans-Searles FT. We have proved that if we start from the specified initial state, then time integrals of the ensemble average of the dissipation function *cannot* be negative. In thermostatted steady states the ensemble average of the dissipation function is equal to the entropy production. Thus, we have proved that time averages of the entropy production are non-negative. This is in contradistinction to the usual (erroneous) statement of irreversible thermodynamics that says that the entropy production is always positive. This usual statement is wrong as any simple consideration of viscoelastic systems reveals. Our proof of the Second Law Inequality shows that time averages of the entropy production are always non-negative. This is an exact consequence of the Evans-Searles FT. *(With D J Searles [Griffith U])*

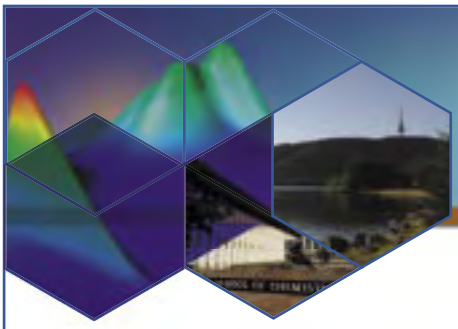
Experimental Confirmation of the Transient FT

Two years ago we conducted the first experimental test of an Evans-Searles FT. However, experimental difficulties meant that we could only test the integrated form of the theorem. This year we conducted the first experimental verification of the distinct version of the Evans-Searles Transient FT. The experiment involved a stationary optical trap in which the trap strength was suddenly changed. The FT was tested for the transient relaxation of the system to its new equilibrium state. *(With E M Sevick, and D J Searles [Griffith U])*

Stochastic Derivation of a Transient Fluctuation Theorem

It has been known for some time that the dissipation function defined deterministically in the Evans-Searles FT, also obeys the Fluctuation Relation when the dynamics are stochastic. We have now given the first completely stochastic derivation of the FT. This work shows that for some stochastic systems the dissipation function that satisfies a Fluctuation Relation is not unique. *(With E M Sevick, and D J Searles [Griffith U])*

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



Theoretical Quantum Chemistry — Professor Peter Gill

In 1998, Walter Kohn and the late John Pople shared the Nobel Prize for Chemistry for their pioneering contributions to the development of quantum chemistry and density functional theory (DFT) as important tools for chemical scientists. By their actions, the Nobel Committee created a watershed in the history of the field, acknowledging that the classical development of the subjects was drawing to a close and that a new chapter was beginning.

Quantum chemistry is the discipline in which the laws of quantum mechanics are applied to understand and predict molecular behaviour and, as we enter the 21st century, one of the scientific "grand challenges" is to find ways to extend quantum chemistry's realm to the study of large systems, especially those of biological interest, without requiring impracticable amounts of computer time. Broadly speaking, two approaches are available. Either one may try to find shortcuts that will allow existing theoretical models to be applied, or one may invent completely new models that are tailor-made for application to systems with lots of atoms. Our group pursues both courses and, despite the inevitable interruption as we relocated from Nottingham to Canberra, we have recently made useful progress on both fronts.

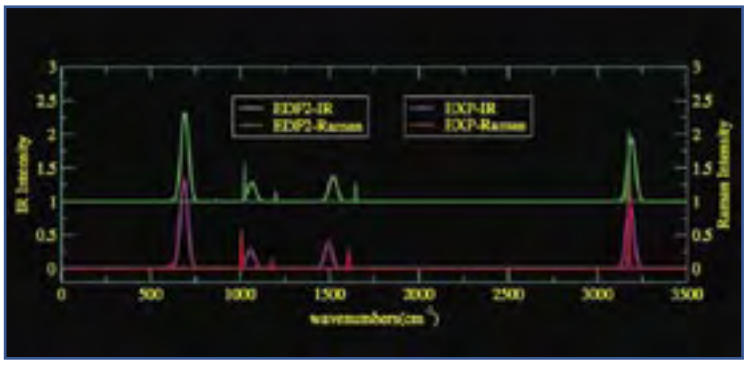
Wigner and Action Intracules

The Heisenberg Uncertainty Principle informs us that it is not possible to simultaneously measure exactly both the position and momentum of a particle. However, we have introduced the Wigner intracule $W(u,v)$, a function that gives the quasiprobability of finding two electrons whose separation r_{12} in position space is u and whose separation p_{12} in momentum space is v. From this, we can derive the action intracule $A(w)$ which gives the quasiprobability that the separation product $r_{12}p_{12}$ is w. These functions give a more detailed picture of the motion of electron pairs than has been previously available and we have recently calculated the intracules for a variety of atoms and molecules, in both the ground and excited states. (The cover of this year's Report shows the Wigner intracule of the Li_2 molecule as it dissociates.) We have also conjectured that the correlation energy – a component of the total energy that is essential for an accurate understanding of bond formation – is related to the action intracule through the equation

$$E_{\mathrm{corr}} = \int_0^\infty A(w)\, G(w)\, \mathrm{d}w$$

where G(w) is a universal (but as yet unknown) function. If this is true, and useful approximate G(w) functions can be discovered, it will have a major impact on the field. *(With D P O'Neill, and N A Besley [U Nottingham, UK])*

DFT for harmonic vibrational frequencies



DFT is often used to predict the vibrational (*i.e.* infra-red or Raman) spectra of molecules but the distinction between harmonic and anharmonic modes is not always made: when a calculated harmonic frequency agrees with an experimental anharmonic one, one is obviously getting the right answer for the wrong reason. We have therefore constructed a new density functional (EDF2) that is designed to give accurate harmonic frequencies and this has been incorporated into the Q-CHEM program. The figure compares the experimental harmonic frequencies of the benzene molecule with the EDF2 harmonic values. We are now extending this work to treat anharmonic frequencies. *(With C Y Lin, and M W George [U Nottingham, UK])*

Do Molecules Contain Atoms?

When atoms bond to form molecules, their atomic identity is partly lost. Where, for example, is the boundary between the hydrogen and oxygen atoms in a water molecule? We are interested in the problem of extracting atoms from a molecule's electron density and we have devised a method based on integral equations for achieving this. At this stage, the method is practical only for diatomics but we hope to extend this in the future. If this can be accomplished, it may allow us to perform complicated calculations on large molecules by first using our approach to partition the electron density into well-defined atomic pieces. *(With A T B Gilbert, and S W Taylor [U Auckland, NZ])*

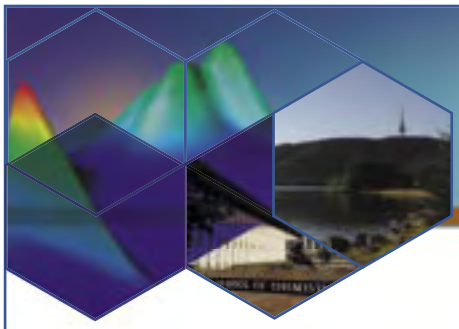
Density Functional Theory Without the Noise

Traditionally, DFT calculations use quadrature (numerical integration) to compute the exchange-correlation energy. Unfortunately, quadrature inevitably introduces numerical errors ("noise") into the calculations and these can cause both technical and chemical problems. Accordingly, we have tried to devise exchange-correlation functionals that can be evaluated without resort to quadrature and recently, using the Hölder inequality, we have constructed the first such functionals. *(With S H Chien)*

Positron Annihilation

Positron annihilation rates in many polyatomic molecular gases are anomalously high. Qualitatively, this can be explained by positron capture in vibrational Feshbach resonances, which can occur for molecules with positive positron affinities. To verify this idea quantitatively, we examined the densities of the vibrational excitation spectra of the *n*-alkanes from propane to nonane and proposed that positron capture is mediated by vibrational doorway states, in which positron binding is accompanied by the excitation of fundamentals. *(With G F Gribakin [Queen's U, Belfast])*

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



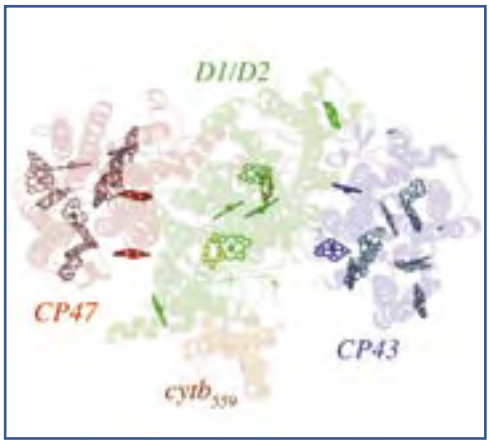
Laser and Optical Spectroscopy — Professor Elmars Krausz

Light, chemistry and photophysics are the most natural and cooperative of partners. The energy in a single particle (photon) of visible light is just that amount needed to perform a chemical transformation. Nature takes ruthless advantage of this synergy in the single most important chemical process on earth. This is the amazingly efficient, yet fascinatingly complex process of photosynthesis. Photosynthesis is the driving force for all life on our planet.

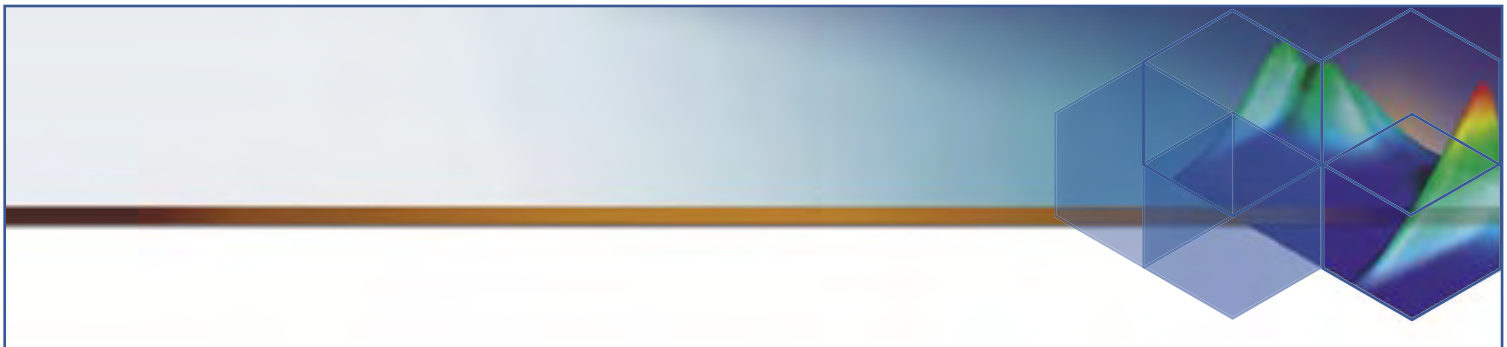
We specialise in spectroscopy. This delves into the subtle yet totally distinctive interactions of light, both visible and invisible, with the many forms of matter. Light, when impinging on a sample, is usually absorbed, emitted or just scattered. We often use lasers, and, *via* their special properties of intensity, purity and coherence, other much less familiar processes become possible. A very wide range of spectroscopic techniques is now available. These techniques may be utilised as either analytical or diagnostic tools, right down to the ultimate limit of chemistry of measurements on *single* molecules, or used to probe fundamental processes.

When spectroscopy is applied at a fundamental level, it is the most potent method with which to probe the innermost secrets of systems. Spectroscopy can map out the detailed electronic structure of the very many different forms of matter: crystals, liquids, glasses, proteins *etc*. In each case, information can be gained on how their constituents bind together and how they interact and transform.

Laser technology has become more familiar to us all with the advent of laser pointers and alignment devices, CDs, DVDs etc. Lasers have also revolutionised spectroscopy and indeed continue to do so. Laser light is *very different* to "ordinary" light (*e.g.* sunlight or lamplight). The spectral purity of a laser can be made better than one part in a billion. Laser pulses can be made shorter than one billionth of one billionth of a second (a femtosecond) or amplified to a level where the very distinction between light and matter becomes blurred. Put simply, lasers induce processes to occur that are just not seen with "ordinary" light sources.



Our group has a well-equipped lab and performs a wide range spectroscopic measurements; absorption, dichroism, emission, Raman, excitation, hole-burning, line-narrowing, on a range of materials. The systems studied can be organic and inorganic, molecular, ionic, amorphous, crystalline, and now predominantly, biological. Our strength is the ability to design, develop and invent special experiments and apparatus to target fundamentally important questions in a particular area of interest. One broad theme we have is that molecules can behave quite differently in solution to when they are 'trapped' or enclosed in a protein or crystal. These critical environmental influences are ideally probed *via* laser-selective spectroscopy.



Photosystem II remains at the centre of our gaze. The figure (PSII) shows its pigments imbedded in its trans-membrane proteins. This year, we have made outstanding discoveries on the nature of P680, the charge-separating assembly and also in the way in which excitation is transferred into the reaction centre. This led to an ANU press release in June, national coverage and invited articles. The group attended the Australasian Conference on Physical Chemistry in Hobart in February and reported some preliminary results. Professor Elmars Krausz and Mr Joseph Hughes attended the International Congress on Photosynthesis in Montreal and the Satellite Conference on Photosystem II in Trois Rivieres where Joseph spoke on some of our key results. Ensuing interest and discussion identified our work as one of the highlights of the congress. Mr Lesley Debono also spoke at the Student Conference on Physical Chemistry at Wagga.

The group hosted a number of visitors. These included the AAS Lemberg Fellow, Professor Charles Dismukes from Princeton and Professor Jim Barber from Imperial College. Joint ARC Linkage PhD student Andrew Dick came to develop our new MCD spectrometer system. Mr Richard Baxter, performed critical experiments towards his University of Chicago PhD on crystalline bacterial reaction centres. Dr Sindra Peterson Årsköld, now at Lund University, returned last summer to perform magneto-optical measurements on cytochrome b_6f. Ms Hendrike Thauern came from the University of Bonn in May to work on chromium and cobalt phosphate crystals.

A New Paradigm for PSII

Exciting developments have evolved from our discovery that PSII undergoes efficient charge separation and hole-burning with long wavelength excitation. Measurements of homogeneous hole-widths establish that excitation transfer from CP43 and CP47 light harvesting assemblies to the reaction centre is remarkably slow. Charge separation occurs with excitation longer than 700 nm, and thus at far lower energy than previously thought. We have been able to establish the source of PSII fluorescence, and develop new paradigm for this system. *(With J Hughes, L Debono, and R Pace, P Smith [Dept Chemistry, ANU], H Riesen [UNSW College, ADFA])*

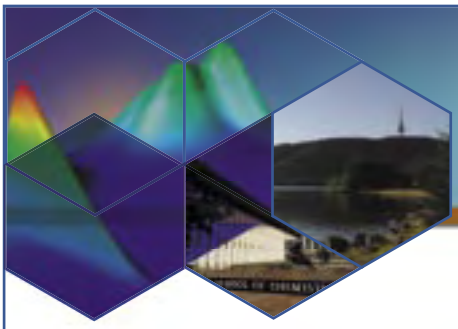
Magneto-enzyme Spectrometer Development

The ARC LEIF- and MEC-funded spectrometers for ANU and the University of Queensland are now a reality. Software development is proceeding at UQ with sample handling and detector systems being further developed and refined at ANU. *(With M Riley, A Dick [U Qld], Lastek [Adelaide])*

Multidimensional Spectral Characterisation of Art Works

A new project has been initiated taking advantage of high performance and inexpensive broad wavelength-sensitive CCD arrays to create wavelength-dependent spectral images of art works, from the UV to the near IR. Such images will establish unique signatures of both the pigments and the methodologies used by the artist. *(With M Kubik, and D Creagh [U Canberra])*

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



Computational Quantum Chemistry — Professor Leo Radom

Chemistry is traditionally an experimental science. However, recent advances in computer technology and the development of highly efficient computer algorithms have opened the way for a viable alternative approach to experimental chemistry: chemistry by computer. We use such computer calculations to determine the structures of molecules and to help understand how molecules react with one another. The procedure employed is called *ab initio* molecular orbital theory, the term *ab initio* signifying that the calculations are carried out from first principles using the laws of quantum mechanics. No experimental data other than values of fundamental physical constants are used. An important feature is that the calculations can be carried out as readily for reactive or hazardous species as for normal, stable molecules. They are therefore particularly useful in cases where experimental studies might be difficult or impossible. Properties that may be examined include molecular structures and reaction pathways, as well as many thermodynamic and spectroscopic properties.

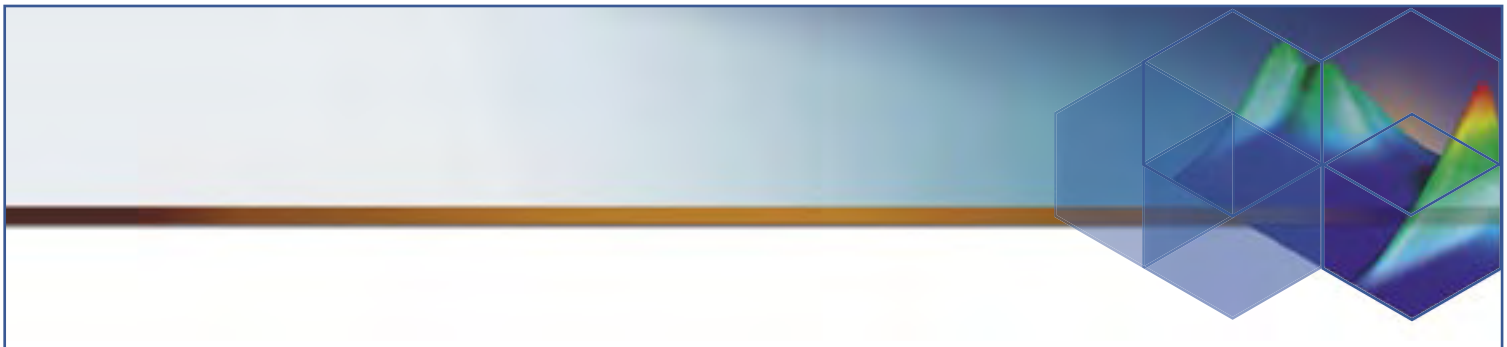
I spent the early part of the year on leave in the School of Chemistry at the University of Sydney, and subsequently made the move a permanent one by resigning from the ANU in October. However, I am hoping to continue my productive links with the RSC through my current appointment as Adjunct Professor.

Free Radical Chemistry

Radicals are ubiquitous in chemistry, biology, and polymer science. Because they are reactive species, they are often difficult to study experimentally and therefore theory has a potentially useful role to play in their characterisation. We have been using theory to determine radical stabilisation energies, with the important aim of seeing how individual substituents stabilise or destabilise a radical centre. We have also been examining the details of radical addition, abstraction and rearrangement reactions, which are of particular importance in biological chemistry and polymer chemistry. *(With M L Coote, D J Henry, and R Gomez-Balderas, G P F Wood, D Moran [U Sydney])*

Enzyme-catalysed Reactions

Vitamin B_{12} is one of nature's essential vitamins. We have used *ab initio* calculations to model reactions mediated by coenzyme B_{12}. Although these reactions have been extensively studied experimentally, there is certainly no consensus as to how they proceed. We find that protonation and/or deprotonation at appropriate sites facilitates the reactions, and that reactions that are facilitated by protonation (or deprotonation) are facilitated by the partial-proton-transfer that enzymatic hydrogen bonding can provide. Supporting evidence for our proposals has come from site-directed mutagenesis experiments. This and other recent examples provide strong encouragement for the use of computer calculations in a predictive manner in the study of enzyme reactions. Our most



recent studies are being directed at the abstraction steps in these B_{12}-mediated reactions, including the deactivation of the enzymes through the addition of substrate analogues, leading to so-called suicide inactivation. *(With G M Sandala, M L Coote, and B T Golding [U Newcastle-upon-Tyne], D M Smith [Rudjer Boskovic Institute, Zagreb, Croatia], S D Wetmore [Mount Alison U, Canada])*

Oxidative Damage to Proteins

An understanding of the oxidation of proteins by free radicals is of great importance because of its implication in a number of human disorders such as Alzheimer's disease, atherosclerosis, and diabetes, as well as aging. We have been using *ab initio* molecular orbital calculations to address the problem. Initial targets have included the cleavage of the peptide backbone following radical formation, and migration of the radical site within the peptide. *(With C J Easton, M L Coote, and G P F Wood, D Moran [U Sydney], R Jacob [RMIT], M Davies [Heart Research Institute, Sydney], R A J O'Hair [U Melbourne], A Rauk [U Calgary, Canada])*

Oxides and Hydroxides of Alkali and Alkaline Earth Metals

We have been examining the alkali metal oxides and hydroxides as a preliminary to investigating their interesting acid and base properties. Reliable experimental data are very sparse for these molecules. Their theoretical description is not entirely straightforward either and has necessitated incorporation of several new features and the development of new basis sets. *(With M B Sullivan, and N L Haworth [U Sydney], A K Wilson [U North Texas, USA], J M L Martin [Weizmann Institute, Israel])*

Development of Improved Theoretical Procedures

The ability to predict reliable thermochemistry represents a very important application of *ab initio* molecular orbital theory. We have recently been designing and assessing methods that are suited for predicting accurate thermochemistry for free radicals because these represent particular challenges for theoretical investigation. Our latest work has been concerned with methods designated R-CBS-QB3. *(With G P F Wood [U Sydney], G A Petersson [Wesleyan U, USA])*

Interaction of Metal Ions with Biological Systems

Metal ions are of great importance in biological function. We have embarked on a theoretical study to probe the interaction of metal ions with prototypical biological molecules. Our initial studies have focussed on the interaction of calcium dications with simple model systems in order to establish suitable theoretical procedures that can be applied to larger molecules. *(With I Corral, O Mó, M Yáñez [Autonoma U, Madrid, Spain])*

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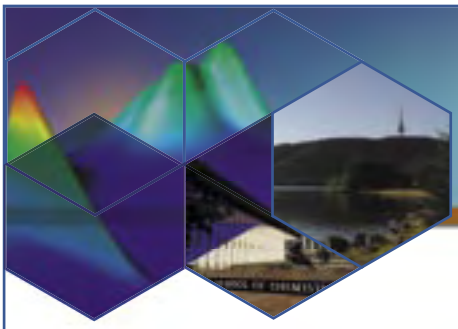


Polymers and Soft Condensed Matter — Dr Edith Sevick

In the past decade, Atomic Force Microscopy (AFM) and Optical Tweezers (OT) have revolutionised molecular science by measuring picoNewton forces over lengthscales from 1 to 10^4 Å. In our laboratory, we have an Optical Tweezer Apparatus which has been extensively modified for our force measurement experiments in polymer and colloids science. The apparatus consists of an optical trap that weakly "holds" a micron-sized bead. The trap is formed by a focused laser beam that is refracted through the transparent bead. The refracted rays differ in intensity over the volume of the colloidal bead and exert a force on the bead, drawing it towards the region of highest light intensity. The optical trap is harmonic near the focal point: the optical force acting on a colloidal particle positioned at x from the trap centre is F_{opt}=-kx, where k is the trapping constant which can be tuned by adjusting the laser power. In this way, the optical trap generated by the OT serves to both localise a colloidal particle and to measure the small, sub-picoNewton scale forces acting on the particle. With substantial modifications, our OT apparatus probes forces at small lengthscales and over small timescales that are necessary in studies of nonequilibrium statistical mechanics and polymer/biopolymer science.

Probing Thermodynamics of Small Systems over Small Timescales Using Optical Tweezers

The puzzle of how time-irreversible microscopic equations of mechanics lead to the time-irreversible macroscopic equations of thermodynamics has been a paradox since the days of Boltzmann. Boltzmann simply side-stepped this enigma by stating "as soon as one looks at bodies of such small dimension that they contain only very few molecules, the validity of this theorem [the Second Law of Thermodynamics and its description of irreversibility] must cease." Today we can state that the Fluctuation Theorem (FT), first proposed by Denis Evans and colleagues in 1993, is a generalised, Second-Law-like theorem that bridges the microscopic and macroscopic domains and links the time-reversible and irreversible descriptions. The predictions of the FT should be relevant to many nanotechnological applications. Our FT-related work in 2004 had two major themes:

Experimental Demonstrations of the FT using a Colloidal Particle in a Viscoelastic Solvent

Recently the Evans and Sevick groups demonstrated experimentally the FT for the first time using a colloidal particle weakly held in a translating optical trap. This work received considerable attention in the popular press, science journals, and other media primarily because of its implications to nanotechnology. Miniature engines are not simple rescaled versions of their larger counterparts, and if the work performed during the duty cycle of any machine is comparable to thermal energy per degree of freedom, then, according to the FT, one can expect that the machine will operate "in reverse" over short time scales. However, to date the FT has been confirmed only with exceptionally simplified systems that are fully describable using deterministic or stochastic dynamics, such as a single optically-trapped colloidal particle in a Newtonian fluid, or a computational sea of Lennard-Jones particles. Our premise is that the FT holds for any general system, including more complex systems that currently defy exact description, such as biological or molecular motors. To test the application of the FT to more relevant nanosystems, we need to address systems of increasing complexity. Our approach is to increase complexity one-step-at-a-time and a strategic system to investigate is, therefore, a single colloidal bead, optically-trapped in a viscoelastic solution. While an optically-trapped particle in a Newtonian fluid is perfectly describable using Langevin dynamics, the dynamics of the same particle in a viscoelastic solution is far more difficult to describe. We have performed preliminary experiments that show that the particle's trajectories in viscoelastic solution should obey the FT. *(With M A B Baker, D M Carberry, J C Reid, G M Wang, D J Evans)*

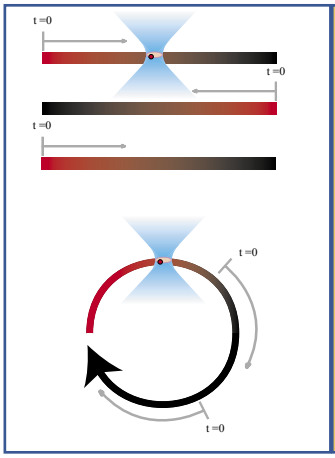


Figure: An illustration of linear (left) and circular (right) translation of an optical trap containing a colloidal particle. The trajectory of the optically-trapped colloidal particle is used to demonstrate the FT under transient and steady-state conditions. Several thousand linear translations are constructed providing transient trajectories (indicated by red portion of the translation) as well as short steady-state trajectories (indicated by black portion). In contrast, a single circular translation provides a single transient trajectory, but a very long steady-state trajectory that can be segmented into "independent" steady-state trajectories.

Application of the FT under Steady-state Conditions

While the FT has been experimentally demonstrated for systems that are perturbed from an initial equilibrium state, there are a number of studies suggesting that the theorem applies asymptotically in the long time limit to systems in a nonequilibrium steady-state. The asymptotic application of the FT to such nonequilibrium steady-states has been referred to in the literature as a separate theorem, the Steady-State Fluctuation Theorem or SSFT. In 2004, we investigated the SSFT and FT under nonequilibrium steady-states using a colloidal particle localised in a linearly-translating optical trap and in a circularly-translating trap. From these colloidal trajectories we demonstrated that the FT holds under nonequilibrium steady-states for all time, and not just in the long time limit, as in the SSFT. We demonstrated experimentally and theoretically that the SSFT holds asymptotically in the long time limit when the argument of the FT, the dissipation function, is derived approximately. However, when the dissipation function is derived exactly, the FT holds for all time, including short times. This suggests that the asymptotic limit in the SSFT is simply due to approximations in the argument of the theorem, and that when the argument of the theorem is derived exactly, the FT is operative over all time. *(With J C Reid, D M Carberry, G M Wang, D J Evans)*

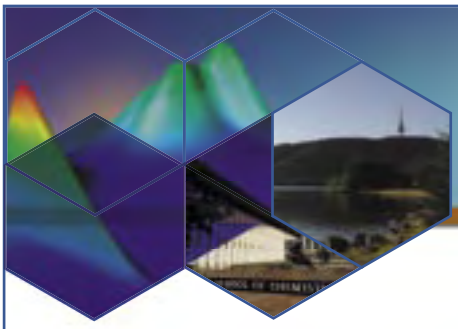
Using Optical Tweezers to Characterise Viscoelasticity of Polymer Solutions

The optical tweezers can also be used as a micro-rheometer to experimentally determine the viscous and elastic response of polymer solutions. By recording the colloidal particle's position in a stationary optical trap over frequencies ranging from 10^{-1} to 10^{4} Hz, we are able to determine viscoelastic properties of the small fluid volume containing the colloidal particle. As the colloidal particle is micron-sized, the volume of fluid probed is very small, in the order of a pico-litre. This year our OT rheometer was used primarily in conjunction with FT experiments. *(With G M Wang)*

Optical Tweezers for Biopolymer Studies

By attaching specially-coated latex beads to the ends of modified DNA, we are able to use an optical trap and micropipette to stretch a single bead-DNA-bead assembly and to construct a force versus extension profiles of several DNA systems. These force profiles are used to study the effect of different salts and the interactions of specific binding proteins on DNA. In conjunction with the Protein Synthesis and Evolution Group headed by Nick Dixon, we focused upon different end-tethering techniques so that we can efficiently stretch double-stranded DNA where one strand is linked to the beads, and where both strands are linked to the beads. *(With G M Wang, D M Carberry, N E Dixon)*

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



Disordered Materials — Professor Richard Welberry

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

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

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

Much of the current effort of the group is concerned with the further development and exploitation of the least-squares method for directly fitting a Monte Carlo (MC) simulation to observed X-ray diffraction data, proposed for the first time in 1997. This work is supported by an ARC Discovery Grant. A second ARC Discovery Grant is held jointly with the Withers Group and supports work to investigate the role of strain in disordered systems.

Diffuse X-ray Scattering and Models of Disorder

A highlight of the year was the publication of the book entitled "Diffuse X-ray scattering and models of disorder" by the Group leader, published by Oxford University Press in the International Union of Crystallography Series of Monographs on Crystallography. The book details the work of the group in developing methods of recording, interpreting and analysing diffuse X-ray scattering.

Refinement of Monte Carlo Models of Disordered Molecular Crystals

The current main emphasis of this work is to develop the techniques whereby the diffuse scattering from a molecular crystal can be measured and analysed on a routine basis. Such analyses provide information on how the molecules interact with each other that is not available from conventional crystal structure determinations. The need to measure very weak intensities in the presence of the very strong Bragg peaks presented nontrivial problems when the synchrotron data that had been collected at the APS in Chicago in 2003 was processed. Considerable effort was required to overcome these problems. The main source of the difficulties was that when Bragg peaks impinge on the detector, locally generated fluorescence produces a 'blooming' artefact. After much work we now have good 3D data sets for the series of flexible molecules 2,2'-, 3,3'- and 4,4'-dimethoxybenzil, each of which has five internal degrees of flexibility.

A number of software tools have been developed to aid the setting up, model design and running of the Monte Carlo (MC) simulation program that is used to analyse the diffuse scattering data. Whereas previously each new project required the setting up of a purpose-built MC program involving many weeks of development, it is now feasible to use a generic program that can be tailored to suit different systems in a much shorter time.

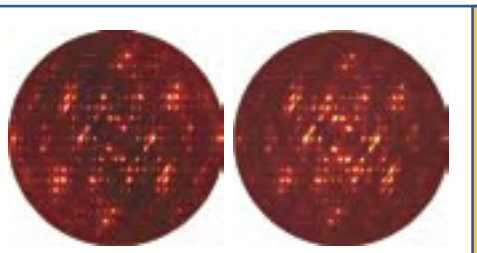


Figure 1: Typical synchrotron data (left) and corresponding calculated diffraction pattern (right) of 3,3'-dimethoxybenzil

Most effort this year has gone into the analysis of 3,3'-dimethoxybenzil. A model that gives excellent agreement with the observed synchrotron data has been developed and the study has provided invaluable experience of how modelling of this kind of system should be carried out. Some preliminary work on the 2,2'-dimethoxybenzil system has also been carried out. This system has presented some unusual new diffraction features which will present new challenges to the methodology. *(With D J Goossens, A P Heerdegen, and D R Haeffner, P L Lee, J Almer [APS, Argonne, USA])*

Diffuse Neutron Scattering from Crystals

Further diffuse neutron scattering data have been recorded for d_{10}-benzil, $C_{14}D_{10}O_2$ using the time-of-flight (tof) Laue technique instrument, SXD, at the ISIS Neutron Source, UK. Data covering a large fraction of the total 3D reciprocal space out to a Q of 15 $Å^{-1}$ has been recorded at four different temperatures. Work has now begun to re-refine the structural model including this new neutron data alongside the original X-ray data. Our work on benzil was featured as a 'Science Highlight' in the ISIS Annual Report for 2004.

Our collaborations with ISIS staff have also led to our involvement with a study of diffuse scattering in the relaxor ferroelectric material PZN ($PbZn_{1/3}Nb_{2/3}O_3$). A renewed interest in the field of ferroelectricity has taken place in recent years since the finding of exceptional piezoelectric properties in the lead-oxide class of relaxor ferroelectric (RF) materials typified by PZN. We have developed a model for PZN that explains the diffuse scattering that is observed. This is based on the supposition that the origin of its properties is the lone-pair electrons of the Pb atoms. *(With D J Goossens, A P Heerdegen, and W I F David, M J Gutmann, M J Bull [ISIS, Oxon, UK])*

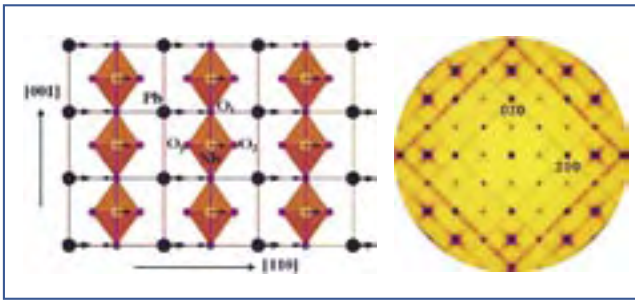


Figure 2: Model for the polar nano-domain structure in PZN (left) together with the calculated (*hk0*) diffraction pattern (right)

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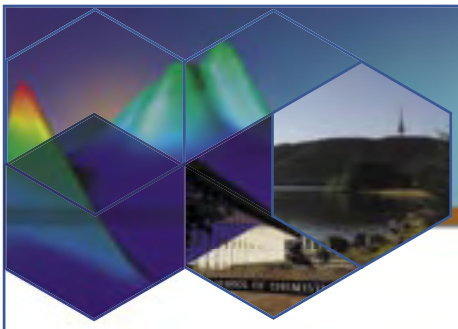


Solid State Molecular Science — Professor John White

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

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

Energy Dispersive X-ray Reflectometry

Reflectometry using X-rays can be used for *in situ* structural analysis during thin-film growth. We are particularly interested in thin films based on oxide networks (TiO_2, ZrO_2 and SiO_2) that could find use in heterogeneous catalysis where high surface area is of the utmost importance. One of the most promising routes to new oxide-based mesostructured materials involves the co-assembly of the oxide precursor with an organic template. Using reflectometry with fast time-resolved energy dispersive X-rays, the interfacial structure of these films can be monitored as they self-assemble at the air/water interface. Surfactants such as cetyltriemethylammonium chloride (CTAC) and sodium dodecyl sulfate (SDS) are used as the organic templates. *(With A Hawley, D King, and A R Rennie [NFL Uppsala Universitet, Sweden], A Gibaud [U the Marne, France])*

Evaporation-induced Self-assembled Thin Films

A collaboration has begun with the University of the Marne (France) and Uppsala University (Sweden) to study evaporation-induced self assembly (EISA). This has been used previously to prepare thin mesostructured silica-based and transition metal oxide-based films including TiO_2 and ZrO_2. Using the micellar template concept followed by calcination, optically uniform mesoporous thin metal oxide films can be realised. *(With A R Rennie [NFL Uppsala Universitet, Sweden], A Gibaud, J-F Bardeau [U the Marne, France])*

Solvent Effects in High Internal Phase Emulsions

Our previous work using small angle neutron scattering (SANS) and neutron and X-ray reflectometry on high internal phase emulsions has concentrated on an archetypal high internal phase emulsions in which surfactant nature, concentration and molecular weight have been varied. We have shown that these consist of polydisperse micron-scale aqueous droplets, 90% by volume, suspended in a continuous 10% by volume hexadecane oil phase. This year we have completed the investigation begun last year of variation in the oil phase by collection of complete sets of SANS data within the

phase space hexadecane-toluene-cyclohexane as a function of temperature, both from emulsions and microemulsions, together with the collection of emulsion rheological data. *(With K J Baranyai, M J Henderson, J Zank, P A Reynolds)*

Ultra Small Angle Scattering from High Internal Phase Emulsions

SANS can only probe scales from *ca.* 1 to 50 nm in high internal phase emulsions, while optical methods probe scales greater than *ca.* 1000 nm. Coverage of this gap between SANS and optical microscopy potentially provides a complete structural description. We have continued and completed experiments detailed in the 2003 Report by further use of the USANS instrument BT-5 at NIST to provide data from 20000 nm down to 60 nm on high internal phase emulsions with various neutron contrasts. *(With K J Baranyai, P A Reynolds, M J Henderson, A J Jackson, J Zank, and J Barker [NIST])*

The Synthesis of New Surfactants

A range of new surfactants have been synthesized to investigate the factors influencing the stability of high internal phase emulsions formed with them at lower surfactant concentrations. They are block oligomers formed from a large variety of monomers with modified headgroups. This new synthetic ability has also allowed us to synthesise partially deuterated surfactants for use in investigations of mixed surfactant emulsions. *(With J Zank, A J Scott)*

Proteins at Surfaces

The effect of interfaces on the thermodynamics and kinetics of protein unfolding is accessible by reflectometry using X-rays and neutrons at interfaces. Present work is directed at following the changes in surface excess of a globular protein adsorbed at the air-water interface in the presence of a chemical denaturant. The experiments probe the equilibrium surface structure of bovine β-lactoglobulin solutions containing increasing concentrations of guanidinium hydrochloride (G•HCl) at constant temperature. A measure has been made of the contribution of the air-water interface to the chemical denaturation enthalpy of β-lactoglobulin. *(With A Perriman)*

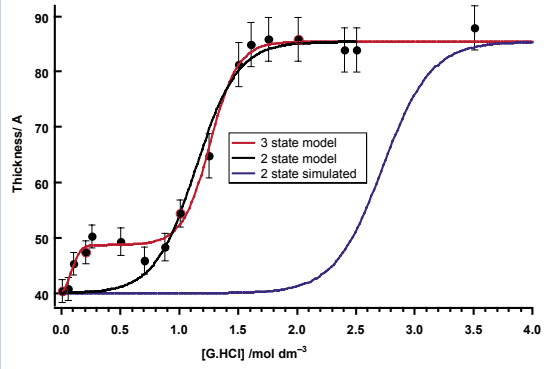
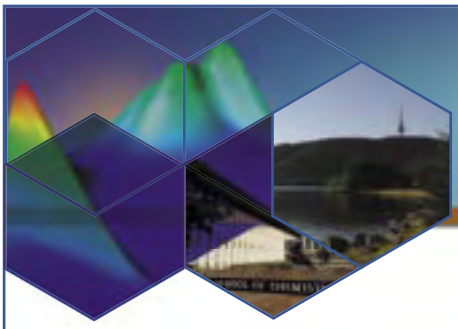


Figure: Thickness parameter as a function of chemical denaturant concentration for β-lactoglobulin at the air-water interface. Solid lines result from application of a 2-state (black), 3-state (red), and solution thermodynamic parameters (blue).

Denaturation of Proteins at Interfaces at the Nanometre Scale

Dried dairy ingredients are an important segment of the Australian dairy market. In the case of high protein content powders a loss of functionality (*e.g.* solubility) is observed on drying. Our aim is to understand the nanoscale structural changes that occur on dehydration and the factors influencing those changes. *(With A J Jackson, and M A Augustin [Food Science Australia])*

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



Electrochemistry — Dr Richard Webster (ARC QEII)

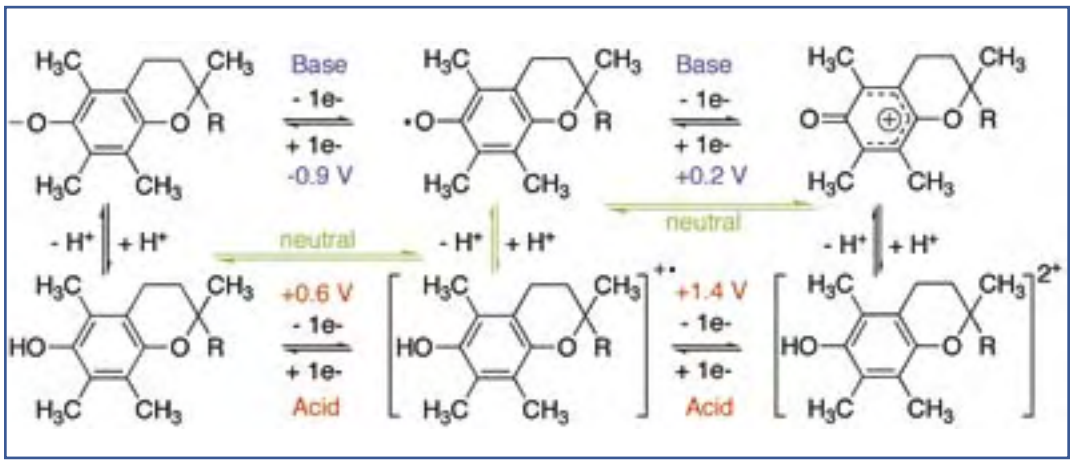
The electrochemical control of oxidation and reduction processes in organic and inorganic systems is an area of extensive research in both academia and industry. Electrochemical techniques are extremely useful in generating interesting species in unusual oxidation states, or for producing reactive intermediates (as, for example in the reductive dimerization 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 to the electrochemical generation, such as in kinetic studies. The focus of this research is developing and utilising spectroscopic techniques (including EPR, UV-VIS, FTIR and NMR) to study processes involving electron transfer, primarily in organic systems.

In situ *Electrochemical-NMR Spectroscopy*

NMR spectroscopy has the capacity for the structural identification of solution-phase species. However, despite widespread interest in both NMR spectroscopy and voltammetry, the compatibility problems that exist between the two procedures have made it extremely difficult to achieve an *in situ* combination, with few published attempts. The principal difficulty is the requirement that a metal electrode be located within the magnet of a NMR spectrometer, with the current flowing simultaneously to spectral acquisition. Recently, we have constructed a three-electrode, two-compartment cylindrical electrochemical cell for *in situ* operation in a 500 MHz 1H NMR spectrometer. The cell was designed around a standard 10 mm sample tube holder and is lowered into position within the magnet by height adjustable aluminum rods that support the wires connecting the potentiostat to the working, auxiliary and reference electrodes. The electrochemical cell functions under diffusion-controlled conditions in non spinning mode and is able to operate under variable temperature and oxygen-free regimes. The working electrode consists of a 10 nm thick gold film deposited onto the surface of a 7.49 mm OD diameter glass NMR tube that is located directly within the radio-frequency (RF) coils of the NMR probe. The NMR spectra were collected simultaneously to the current flowing during the electrolysis with typical NMR linewidths being approximately 2 Hz. The highly symmetrical nature of the cell design meant that probe tuning and gradient shimming changed minimally between each experiment, which allowed standard shim sets to be saved and recalled for later use, thereby greatly reducing the time taken for tuning processes. Insertion and removal of the cell from within the magnet is achieved within a few seconds, which combined with the rapid shimming process, makes the cell suitable for routine operation. The cell was used to study the *in situ* reduction of 9-bromoanthracene, 9-chloroanthracene and 4-bromobenzophenone in deuterated acetonitrile with tetrabutylammonium hexafluorophosphate as the supporting electrolyte.

The Redox Chemistry of α-Tocopherol (Vitamin E)

α-Tocopherol (α-TOH) is the most naturally abundant, extensively methylated, and biologically active of the four (α, β, γ and δ) structurally related phenolic compounds that are labelled vitamin E. α-TOH is thought to play an important role as an antioxidant in mammalian tissues by inhibiting the free radical chain autoxidation of polyunsaturated fatty acid esters (LH) in two principal steps. First, α-TOH reacts with an oxidised site on a lipid cell wall (LOO•) to yield a molecule of lipid hydroperoxide (LOOH) and the tocopheroxyl radical (α-TO•). Second, the α-TO• radical reacts with another LOO• radical so that overall one α-TOH molecule is able to inhibit two LOO• sites. To date, the important biological chemistry of vitamin E is thought to involve only the neutral compound (α-TOH) and phenoxyl radical (α-TO•).



However, electrochemical and spectroelectrochemical experiments performed in our laboratory have demonstrated the existence of several other forms of vitamin E that are linked through proton and electron transfers; the monocation radical (α-TOH^{+}•), the dication (α-TOH^{2+}) and the phenoxonium cation (α-TO^{+}). Surprisingly, the phenoxonium cation was found to be very stable in dry organic solvents and readily undergoes a chemically reversible two-electron/one-proton (ECE) process with the neutral phenolic starting material. The interesting possibility that α-TO^{+} has biological significance is currently under investigation.

Electrochemistry and EPR Spectroscopy of Transition Metal Compounds Containing Bridging Thiolate Ligands

Various bi- and tri-metallic transition metal compounds with sulfur-containing ligands have been investigated using electrochemistry to probe the degree of electron delocalisation between the metal centres. Electrochemistry and EPR spectroscopy have been used to identify reversible homolytic S-S bond formation/cleavage in a pentamethylcyclopentadienyl ruthenium(III) thiolate-thioether system. *(With L Y Goh, [National U Singapore])*

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

VISITING FELLOWS (POST-RETIREMENT)

There are eight post-retired staff members of the RSC who are continuing independent research programs and have been appointed as Visiting Fellows by invitation of the School:

Emeritus Professor Athelstan L J Beckwith AO BSc *WA* DPhil *Oxford*, FRACI, FAA, FRS (retired 1996) is continuing his work on the structure, stability and reactions of organic free radicals. Papers published during this year describe a number of highly stereoselective radical reactions of considerable synthetic utility. The factors that underlie such high diastereoselectivity are being studied, as is the utility of ESR spectroscopy for the estimation of radical stability. A major collection of ESR data for organic radicals is in the hands of the publisher. During the year, Athel was invited to attend a major symposium held in Ottawa to honour Dr K U Ingold. The award of Officer of the Order of Australia (AO) was included in the Queen's Birthday Honours list for '*Service to science in the field of organic chemistry as a leading researcher and through advice to government and the wider community on scientific matters*'.

Emeritus Professor Martin A Bennett BSc PhD DIC DSc *London*, ARCS, FRACI, FAA, FRS (retired 2000) During 2004, Martin continued collaboration with Professor S Bhargava at RMIT University. He has also been co-supervising a PhD student, Steven Privér, who submitted his thesis a few months ago, and was awarded the PhD degree. A full paper based on part of this thesis work has just appeared in *Inorg. Chem*. Also, as part of this collaboration, a PhD student, Kunihiko Kitadai, from the group of Professor Takahashi, Toho University, Japan, spent three weeks with Martin carrying out experiments on gold-tertiary arsine complexes. Martin continues to work through the backlog of publications resulting from work done by his previous co-workers. An invited review based on the work of Matthew Byrnes and Ivan Kovacik has just appeared in the 40th anniversary issue of *J. Organomet. Chem*., in honour of (the late) Professor Colin Eaborn. Martin also continues to referee extensively for international journals, including *Organometallics, J. Chem. Soc., Dalton Trans., Inorg. Chem., J. Organomet. Chem., and Inorg. Chim. Acta*.

Dr Richard Bramley MSc *Sydney*, PhD *London*, MRACI (retired 1997) During the year, Richard has had consultations with Ms Joanne Harrison, PhD scholar in the Laser Physics Group, RSPhysSE, on colour centres in diamonds, a project concerned with coherence times in candidate materials for quantum cubits. He has also consulted with, and provided facilities for, Ms Harrison and Dr Andrei Rode (also Laser Physics Group) in their studies of carbon nanofoam, a fascinating new form of carbon. Consultations have also taken place with staff at Caltech in their attempts to pursue zero-field EPR spectroscopy, a field in which the RSC is a world leader. Comments on the theory underlying the relevance and complications of using standard Hamiltonians were provided along with instrument design features. Richard continues to collaborate with UNSW College ADFA, and indirectly with the Quantum Computing group, UNSW, on ways of reading out data bits without destroying them in the

process. Work has focussed on electric field rather than magnetic field readout in P doped silicon. Experiments are in hand to circumvent an effect which has thwarted an initial simple experiment, an effect which is now understood and has been proven experimentally. A simple way around the problem will be tried shortly. Richard has been consulted and provided assistance in setting up a vibrating sample magnetometer in the Physics, Environment and Mathematical Science Department at UNSW College ADFA. A condition of the transfer to ADFA was that RSC would have access to the instrument and its extended facilities at low temperatures.

Dr Desmond J Brown BSc MSc *Sydney* PhD DSc *London* (retired 1986), formerly of the JCSMR, is nearing completion of a critical review of research in the cinnoline and phthalazine areas of heterocyclic chemistry during the last 30 years, for publication as a companion volume to his book *Qinoxalines: Supplement II*.

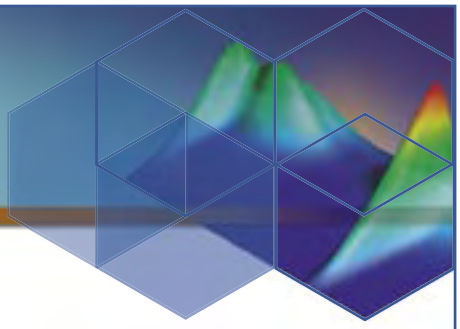
Dr John K MacLeod BSc PhD *Queensland*, FRACI (retired in 1999) continued to be involved in writing papers resulting from work carried out by two of his former PhD students and from a collaborative project with Dr Murali Nayudu, Division of Botany and Zoology (BOZO), School of Life Sciences, ANU.

Emeritus Professor Rodney W Rickards BSc *Sydney* FRACI, FAA (retired in 1999) is also a Visiting Scientist at CSIRO Entomology, and continued his research collaboration there with Dr Stephen Trowell. The work is directed towards the discovery of new antibiotics for human use from novel sources such as termites, sawflies, and other insects and terrestrial invertebrates selected from Australia's unique biodiversity. The four million species of insects which exist on Earth constitute a virtually untapped pharmaceutical resource, in contrast to plants and microoganisms which have long been targets for drug discovery. Work to date has resulted in two international patent applications, and was continued during 2004 by Professor Weiping Yin, a Visiting Scientist from China. Collaboration continued with Dr Geoffrey Smith in the Division of Biochemistry and Molecular Biology (BaMBi), Faculty of Science, on biologically-active cyanobacterial metabolites. The highlight of this work was the isolation and structural analysis of the calothrixins, pentacyclic heterocycles unique among natural products, with potent antitumor and antimalarial activity which is currently being explored for possible application by an international pharmaceutical company under agreement with ANU. 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 Research School of Biological Sciences. This material is available only at mass spectrometric levels, and presents a major structural challenge. Joint research also continued with the University of Queensland and the Australian company Bio-Care Technology Pty Ltd on the characterisation of complex cyclic peptide antibiotics produced by certain biocontrol bacteria. A Commemorative Issue of *ARKIVOC* [2004, Part x, 1–177], Archive for Organic Chemistry, with a forward written by a previous RSC Research Fellow Dr Melvyn Gill, was published in recognition of Rod's 70th birthday.

Emeritus Professor Alan M Sargeson BSc PhD DipEd *Sydney*, FRACI, FAA, FRS (retired 1996) is collaborating with Dr S V Smith, ANSTO, Biomedicine and Health, and with Professor B T Golding, University of Newcastle-upon-Tyne, UK, on the development of detecting therapeutic agents for cancer. Currently, Dr Sue Smith and Alan are also collaborating with Addenbrook's Hospital of Cambridge University, UK, on developing reagents to image breast cancer with the SarAr technology. A recently initiated project with Dr Kevin Brindal, Biochemistry Department, Cambridge University, UK, is aimed at imaging apoptosis with the Cu-reagent. In addition, a study has also commenced with the Boston Children's Hospital, Harvard Medical School, to label a humanised antibody to target neuroblastoma. This last project is also in collaboration with Lexigen, a subsidiary of Merck.

Emeritus Professor John F Williams MSc PhD *NSW* MA *Oxford* DSc *ANU*, FRACI, FAIFT (retired 1992), formerly of the Department of Biochemistry, The Faculties has completed an invited article entitled *Pentose Phosphate Pathway, History of*, which has been published by Elsevier Science in the ***Encyclopedia of Biological Chemistry***, a new four-volume encyclopedia covering *all* contemporary Biochemistry (Normal and Pathabolic) and Molecular Biology. He has also completed Paper 1 of a two paper set, with Dr John MacLeod, describing biochemical studies on Octulose phosphates in the path of carbon in photosynthesis. Paper 2 is well advanced following a time consuming recalculation of most of the primary data. Both papers are planned for submission in the New Year to *Photosynthesis Research* for side-by-side publication.

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



ADJUNCT PROFESSORS

Professor Roger Amos

Uses quantum chemistry to calculate molecular properties from first principles. Calculation of electromagnetic properties. A particular interest in Density Functional Theory, and its application to excited states using time-dependent DFT.

Professor Veronica J James OAM

Fibre diffraction of hair can be used as a totally noninvasive screening test for breast cancer for women of all ages. *(With Professor J Kearsley [Cancer Care, St George Hospital, Sydney], Dr B E Willis [Eastmoreland Hospital, Portland Oregon], Dr Osmo Räsänen [Breast Cancer Centre, Turku, Finland])*

Fibre diffraction is able to diagnose the presence of these cancers at an earlier stage than any other cancer. *(With Dr T Robertson, Dr A Boyd, Professor J Papadimitriou [Division of Pathology, School of Surgery and Pathology, UWA])*

Fibre diffraction of hair can be used as a totally noninvasive screening test for colon cancer. *(With Dr A Polyglase [Monash U Medical School])*

Fibre diffraction of hair may be able to be used as a totally noninvasive screening test for some forms of liver, lung and skin cancer. *(With Professor D Morris [St George Hospital, Sydney], Professor P Heenan [UWA], Professor B McCaughan [Royal Prince Alfred Hospital, Sydney])*

Fibre diffraction of hair may be used as a relatively inexpensive, noninvasive gene test. *(With Professor R Scott [Molecular Genetics and Cytogenetics, Hunter Area Pathology Service, NSW])*

Chemical analysis to determine the origin of the change in the α-keratin structure of hair in breast cancer. *(With Dr G Corino [CSIRO Fibre Technology, Geelong], Dr J Ouwagie [Innogenetics, Belgium])*

Fibre diffraction of hair can be used as a totally noninvasive screening test for Alzheimer's Disease. *(With Dr T Robertson and Professor J Papadimitriou [Division of Pathology, School of Surgery and Pathology UWA], Professor R Martins [Alzheimer's and Ageing, School of Biomedical and Sports Science, Edith Cowan U, Sir James McCusker Alzheimer's Disease Research Unit, School of Psychiatry and Clinical Neurosciences, U WA, Hollywood Private Hospital, Perth])*

HONOURS AND AWARDS

Ms Robyn J Abernathy was awarded second prize for a student contribution at the 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, New Zealand, in December. Her talk was entitled: *Solvent-mediated reactions of ruthenium complexes with poly(pyrazolyl) borates.*

Mr Matthew A B Baker, has been awarded the 2004 General Sir John Monash award for excellence The scholarship will allow Matthew to attend Vrije Universiteit in the Netherlands to study biological nanomotors.

Professor Martin G Banwell

- was awarded the 2003 Royal Society of Chemistry, Industrially Sponsored Award for Synthetic Organic Chemistry. This award was made for Martin's "elegant use of chemoenzymatic methods for the preparation of a wide variety of complex natural products including alkaloids and sesquiterpenes, as well as versatile strategies for the synthesis of troponoids and the lamellarins";
- was awarded the Novartis Chemistry Lectureship for 2004-2005;
- was the 2004 Boehringer-Ingleheim Lecturer of the Ohio State University;
- was the 2004 Nanjing University of Science and Technology International Exchange and Co-operation Lecturer;
- awarded the 2004 Royal Australian Chemical Institute (RACI) Birch Medal – this is the premier medal awarded for organic chemistry by the RACI;
- was elected Fellow of the Australian Academy of Science.

Professor Athelstan L J Beckwith was honoured with the award of Officer of the Order of Australia in the Queen's Birthday Honours list.

Ms Lorraine M Caldwell was awarded a National Institute of Physical Sciences Travel Assistance Grant for her poster presentation entitled: *Cytotoxic iron chelators: iron complexes of di-2-pyridyl keton isonicotonyl hydrazone (HPKIH) analogues*, at the International Conference on Coordination Chemistry (ICCC 36), Mérida, Yucatán, México, in July.

She was also awarded a National Institute of Physical Sciences Travel Assistance Grant for her poster presentation entitled: *Group 6 selenoaroyl complexes: isoselenocyanates as single atom selenium transfer reagents*, at the International Conference on Organometallic Chemistry (ICOMC 21), Vancouver, Canada, in July.

Mr David M Carberry was awarded 3rd prize plus a certificate and $500 off his next National Instrument purchase in the 2004 Oceania Customer Solution Competition for his design of a customer solution article detailing a problem and how it could be solved using one or more NI products. The competition was organised by National Instruments and was open to anyone using any NI product.

Professor Michael A Collins was awarded the Physical Chemistry Division Medal of the Royal Australian Chemical Institute.

Mr Ryan E Dawson was awarded best poster prize at the 20th Royal Australian Chemical Institute Conference and the 29th International Symposium on Macrocyclic Chemistry, Cairns, in July. The poster title was: *Stilbene and cyclodextrins as the basis of molecular shuttles.*

Mr Rian D Dewhurst presented the talk: *Simple convergent routes to Heterobimetallic C_3 complexes*, at the International Conference on Organometallic Chemistry (ICOMC 21), Vancouver, Canada, in July, for which he was awarded a National Institute of Physical Sciences Travel Assistance Grant.

Professor Christopher J Easton

- was elected as a Fellow of the World Innovation Foundation;
- was elected as Fellow of the Australian Academy of Science.

Professor Denis J Evans was awarded the 2004 Moyal Medal from Macquarie University "for distinguished contributions to research in mathematics, physics and statistics".

Mr Gwion Harfoot was awarded an Alexander von Humboldt Postdoctoral Research Fellowship to study in Germany.

Ms Elizabeth H Krenske was selected to present a student lecture at the Southern Highlands Conference on Heterocyclic Chemistry, 7-9 September 2003. The lecture was entitled *Alkyne Exchange in Phosphirenium Salts*.

She also won the prize for the best student lecture at the Second Australia and New Zealand Symposium on Organometallic Chemistry at the University of Adelaide, 11-14 January, entitled *Phosphine-stabilised Arsenium Salts as Precursors for the Asymmetric Synthesis of Tertiary Arsines*.

Mr Lawrence C H Kwan was the co-recipient of the award for the best student lecture entitled *Towards an efficient construction of steroids using a domino IMDA reaction*, presented to the Royal Australian Chemical Institute NSW Organic Group 25th Annual One-day Symposium, University of New South Wales in December.

Mr David W Lupton was the co-recipient of the award for the best student lecture entitled *A total synthesis of the alkaloid aspidospermidine*, presented to the Royal Australian Chemical Institute NSW Organic Group 25th Annual One-day Symposium, University of New South Wales in December.

Professor Lewis N Mander — A One-day Synthesis Symposium in honour of Professor Mander was held at the Shine Dome on 8 September, on the occasion of his 65th birthday. The symposium featured ten presentations from his colleagues and former students. The program concluded with the presentation of the 2004 Birch Lecture by Professor Robert Grubbs, and a dinner honouring both Professors Mander and Grubbs followed. During the dinner, glassblower Chris Tomkins presented Professor Mander with a model of Gibberellin A3. Chris made this model while Ray Filardo constructed the perspex casing and Ian Clarke the timber base.

Ms Natalie A Miller won a prize for best student poster at the Royal Australian Chemical Institute NSW Organic Chemistry Group 25th Annual One-day Symposium, University of New South Wales, in November, and also the best poster prize at the IUPAC ICOS-15, 15th International Conference on Organic Synthesis, Nagoya, Japan, in August. The poster title was: *Synthesis and reactions of substituted dendralenes*.

Dr Hideki Onagi

- was awarded the Dean's Prize 2004 for the best PhD thesis, entitled *Cyclodextrins as Building Blocks for Supramolecular Chemistry*;
- was awarded the JG Crawford Prize of the ANU.

Ms Lisa A Sharp won a prize for best student presentation at the 20th Royal Australian Chemical Institute Conference and the 29th International Symposium on Macrocyclic Chemistry, Cairns, July, for her talk entitled: *The intramolecular radical carboxyarylation reaction: scope and application to natural product synthesis.*

Ms Christine Sharrad was awarded the 2004 Dean's Prize for General Staff Excellence for her outstanding work on the School's contribution to the ANU Quality Review.

Mr Andrew J Scott won a prize for best student poster at the 20th Royal Australian Chemical Institute Conference and the 29th International Symposium on Macrocyclic Chemistry, Cairns, July.

Mr Never Tshabang was highly commended for his student contribution at the 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, New Zealand, in December. His talk was entitled: *Heterobimetallic complexes of poly(methimazolyl)borate ligands.*

Mr Peter Wu was invited to give an oral presentation of his poster, entitled: *Measurement and Φ angle dependence of CSA/DD cross-correlation effects between H^{α} and H^{N}*, at the **ANZMAG 2004,** Barossa Valley, South Australia, in February

PUBLICATIONS

Key to Symbols Used to Identify Research Workers

The following symbols have been used to indicate the status of individuals who were not regular members of the RSC during 2004.

- * Not a member of The Australian National University
- ≠ Visiting Fellow (during that year)
- # Member of the IAS◇
- \+ Member of the Faculties, Central Areas, or attached Centres◇

◇ Research workers with the same symbol, but from different Schools/Faculties, are numbered: #1, #2/+1, +2. A note is made of their affiliation at the end of the publication list.

Biological Chemistry

Protein Structure and Function

Dixon, N. **DNA replication: the fellowship and the rings.** *Aust. Biochemist* (2004), 35(1), 4.

Gupta, R.*, Hamdan, S.M., Dixon, N.E., Sheil, M.M.*, Beck, J.L.* **Application of electrospray ionization mass spectrometry to study the hydrophobic interaction between the ε and θ subunits of DNA polymerase III.** *Protein Sci.* (2004), 13(11), 2878–2887.

Loscha, K., Oakley, A.J., Bancia, B., Schaeffer, P.M., Prosselkov, P., Otting, G., Wilce, M.C.J.*, Dixon, N.E. **Expression, purification, crystallization, and NMR studies of the helicase interaction domain of *Escherichia coli* DnaG primase.** *Protein Expr. Purif.* (2004), 33(2), 304–310.

Ozawa, K., Headlam, M.J., Schaeffer, P.M., Henderson, B.R., Dixon, N.E., Otting, G. **Optimization of an *Escherichia coli* system for cell-free synthesis of selectively ^{15}N-labelled proteins for rapid analysis by NMR spectroscopy.** *Eur. J. Biochem.* (2004), 271(20), 4084–4093.

Pintacuda, G., Keniry, M.A., Huber, T.*, Park, A.Y., Dixon, N.E., Otting, G. **Fast structure-based assignment of ^{15}N HSQC spectra of selectively ^{15}N-labeled paramagnetic proteins.** *J. Am. Chem. Soc.* (2004), 126(9), 2963–2970.

Schaeffer, P., Headlam, M., Dixon, N. **Protein-protein interactions in the bacterial replisome.** *Aust. Biochemist* (2004) 35(1), 9–12.

Sheil, M.M.*, Beck, J.L.*, Gupta, R.*, Watt, S.*, Brown, S.E., Dixon, **N.E. Electrospray mass spectrometry of gas phase macromolecular complexes.** *Adv. Mass Spectrom.* (2004), 16, 295–313.

Wijffels, G.*, Dalrymple, B.P.*, Prosselkov, P., Kongsuwan, K.*, Epa, V.C.*, Lilley, P.E., Jergic, S., Buchardt, J.*, Brown, S.E., Alewood, P.F.*, Jennings, P.A., Dixon, N.E. **Inhibition of protein interactions with the β_2 sliding clamp of *Escherichia coli* DNA polymerase III by peptides from β_2-binding proteins.** *Biochemistry* (2004), 43(19), 5661–5671.

Nuclear Magnetic Resonance

Pintacuda, G., Keniry, M.A., Huber, T.*, Park, A.Y., Dixon, N.E., Otting, G. **Fast structure-based assignment of ^{15}N HSQC spectra of selectively ^{15}N-labeled paramagnetic proteins.** *J. Am. Chem. Soc.* (2004), 126(9), 2963–2970.

Structural Biology

Bogoyevitch, M.A.*, Boehm, I.*, Oakley, A., Ketterman, A.J.*, Barr, R.K.* **Targeting the JNK MAPK cascade for inhibition: basic science and therapeutic potential.** *Biochim. Biophys. Acta* (2004), 1697(1–2), 89–101.§

Loscha, K., Oakley, A.J., Bancia, B., Schaeffer, P.M., Prosselkov, P., Otting, G., Wilce, M.C.J.*, Dixon, N.E. **Expression, purification, crystallization, and NMR studies of the helicase interaction domain of *Escherichia coli* DnaG primase.** *Protein Expr. Purif.* (2004), 33(2), 304–310.

Oakley, A.J., Klvana, M.*, Otyepka, M.*, Nagata, Y.*, Wilce, M.C.J.*, Damborsk, J.* **Crystal structure of haloalkane dehalogenase LinB from *Sphingomonas paucimobilis* UT26 at 0.95 Å resolution: dynamics of catalytic residues.** *Biochemistry* (2004), 43(4), 870–878.§

§ Research conducted prior to commencement at RSC

Protein Crystallography and Engineering

Murphy, J.M., Ford, S.C.[#1], Olsen, J.E.[#1], Gustin, S.E.[#1], Jeffrey, P.D.[#1], Ollis, D.L., Young, I.G.[#1] **Interleukin-3 binding to the murine β_{IL-3} and human βc receptors involves functional epitopes formed by domains 1 and 4 of different protein chains.** *J. Biol. Chem.* (2004), 279(25), 26500–26508.

Xu, Y.*, Wen, D.*, Clancy, P.*, Carr, P.D., Ollis, D.L., Vasudevan, S.G.* **Expression, purification, crystallization, and preliminary X-ray analysis of the N-terminal domain of *Escherichia coli* adenylyltransferase.** *Protein Expr. Purif.* (2004), 34(1), 142–146.

Xu, Y.*, Zhang, R.*, Joachimiak, A.*, Carr, P.D., Huber, T.*, Vasudevan, S.G.*, Ollis, D.L. **Structure of the *N*-terminal domain of *Escherichia coli* glutamine synthetase adenylyltransferase.** *Structure* (2004), 12(5), 861–869.

Yu McLoughlin, S., Jackson, C., Liu, J.-W., Ollis, D.L. **Growth of *Escherichia coli* co-expressing phosphotriesterase and glycerophosphodiester phosphodiesterase, using paraoxon as the sole phosphorus source.** *Appl. Environ. Microbiol.* (2004), 70(1), 404–412.

Yu McLoughlin, S., Ollis, D.L. **The role of inhibition in enzyme evolution.** *Chem. Biol.* (2004), 11(6), 735–737.

[#1] IAS (John Curtin School of Medical Research)

Biomolecular NMR

Hoshino, M., Otting, G. **Sensitivity-enhanced double-TROSY experiment for simultaneous measurement of one-bond ^{15}N–^{1}H, ^{15}N–$^{13}C'$ and two-bond ^{1}H–$^{13}C'$ couplings.** *J. Magn. Reson.* (2004), 171(2), 270–276.

Liepinsh, E.*, Rakonjac, M.*, Boissoneault, V.*, Provost, P.*, Samuelsson, B.*, Rådmark, O.*, Otting, G. **Letter to the Editor: NMR structure of human coactosin-like protein.** *J. Biomol. NMR* (2004), 30(3), 353–356.

Loscha, K., Oakley, A.J., Bancia, B., Schaeffer, P.M., Prosselkov, P., Otting, G., Wilce, M.C.J.*, Dixon, N.E. **Expression, purification, crystallization, and NMR studies of the helicase interaction domain of *Escherichia coli* DnaG primase.** *Protein Expr. Purif.* (2004), 33(2), 304–310.

Modig, K.*, Liepinsh, E.*, Otting, G., Halle, B.* **Dynamics of protein and peptide hydration.** *J. Am. Chem. Soc.* (2004), 126(1), 102–114.§

Ozawa, K., Headlam, M.J., Schaeffer, P.M., Henderson, B.R., Dixon, N.E., Otting, G. **Optimization of an *Escherichia coli* system for cell-free synthesis of selectively ^{15}N-labelled proteins for rapid analysis by NMR spectroscopy.** *Eur. J. Biochem.* (2004), 271(20), 4084–4093.

Pintacuda, G., Kaikkonen, A.*, Otting, G. **Modulation of the distance dependence of paramagnetic relaxation enhancements by CSA×DSA cross-correlation.** *J. Magn. Reson.* (2004), 171(2), 233–243.

Pintacuda, G., Keniry, M.A., Huber, T.*, Park, A.Y., Dixon, N.E., Otting, G. **Fast structure-based assignment of ^{15}N HSQC spectra of selectively ^{15}N-labeled paramagnetic proteins.** *J. Am. Chem. Soc.* (2004), 126(9), 2963–2970.

Pintacuda, G.*, Moshref, A.*, Leonchiks, A.*, Sharipo, A.*, Otting, G. **Site-specific labelling with a metal chelator for protein-structure refinement.** *J. Biomol. NMR* (2004), 29(3), 351–361.

[§] Research conducted prior to commencement at RSC

Inorganic Chemistry

Coordination Chemistry and Spectro-electro Chemistry

Bernardo, P.H.[+1], Chai, C.L.L.[+1], Heath, G.A., Mahon, P.J., Smith, G.D.[+2], Waring, P.[+1], Wilkes, B.A.[+1] **Synthesis, electrochemistry, and bioactivity of the cyanobacterial calothrixins and related quinones.** *J. Med. Chem.* (2004), 47(20), 4958–4963.

Mahon, P.J., Oldham, K.B.* **Convolutive modelling of the disk electrode geometry under reversible conditions.** *Electrochim. Acta* (2004), 49(28), 5049–5054.

Mahon, P.J., Oldham, K.B.* **The transient current at the disk electrode under diffusion control: a new determination by the Cope-Tallman method.** *Electrochim. Acta* (2004), 49(28), 5041–5048.

[+1] Faculty of Science (Chemistry)

[+2] Faculty of Science, (Biochemistry and Molecular Biology)

Synthetic Organometallic and Coordination Chemistry

Anderson, S.*, Berridge, T.E.*, Hill, A.F., Ng, Y.T.*, White, A.J.P.*, Williams, D.J.* **Dihapto carbamoyl (carboxamide) complexes of Iron(II).** *Organometallics* (2004), 23(11), 2686–2693.

Anderson, S.*, Cook, D.J.*, Hill, A.F., Malget, J.M.*, White, A.J.P.*, Williams, D.J.* **Reactions of tungsten alkylidynes with thionyl chloride.** *Organometallics* (2004), 23(11), 2552–2557.

Crossley, I.R., Hill, A.F. **Di- and zerovalent platinaboratranes: The first pentacoordinate d^{10} platinum(0) complex.** *Organometallics* (2004), 23(24), 5656–5658.

Crossley, I.R., Hill, A.F., Humphrey, E.R., Smith, M.K., Tshabang, N., Willis, A.C. **Caveats for poly(methimazolyl)borate chemistry: the novel inorganic heterocycles [$H_2C(mt)_2BR_2$]Cl (mt = methimazolyl; BR_2 = BH_2, BH(mt), 9–BBN).** *Chem. Commun.* (2004), (16), 1878–1879.

Dewhurst, R.D., Hill, A.F., Smith, M.K. **Heterobimetallic C_3 complexes through silylpropargylidyne desilylation.** *Angew. Chem.* (2004), 116(4), 482–484; *Angew. Chem.*, Int. Ed. (2004), 43(4), 476–478.

Dewhurst, R.D., Hill, A.F., Willis, A.C. **A bis(tricarbido) complex of iridium and tungsten: [IrH($C{\equiv}CC{\equiv}W(CO)_2${HB(pz)$_3$})$_2$(CO)(PPh$_3$)$_2$].** *Organometallics* (2004), 23(8), 1646–1648.

Dewhurst, R.D., Hill, A.F., Willis, A.C. **A mercury bis(tricarbido) complex: [Hg{$C{\equiv}C{-}C{\equiv}W(CO)_2$Tp}$_2$-(dmso)$_4$](dmso)$_2$(Tp = hydrotrispyrazolylborate).** *Chem. Commun.* (2004), (24), 2826–2827.

Dewhurst, R.D., Hill, A.F., Willis, A.C. **Bi- and tetranuclear tricarbido complexes: $\mu,\sigma{:}\sigma'$ and $\mu,\sigma{:}\sigma'{:}\pi_\perp$ coordination of bridging C_3 ligands.** *Organometallics* (2004), 23(25), 5903–5906.

Foreman, M.R.St.-J.*, Hill, A.F., White, A.J.P.*, Williams, D.J.* **Polyazolyl chelate chemistry. 13. An osmaboratrane.** *Organometallics* (2004), 23(4), 913–916.

Hill, A.F., Malget, J.M.*, White, A.J.P.*, Williams, D.J.* **Dihydrobis(pyrazolyl)borate alkylidyne complexes of tungsten.** *Eur. J. Inorg. Chem.* (2004), (4), 818–828.

Hill, A.F., Rae, A.D., Schultz, M., Willis, A.C. **Organometallic macrocyclic chemistry. 6. Chelate-assisted macrocyclization of 4,7,10-trithiatrideca-2,11-diyne.** *Organometallics* (2004), 23(1), 81–85.

Hill, A.F., Schultz, M., Willis, A.C. **Reactions of ruthenium(0) phosphine complexes with diphenylacetylene.** *Organometallics* (2004), 23(24), 5729–5736.

Hulkes, A.J.*, Hill, A.F., Nasir, B.A.*, White, A.J.P.*, Williams, D.J.* **Reactions of μ-alkylidyne complexes with tellurium. Telluroacyl versus μ-telluride formation.** *Organometallics* (2004), 23(4), 679–686.

Inorganic Stereochemistry and Asymmetric Synthesis

Brasch, N.E., Hamilton, I.G., Krenske, E.H., Wild, S.B. **π-Ligand exchange on phosphenium ions: reversible exchange between free and coordinated alkynes in phosphirenium salts.** *Organometallics* (2004), 23(2), 299–302.

Kitto, H.J., Rae, A.D., Willis, A.C., Zank, J., Wild, S.B. **Synthesis and structure of the helicate (M)-(–)-$[Pt_2\{(R,R)\text{-tetraphos}\}_2](CF_3SO_3)_4 \bullet 4.5H_2O$.** *Z. Naturforsch., B: Chem. Sci.* (2004), 59b(11&12), 1458–1461.

Solid State Inorganic Chemistry

2003:

Onagi, H., Carrozzini, B.*, Cascarano, G.L.*, Easton, C.J., Edwards, A.J., Lincoln, S.F.≠, Rae, A.D. **Separated and aligned molecular fibres in solid state self-assemblies of cyclodextrin [2]rotoxanes.** *Chem. Eur. J.* (2003), 9(24), 5971–5977.

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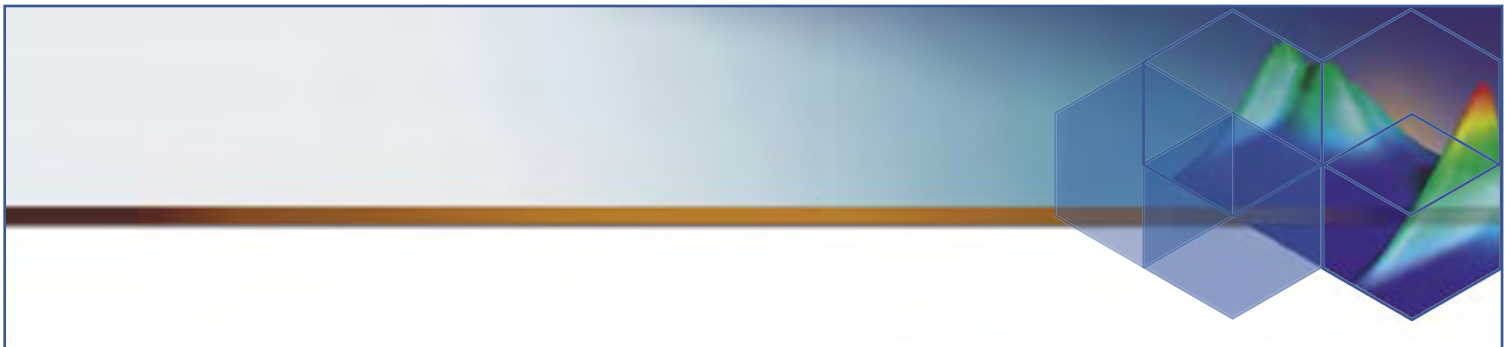

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NATIONAL AND INTERNATIONAL LINKS

Collaborative Research Projects with Universities, CSIRO and Other Institutions

Biological Chemistry

Protein Structure and Function

Carbohydrate binding by C-type lectins by DR N E DIXON with Drs J E Gready, M Hulett and Mr Y-M Hyun, John Curtin School of Medical Research, ANU

Cleavage of DNA by chromium(V) complexes by DR N E DIXON and MS P E LILLEY with Professor P A Lay and Dr A Levina, School of Chemistry, University of Sydney

Expression, isolation and structures of the *Bacillus subtilis* DnaC helicase and DnaI proteins by DRS N E DIXON, P M SCHAEFFER, X-C SU and MS K V LOSCHA with Professor R G Wake, and Drs D B Langley and J M Guss, School of Molecular and Microbial Biosciences, University of Sydney

Evolution of new protein functions by DRS N E DIXON and P M SCHAEFFER with Dr G Coia, Evogenix Pty Ltd, Melbourne

In vitro protein synthesis by DRS N E DIXON, M J HEADLAM, K OZAWA and PROFESSOR G OTTING with Professor R Dean, University of Canberra; Dr K Rogers, Heart Research Institute, Sydney; Dr A V Kralicek, HortResearch, Auckland, NZ; and Dr M Pavlov and Professor M Ehrenberg, University of Uppsala, Sweden

Mass spectrometry of protein-protein and protein-DNA complexes by DRS N E DIXON, P M SCHAEFFER, MS K V LOSCHA and MS A Y PARK with Dr J L Beck, Mr S J Watt and Professor M M Sheil, Department of Chemistry, University of Wollongong

Mechanisms of termination of DNA replication by DRS N E DIXON, P M SCHAEFFER, A J OAKLEY and MR M MULCAIR with Dr D C Neylon, Department of Chemistry, University of Southampton, UK; Dr A V Kralicek, HortResearch, Auckland, NZ; and Professor T M Hill, School of Medicine and Health Sciences, University of North Dakota, USA

Near-perfect rubber by DR N E DIXON with Dr C M Elvin, CSIRO Division of Livestock Industries, Brisbane

Properties and structures of proteins circularised by intein-mediated reactions by DRS N E DIXON, P PROSSELKOV, N K WILLIAMS, P D CARR, MS A Y PARK, MR B BANCIA, PROFESSOR G OTTING and PROFESSOR D L OLLIS with Dr J M Matthews, School of Molecular and Microbial Biosciences, University of Sydney; Dr J L Beck, Mr S J Watt and Professor M M Sheil, Department of Chemistry, University of Wollongong; Dr E Liepinsh, Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm, Sweden; Mr D Spencer and Dr H-X Zhou, Institute of Molecular Biophysics, Florida State University, USA; and Drs A Rak and K Alexandrov, Department of Physical Biochemistry, Max-Planck-Institute for Molecular Physiology, Dortmund, Germany

QOR quinone reductase structure and mechanism by DRS N E DIXON, P PROSSELKOV and R D WEBSTER with Dr J-I Mano, Faculty of Agriculture, Yamaguchi University, Japan

Spectroscopic studies of the proofreading exonuclease subunit of DNA polymerase III by DR N E DIXON and MS A Y PARK with Dr G Schenk, Department of Chemistry; and Professor G R Hanson, Centre for Magnetic Resonance, University of Queensland

Structural genomics of integron proteins by DRS N E DIXON, P M SCHAEFFER, MR P WU and PROFESSOR G OTTING with Drs B Mabbutt, H Stokes and Mr A Robinson, Department of Chemistry, Macquarie University; and Dr Zs Dosztányi, Institute of Enzymology, Budapest, Hungary

Structure and mechanism of action of proline aminopeptidase by DRS N E DIXON, P M SCHAEFFER and MS P E LILLEY with Professor H C Freeman and Dr J M Guss, School of Molecular and Microbial Biosciences, University of Sydney

Structure of DnaG primase by DRS N E DIXON, A J OAKLEY, P PROSSELKOV, P M SCHAEFFER, MR B BANCIA, MS K V LOSCHA and PROFESSOR G OTTING with Dr M C J Wilce, University of Western Australia; and Dr E Liepinsh, Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm, Sweden

Structures and functions of the *Escherichia coli* replicase by DRS N E DIXON, A J OAKLEY, K OZAWA, P PROSSELKOV, MR S JERGIC, MS A Y PARK and PROFESSOR G OTTING with Drs K Kongsuwan and G Wijffels, CSIRO Division of Livestock Industries, Brisbane; and Drs R Rothnagel and B Hankamer, Institute for Molecular Biosciences, University of Queensland

Structures of complexes of the proofreading exonuclease subunit of DNA polymerase III by DRS N E DIXON, M A KENIRY, G PINTACUDA, PROFESSOR G OTTING and MS A Y PARK with Dr E Liepinsh, Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm, Sweden

Structures of the *Escherichia coli* DnaB helicase protein and the DnaB•DnaC complex by DRS N E DIXON, P M SCHAEFFER and MS K V LOSCHA with Professor J M Carazo, Drs L E Donate, M Barcéna and Ms Y Robledo, Centro Nacional de Biotecnologia, Universidad Autonoma, Madrid, Spain

Nuclear Magnetic Resonance

Defining the structure of a proteins involved in the onset of breast cancer by DR M A KENIRY with Professor C C Benz and Dr G Scott, Buck Institute for Age Research, Novato, California, USA Supported by a travel grant from the International Union Against Cancer

The association of calothrixin with DNA by DR M A KENIRY and MS E A OWEN with Drs C Chai, M Waring and G Smith, Department of Chemistry, ANU

Structural Biology

Glutathione transferases from the malaria vector *Anopheles dirus* Their pesticide binding and detoxifying properties by DR A J OAKLEY with Dr Albert Ketterman, Mahidol University, Thailand

Haloalkane dehalogenases-structure and function of bioremediation enzymes of the α/β hydrolase family by DR A J OAKLEY with Dr Jiri Damborsky, Masaryk University, Brno, Czech Republic

Structure of cofactor-free oxygenases by DR A J OAKLEY with Professor S Fetzner, University of Oldenburg, Germany

Structure of tomato *endo*-β-mannanase by DR A J OAKLEY with Dr R Bourgault and Professor J D Bewley, University of Guelph, Canada

Protein Crystallography and Engineering

Structural studies of the β IL5 receptor by PROFESSOR D L OLLIS, MR J M MURPHY and DR P D CARR with Professor I G Young, John Curtin School of Medical Research, ANU

Structural studies of the PII and GlnK proteins by PROFESSOR D L OLLIS and DR P D CARR with Drs S G Vasudevan and Y Xu, James Cook University, Queensland

Structure function studies with esterases by PROFESSOR D L OLLIS with Dr J Oakeshott, CSIRO, Department of Entomology, Canberra, ACT

Biomolecular NMR

Analysis of the oligomerisation interface of the PYRIN domain by PROFESSOR G OTTING and MR P WU with Dr J Sagara, M Moriya and S Taniguchi, Osaka University, Japan; and Dr E Liepinsh, Karolinska Institute, Stockholm, Sweden

Cross-correlated DSA/CSA relaxation by PROFESSOR G OTTING and DR G PINTACUDA with Dr A Kaikkonen, Karolinska Institute, Stockholm, Sweden

Determination of the three-dimensional structure of pig Cox-17 by PROFESSOR G OTTING, with Drs E Liepinsh and R Sillard, Karolinska Institute, Stockholm, Sweden

Determination of the three-dimensional structure of WIF-1 by PROFESSOR G OTTING, with Dr E Liepinsh, Karolinska Institute, Stockholm, Sweden; and Professor L Patthy, Hungarian Academy of Sciences, Budapest, Hungary

Fast structure-based assignment of ^{15}N-HSQC spectra of selectively ^{15}N-labeled paramagnetic proteins by PROFESSOR G OTTING, DRS G PINTACUDA, M A KENIRY, N E DIXON and MS A Y PARK with Dr T Huber, University of Queensland

Protein-labelling with paramagnetic ions by PROFESSOR G OTTING and DR G PINTACUDA with Dr A Moshref, Karolinska Institute, Stockholm; and Drs A Leonchicks and A Sharipo, University of Latvia

Study of protein hydration by high-resolution NMR and MRD by PROFESSOR G OTTING with Dr E Liepinsh, Karolinska Institute, Stockholm, Sweden; Dr K Modig and Dr B Halle, University of Lund, Sweden

Thermodynamic and kinetic analysis of a cyclized protein by PROFESSOR G OTTING, DRS N E DIXON, N K WILLIAMS and P PROSSELKOV with Drs J M Matthews and P Attard, University of Sydney; Mr S J Watt and Dr J L Beck, University of Wollongong; and Dr E Liepinsh, Karolinska Institute, Stockholm, Sweden

3D structure determination of human coactosin-like protein by PROFESSOR G OTTING with Drs E Liepinsh, M Rakonjac, B Samuelsson and O Rådmark, Karolinska Institute, Stockholm, Sweden; and Dr O Provost and V Boissoneault, Centre de Recherche du CHUL, Ste-Foy, QC, Canada

3D structure determination of the helicase-binding domain of *E coli* primase by PROFESSOR G OTTING, DRS N E DIXON, P M SCHAEFFER, A J OAKLEY, G PINTACUDA and MS K V LOSCHA with Dr M C J Wilce, University of Western Australia; and Dr E Liepinsh, Karolinska Institute, Stockholm, Sweden

Inorganic Chemistry

Coordination Chemistry and Spectro-electro Chemistry

Computational modelling of electrochemical responses by DR P J MAHON with Assoc. Professor D K Cope, North Dakota State University, USA; and Professor K B Oldham, Trent University, Ontario, Canada

Corrosion analysis and conservation treatments by DRS G A HEATH and P J MAHON with Professor D C Creagh, University of Canberra; and Dr V Otiengo-Alego, AFP Forensic Laboratories, Weston, ACT

Paintings and textiles; spectroscopic means of analysis by DRS G A HEATH, P J MAHON and MS M E KUBIK with Dr R Maxwell, Art History, ANU; Dr M Sterns, Chemistry, ANU; Ms D Ward, Australian National Gallery; Professor D C Creagh, University of Canberra; Dr V Otiengo-Alego, AFP Forensic Laboratories, Weston, ACT; and Dr D J Fyffe, Varian Analytical Instruments, Melbourne

Redox-modulation of metal cluster compounds by DRS G A HEATH, A J EDWARDS, P J MAHON and MR S B LEE with Dr S P Best and Mr M Bondin, University of Melbourne; and Dr G Foran, Australian National Beamline Facility, KEK, Tsukuba, Japan

Spectro-electrochemical and theoretical investigation of binuclear and tetranuclear arrays by DR G A HEATH with Dr J E McGrady and Dr S Z Knottenbelt, University of York, UK

Inorganic Stereochemistry and Asymmetric Synthesis

Tertiary arsine adducts of iodoarsines: A structural and theoretical investigation by PROFESSORS A D REA, S B WILD, DRS A C WILLIS and X-T ZHOU with Drs S Petrie and R Stranger, Department of Chemistry, The Faculties

Solid State Inorganic Chemistry

A composite modulated structure approach to hollandites by PROFESSOR R L WITHERS with Ms M Carter, Australian Nuclear Science and Technology Organisation, Menai, NSW

A low temperature electron diffraction study of structural disorder and its relationship to the Kondo effect in UAsSe by PROFESSOR R L WITHERS with Professor J Schoenes, Technical University Braunschweig, Germany

Atomic ordering in doped, rare earth cobaltates by PROFESSOR R L WITHERS with Dr M James, Australian Nuclear Science and Technology Organisation, Menai, NSW

Composition induced structural phase transitions in the $(Ba_{1-x}La_x)_2In_2O_{5+x}$ ($0 \leq x \leq 0.6$) system by PROFESSOR R L WITHERS and DR Y LIU with Drs A Pring and C Tenailleau, South Australian Museum; and Professor M Carpenter, University of Cambridge, UK

Constrained refinement techniques for problem crystal structure refinements by PROFESSOR A D RAE with Dr K J Haller and Ms W Somphon, Suranaree University of Technology, Nakhon Ratchisima, Thailand

Oxygen/fluorine ordering in $Nb_3O_5F_5$ by PROFESSOR R L WITHERS and MR F BRINK with Mr S Cordier, University of Rennes, France

Refinement of crystal structures showing twinning and disorder by PROFESSOR A D RAE with Dr S W Ng, University of Malaya, Kuala Lumpur, Malaysia

Organic Chemistry

Synthesis and Mechanism

Biotransformations by PROFESSOR M G BANWELL and MR D W LUPTON with Dr G M Whited, Genencor International Inc, Palo Alto, California, USA

Chemoenzymatic routes to novel dendritic architectures suitable for pharmaceutical applications by PROFESSOR M G BANWELL and MS L FEARNSIDE with Drs G Krippner and T McCarthy, Starpharma Ltd, Melbourne

Studies in biologically active alkaloid analogue synthesis by PROFESSOR M G BANWELL and MR M O SYDNES with Dr C Burns, Cytopia Pty Ltd, Melbourne; and Professor C Parish, John Curtin School of Medical Research, ANU

The development of chemoenzymatic methods for the selective elaboration of polyfunctionalised therapeutic agents to oligomers with improved efficacy by PROFESSOR M G BANWELL and MR M P FRIEND with Dr J Lambert, Biota Chemistry Laboratories, Melbourne

The development of new, non-steroidal anti-asthma drugs with novel modes of action by PROFESSOR M G BANWELL with Dr A Stewart, Cryptopharma Pty Ltd, Melbourne

The development of novel carbohydrate-like drugs by PROFESSOR M G BANWELL, DRS M BONNET, A KREIPL and J RENNER with Drs R H Don and V Ferro, Progen Industries Ltd, Brisbane

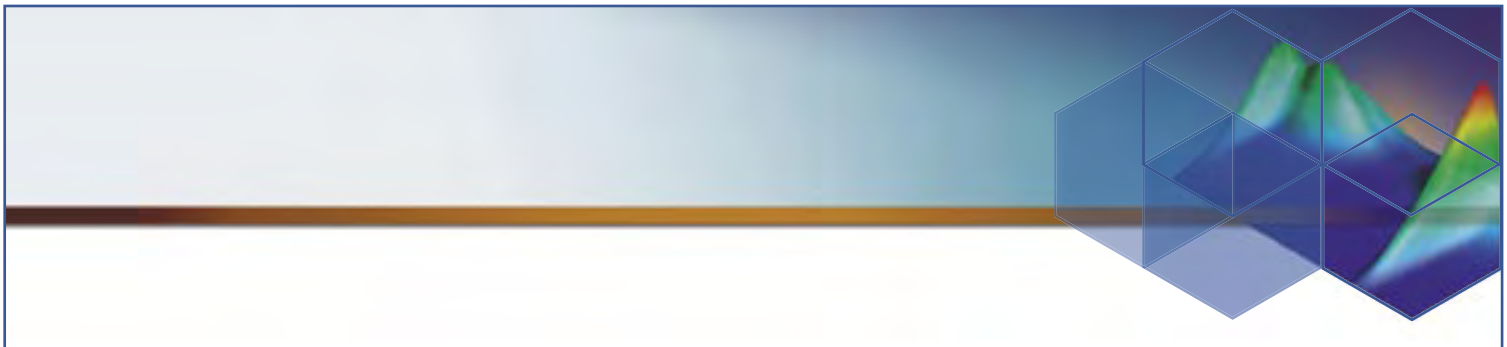
The total synthesis of biologically active marine alkaloids from the Great Barrier Reef by PROFESSOR M G BANWELL, DRS M BACKES and S GROSS with Assoc. Professor M J Garson, Department of Chemistry, University of Queensland; and Dr C Burns, Cytopia Pty Ltd, Melbourne

The total synthesis of biologically active natural products by PROFESSOR M G BANWELL and MR S CHAND with Dr G P Savage, CSIRO Molecular Science, Melbourne; Professor C Parish, John Curtin School of Medical Research, ANU; and Professor G Dannhardt, Institute of Pharmacy, University of Mainz, Germany

Biochemical Reactions and Molecular Recognition

Activators and inhibitors of ryanodine receptor calcium ion channels by PROFESSOR C J EASTON and DR J K ROBINSON with Professor A Dulhunty and Dr M Casarotto, John Curtin School of Medical Research, ANU; and Dr M Miller, Biotron, Canberra

Cycloaddition reactions of nitrile oxides by PROFESSOR C J EASTON with Drs G P Savage and G W Simpson, CSIRO Molecular Science, Melbourne



Free radical reactions by PROFESSOR C J EASTON, MR B J W BARRATT, MR A J HERLT, MS I LI, MR A J MORTIMER, DR J S SIMPSON, MS Y-C TSAI, MR Z WATTS and DR A WRIGHT with Mr M Taylor, ANUTECH Pty Ltd; Business ACT; Professor L Radom, University of Sydney; Dr R O'Hair, University of Melbourne; and Professor C Schofield, Oxford University, UK

Lipid chemistry by PROFESSOR C J EASTON with Professors A Ferrante and A Poulos, Adelaide Medical Centre for Women and Children, SA

Lipid modified coordinating ligands by PROFESSOR C J EASTON and DR M R NAIRN with Dr J Altin, Division of Biochemistry and Molecular Biology, ANU; and Lipotek Pty Ltd, Canberra

Macrocyclic chemistry by PROFESSOR C J EASTON with Professor R Keene, James Cook University; and Professor L Lindoy, University of Sydney

Supramolecular chemistry of cyclodextrins by PROFESSOR C J EASTON, MS L BARR, MS S BOWEN, MS M M CIESLINSKI, MR R DAWSON, MR A J HERLT and DR J S SIMPSON with Professor S F Lincoln, Ms J S Locke, Mr B L May and Ms J Patrick, University of Adelaide

Synthetic enzymes for synthetic chemistries by PROFESSOR C J EASTON with Dr J Oakeshott and Dr R Russell, CSIRO Entomology; and Dr G W Simpson, CSIRO Molecular Science

Towards improved melamine-urea-formaldehyde resins by PROFESSOR C J EASTON and MS A PHILBROOK with Dr N Dunlop, Orica Adhesives and Resins, Melbourne, through the UnIChe program

Organic Synthesis

Biosynthetic, structural and metabolic studies on gibberellins by PROFESSOR L N MANDER and MR B TWITCHIN with Professor R P Pharis, Department of Biology, University of Calgary, Canada; Drs M Koshioka and M Nakayama, Department of Genetics and Physiology, National Institute of Floricultural Science, Tsukuba, Japan

Structural and biosynthetic studies on antheridiogens from fern gametophytes by PROFESSOR L N MANDER with Dr J Banks, Department of Botany and Plant Pathology, University of Purdue, USA; Dr J Nester, Department of Biological Sciences, Sam Houston State University, Texas, USA

Studies on gibberellin receptors by PROFESSOR L N MANDER and MR J R CROW with Dr P M Chandler, CSIRO Division of Plant Industry, Canberra, ACT

Studies on growth inhibition and flowering by PROFESSOR L N MANDER and MR B TWITCHIN with Drs L T Evans and R W King, CSIRO Division of Plant Industry, Canberra; and Professor R P Pharis, University of Calgary, Canada

Organic Synthesis, Methodology and Host-guest Chemistry

Cavitand boronic acids by DR M S SHERBURN and MS E S BARRETT with Dr P Duggan, Molecular Engineering Program, CSIRO Molecular Science, Melbourne

Cavitand coordination cages by DRS M S SHERBURN and D J SINCLAIR with Professor P J Stang and Dr H Jude, Department of Chemistry, University of Utah, UT, USA

Himbacine muscarinic receptor antagonists by DRS M S SHERBURN, MR L S-M WONG and MR T N CAYZER with Hon Assoc. Professor F J Mitchelson, Department of Pharmacology, University of Melbourne

New horizons in Diels–Alder chemistry by DRS M S SHERBURN, R TRIPOLI and A D PAYNE with Emeritus Scientia Professor M N Paddon-Row and Dr D Moran, School of Chemical Sciences, University of New South Wales

Physical and Theoretical Chemistry

Theoretical Chemical Physics

Chemical reaction dynamics by PROFESSOR M A COLLINS, with Assoc. Professor D H Zhang, National University of Singapore; Dr M Brouard, Oxford University, UK; and Dr J F Castillo, Universidad Complutense de Madrid, Spain

Construction of the energy surfaces for multiple electronic states by PROFESSOR M A COLLINS, with Professor Mark Gordon and Ms Heather Netzloff, Iowa State University, USA

Nonabiabatic dynamics and coupled potential energy surfaces by PROFESSOR M A COLLINS, with Professor D Yarkony, Johns Hopkins University, USA; and Associate Professor D H Zhang, National University of Singapore

Quantum scattering of hydrogen and methane on a nickel surface by PROFESSOR M A COLLINS, with Dr C Crespos and Professor G-J Kroes, University of Leiden, Netherlands

Computational Quantum Chemistry Polymer Chemistry

Combined experimental/theoretical studies of RAFT polymerization by DR M L COOTE with Professor T P Davis, Dr Achim Feldermann, Dr M H Stenzel, Dr C Barner-Kowollik and Mr H Chaffey-Millar, Centre for Advanced Macromolecular Design, University of New South Wales

Degradation Resistant PVC by DR M L COOTE with Professor A J Schouten, Ms J Purmova, Ms K F D Pauwels, Ms W van Zoelen, and Dr J E Vorenkamp, Department of Polymer Science, University of Groningen, The Netherlands

Copolymerization Kinetics by DR M L COOTE with Professor T P Davis, and Dr C Barner-Kowollik, Centre for Advanced Macromolecular Design, University of New South Wales; Dr P Vana, Georg-August-Universität Göttingen, Germany; and Professor K Matyjaszewski, Carnegie Mellon University, Pittsburg PA, USA

Reactions catalyzed by vitamin B_{12} by PROFESSOR L RADOM, MR G SANDALA and DR M L COOTE with Dr D Smith, Rudjer Boskovic Institute, Zagreb, Croatia

Bond dissociation energies by DR M L COOTE and PROFESSOR L RADOM with Professor A Pross, Ben Gurion University, Israel

Liquid State Chemical Physics

Chaos and nonequilibrium statistical mechanics by PROFESSOR D J EVANS with Professor L Rondoni, Politecnico Di Torino, Italy

Derivation of potential models for phase equilibria by DR J P DELHOMMELLE with Dr P Millie, Laboratoire Francis Perrin, France

Fluctuation theorem by PROFESSOR D J EVANS, DRS E MITTAG, E M SEVICK and G M WANG with Dr D J Searles, Griffith University, Brisbane

Laser and Optical Spectroscopy

Multi-dimensional spectroscopy of PSII protein sub-assemblies by PROFESSOR E KRAUSZ with Dr R Pace, Department of Chemistry, ANU; Dr M Seibert, NREL, Golden Colorado, USA

EPR and optical spectroscopy of thermophillic PSII from *Synechococcus vulcanus* by PROFESSOR E KRAUSZ with Dr R Pace Department of Chemistry, ANU; Professor J-R Shen, Riken Institute, Hyogo, Japan; and Dr S Peterson Årksöld, University of Lund Sweden

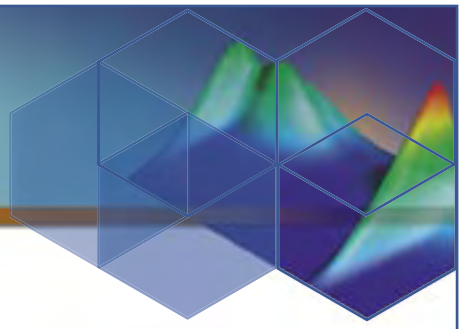
Magneto-optical spectroscopy of cytochrome b_6f by PROFESSOR E KRAUSZ with Professor S Peterson Årksöld, Professor J F Allen, Dr J Ström, University of Lund, Sweden

Spectroscopy of mutants of the *Rhodopseudomonas viridis* bacterial reaction centre by PROFESSOR E KRAUSZ with Professor J Norris, Mr R Baxter, and Dr N Ponomarenko, University of Chicago, USA

Light induced changes in single crystals of *Rhodopseudomonas viridis* by PROFESSOR E KRAUSZ with Professor J Norris, Mr R Baxter, University of Chicago, USA

Spectroscopy of CP47 Mutants of the *syn 6803cyanobacteria*; investigating the trap state by PROFESSOR E KRAUSZ with Professor J Eaton-Rye, Otago University, NZ

Narrow band hole-burning in active Photosystem II by PROFESSOR E KRAUSZ and MR J HUGHES with Professor H Riesen, University College UNSW, ADFA, ACT



Spectroscopy of New Chromium(III) Hole-burning materials by PROFESSOR E KRAUSZ and MR J HUGHES with Professor H Riesen, University College UNSW, ADFA, ACT

Development of the new generation MCD Metallo-Enzyme Spectrometer by PROFESSOR E KRAUSZ with Dr M Riley, University of Queensland; and Alex Stanco, CEO LASTEK Adelaide

Physical and optical properties of self-assembled Si nanocrystals by PROFESSOR E KRAUSZ with Professor R Elliman, RSPhysSE ANU; and Professor S H Choi, Kyung Hee University, Korea

Computational Quantum Chemistry

Solvation of glycyl radicals by PROFESSOR L RADOM, with Mr G P F Wood, University of Sydney; and Professor M S Gordon, Iowa State University, USA

Thermochemistry of metal oxides and hydroxides by PROFESSOR L RADOM with Dr N L Haworth, University of Sydney; Professor A K Wilson, University of North Texas, USA; and Professor J M L Martin, Weizmann Institute, Israel

Oxidative damage to proteins by PROFESSORS L RADOM, C J EASTON and DR M L COOTE with Mr G P F Wood and Dr D Moran, University of Sydney; Dr R Jacob, RMIT University; Dr M Davies, Heart Research Institute, Sydney; Associate Professor R A J O'Hair, University of Melbourne; and Professor A Rauk, University of Calgary, Canada

Reactions catalysed by vitamin B_{12} by PROFESSOR L RADOM and DR M L COOTE with Professor B T Golding, University of Newcastle upon Tyne, UK; Dr D M Smith, Rudjer Boskovic Institute, Zagreb, Croatia; and Dr S D Wetmore, Mount Allison University, Canada

Development of improved theoretical procedures by PROFESSOR L RADOM with Mr G P F Wood, University of Sydney; and Professor G A Petersson, Wesleyan University, USA

Interaction of calcium dications with molecules of biological interest by PROFESSOR L RADOM with Ms I Corral, Professor M Yanez and Professor O Mo, Autonoma University of Madrid, Spain

Carbapenem biosynthesis by PROFESSORS L RADOM, C J EASTON, and MR G M SANDALA with Dr M Topf, University of California, San Francisco, USA; Dr D M Smith, Rudjer Boskovic Institute, Zagreb, Croatia; and Professor C J Schofield, University of Oxford, UK

Disordered Materials

Neutron diffuse scattering and Monte Carlo study of the relaxor ferroelectric $PbZn_{1/3}Nb_{2/3}O_3$ (PZN) by PROFESSOR T R WELBERRY and DR D J GOOSSENS with Dr M J Gutmann, ISIS Facility, Rutherford Appleton Laboratory, Oxfordshire, UK; Dr H Woo and Dr G Xu, Physics Department, Brookhaven National Laboratory, New York, USA; and Dr C Stock, Department of Physics, University of Toronto, Ontario, Canada

Diffuse scattering from benzil, $C_{14}H_{10}O_2$ by PROFESSOR T R WELBERRY and DR D J GOOSSENS with Professor W I F David and Dr M J Gutmann, ISIS, Rutherford Appleton Laboratory, Oxfordshire, UK

Diffuse scattering in zeolites by PROFESSOR T R WELBERRY with Dr B Campbell, Department of Physics and Astronomy, Brigham Young University, Utah, USA

High-pressure X-ray scattering of oxides with a nanoscaled local structure by PROFESSOR T R WELBERRY with Dr J Kreisel, Laboratoire Matériaux et Génie Physique, ENS de Physique de Grenoble, France; Professor A M Glazer, Clarendon Laboratory, Oxford, UK; and Dr P A Thomas, Department of Physics, University of Warwick, UK

Phonon softening in benzil by DR D J GOOSSENS with Dr M E Hagen, SNS, Oak Ridge, USA

Structure and magnetism in disordered perovskite oxides, focussing on cobaltates by DR D J GOOSSENS and PROFESSOR R L WITHERS with Dr M James, ANSTO, Sydney; and Dr K F Wilson, Physics Department, ANU

Magnetic Structure in $RNiAl_4$ (R = rare earth) by DR D J GOOSSENS with Dr W Hutchison, University College, UNSW (ADFA) ACT

Diffuse neutron scattering and structural phase transition in *p*-terphenyl, by DR D J GOOSSENS and PROFESSOR T R WELBERRY with Dr M J Gutmann, ISIS, UK

Magnetic ordering in dicyanamide coordination polymers by DR D J GOOSSENS with Dr S Batten, Monash University

Solid State Molecular Science

The interface between complex fluids and solids by DR P A REYNOLDS, PROFESSOR J W WHITE, DRS M J HENDERSON, J ZANK and MR K BARANYAI with Dr S A Holt, Rutherford Appleton Laboratory, Oxford, UK; and Dr D Tunaley, Orica Ltd, Australia

Making film stars-nanocomposite films for solar energy capture by DR M J HENDERSON, and PROFESSOR J W WHITE with Dr A Gibaud and Dr J-F Bardeau, Laboratoire de Physique de l'Etat Condensé, Le Mans, France; and Dr A R Rennie, Uppsala University, The Studsvik Neutron Research Laboratory, Sweden — Innovation Access Programme (CG050120)

Conformation of proteins at interfaces by PROFESSOR J W WHITE and DR M J HENDERSON with Dr S A Holt, Rutherford Appleton Laboratory, Oxford, UK

Kinetics of template action in silicalite synthesis by PROFESSOR J W WHITE with Dr L Iton, Argonne National Laboratory, Chicago, USA

Millisecond X-ray reflectometer for ChemMatCARS by PROFESSOR J W WHITE and DR M J HENDERSON with Dr R Garrett, ANSTO, Sydney; and Dr J Viccaro, University of Chicago, USA

Nanostructure of milk membrane and proteins by PROFESSOR J W WHITE with Dr S A Holt, Rutherford Appleton Laboratory, UK; and Dr B Cox, Dairy Research Corporation, Melbourne

Structure of high internal phase emulsions by PROFESSOR J W WHITE, DRS P A REYNOLDS, M J HENDERSON, J ZANK and MR K BARANYAI with Drs R Goodridge, C Such, Orica Ltd, Australia; and Mr A Fontaine, FIUPSO, France

Structure of polymer surfactant films by PROFESSOR J W WHITE with Dr J Penfold, Rutherford Appleton Laboratory, Oxford, UK

X-ray small angle scattering from whole blood and haemoglobin by PROFESSOR J W WHITE with Dr C Garvey, Department of Biochemistry, University of Sydney

Titania and zirconia composite thin films by PROFESSOR J W WHITE and DR M J HENDERSON with Professor A R Rennie, NFL, Studsvik, Uppsala Universitet, Sweden; and Mr N Rosier, FIUPSO, France

Structure of inorganic catalyst films by PROFESSOR J W WHITE with Dr J Bartlett, ANSTO, Sydney

Structure of polymer clay-composites by PROFESSOR J W WHITE with Dr E Gilbert, ANSTO, Sydney

Structure of polymer composites by PROFESSOR J W WHITE with Dr D Martin, Department of Chemical Engineering, University of Queensland

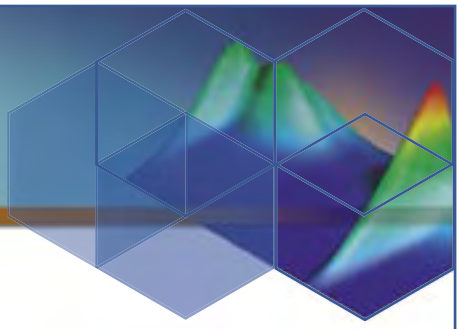
Proposal for an X-ray liquid surface reflectometer by PROFESSOR J W WHITE with Dr M Schlossman, University of Illinois, Chicago and CARS Synchrotron Consortium, Argonne National University, USA

The following collaborators visited the group during 2004 to conduct X-ray reflectometry experiments: Dr W Fullagar University of Queensland; Dr V James Hon Visiting Fellow, RSC; Dr C Garvey University of Sydney; Dr K Latham RMIT University, Melbourne; Drs V Luca and M James, ANSTO, Sydney; Dr D Martin, University of Queensland; Dr A Whittaker, University of Queensland; Dr G Warr, University of Sydney; Dr J Ruggles, University of Queensland; Professor R Amal, University of NSW, and Dr Y Chen, RSPhysSE, ANU; Dr L Graham, CSIRO, Mr B Finnegan, University of Queensland; Ms L Rodgers, UNSW and Dr R Knott, ANSTO

Electrochemistry

Corrosion of copper in potable water systems by DR R D WEBSTER with Dr A G Christy, Department of Geology, ANU; Dr A Lowe and Mr M Stoll, Department of Engineering, ANU; and Dr V OtienoAlego, AFP Forensic Laboratories, Weston, ACT

Electrochemistry and EPR spectroscopy of transition metal complexes containing bridging thiolate ligands by DR R D WEBSTER with Dr L Y Goh, National University of Singapore



Academic Visitors

The David Craig Lecturer

Stang, Professor Peter J BSc *Alberta* PhD, *California Berkeley*. Dean, College of Science, University of Utah. Distinguished Professor of Chemistry, University of Utah; Senior Fellow, Loker Hydrocarbon Research Institute, University of Southern California

The Birch Lecturer

Grubbs, Professor Robert H BSc MSc *University of Florida* PhD *Columbia University*; Victor and Elizabeth Atkins Professor of Chemistry, California Institute of Technology

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:

Adams, Dr Joanne formerly of the Research School of Chemistry

Bosnich, Professor Brice Department of Chemistry, University of Chicago, USA

Brown, Dr Susan CSIRO Entomology (Biotechnology)

Constable, Professor Edwin Institut für Anorganische Chemie, Switzerland

Crossley, Professor Max School of Chemistry, University of Sydney

Dubicki, Dr Lucjan Australian National University

Gilbert, Dr Elliot Neutron Scattering Group, ANSTO

Gordon, Professor Mark Department of Chemistry, Iowa State University, USA

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

Hanley, Professor Howard NIST, Colorado, USA

Harper, Dr Jason School of Chemical Sciences, University of New South Wales

Hoshino, Dr Masaru Institute for Protein Research, Osaka University, Japan

Hueller, Professor Alfred Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen Nürnberg, Germany

Jones, Professor Keith School of Chemical and Pharmaceutical Sciences, Kingston University, UK

Liu, Dr Xiaoheng Materials Chemistry Laboratory, Nanjing University of Science and Technology, China

Loong, Dr David formerly of the Research School of Chemistry

Mahon, Dr Peter Department of Chemistry, University of Canberra

Majewski, Professor Marek Department of Chemistry, University of Saskatchewan, Canada

Netzloff, Dr Heather Department of Chemistry, Iowa State University, USA

Nixon, Professor John School of Chemistry, Physics & Environmental Science, University of Sussex, UK

Schaumann, Professor Dr Ernst Institut für Organische Chemie, Der Technsichen Universität Clausthal, Germany

Schmidbaur, Professor Dr Hubert Technical University of Munich, Inorganic Chemistry Institute, Germany

Storey, Dr John Department of Chemistry, University of Aberdeen

Research Seminars

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

Abell, Professor Chris Cambridge University, UK

Attard, Dr Phil University of Sydney

Berners-Price, Professor Sue University of Western Australia

Biedron, Dr Sandra G Argonne National Laboratory, USA

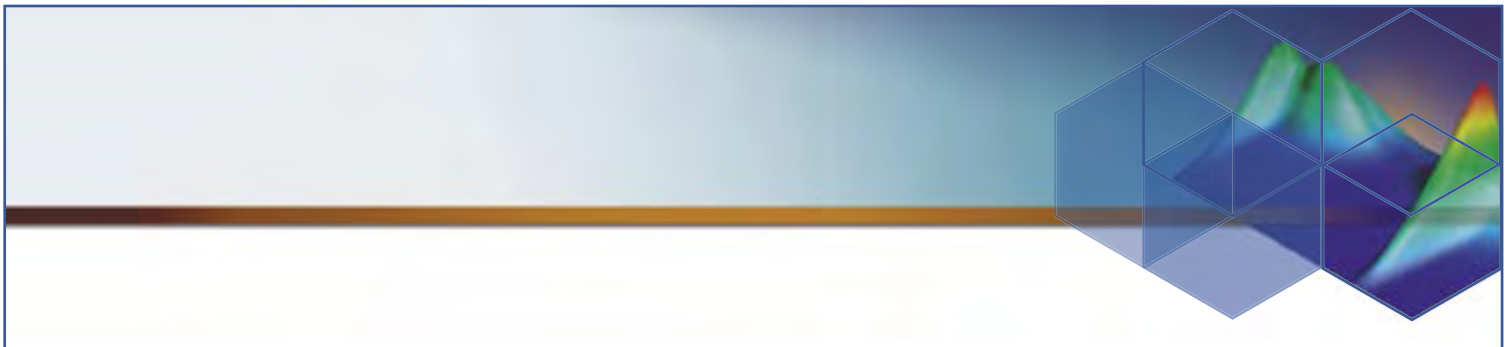
Broeer, Dr Stefan School of Biochemistry and Molecular Biology, ANU

Cavigliasso, Dr German Inorganic Computational Chemistry Group, Dept of Chemistry ANU

Deacon, Professor Glen Monash University, Melbourne

De Voss, Dr James Dept of Chemistry, University of Queensland

Fairlie, Professor David University of Queensland
Georges, Dr Cedric Bio-Logic, Grenoble, France
Gomperts, Dr Roberto Senior Scientist, SGI, Hudson, USA
Griesinger, Professor Christian Director, Max-Planck Institute for Biophysical Chemistry, Göttingen, Germany
Hill, Dr Justine M Institute for Molecular Bioscience, University of Queensland
Jaspars, Professor Marcel University of Aberdeen, UK
Jones, Professor Cameron Dept of Chemistry, Cardiff University, UK
Kepert, Dr Cameron J School of Chemistry, University of Sydney
King, Assoc. Professor Bruce University of Newcastle
Larkins, Professor Frank Deputy Vice Chancellor, University of Melbourne
Maclaga, Dr Robert N University of Canterbury, NZ
Mathesius, Dr Ulrike School of Biochemistry and Molecular Biology, ANU
Milton, Dr Stephen V Argonne National Laboratory, USA
Moore, Dr Evan Dept of Physics, University of Queensland
McLachlan, Dr Matthew Dept of Chemistry, University of Cambridge, UK
Neuman, Dr Dan A Gaithersburg, Maryland, USA
Nugent, Professor Keith University of Melbourne
Richard O'Hair, Assoc. Professor School of Chemistry, University of Melbourne
Paterson, Professor Ian University of Cambridge, UK
Paul, Dr Fred Institute of Chemistry, Dept of Chemistry, University of Rennes, France
Petrosyan, Professor Valery MV Lomonosov University, Moscow
Radt, Dr Benno University of Melbourne
Reimers, Dr Jeff School of Chemistry, University of Sydney
Saint, Professor Robert Research School of Biological Sciences, ANU
Scammells, Professor Peter Monash University
Steel, Professor Peter University of Canterbury, NZ
Takeda, Professor Masuo Toho University, Japan
Taylor, Professor Richard Dept of Chemistry, University of York, UK
Thordarson, Dr Pall School of Chemistry, University of Sydney
Turner, Dr Craig Royal Australian Chemical Institute and 2003 Cornforth Medallist
Tuite, Dr Eimer Physical Chemistry, School of Natural Sciences, University of Newcastle-upon-Tyne, UK
Spackman, Professor Mark Chemistry, School of Biological, Biomedical and Molecular Sciences, University of New England, Armidale
Viau, Dr Lydie Department of Chemistry, ANU
von Itzstein, Professor Mark Institute for Glycomics, Griffith University
Wiley, Dr Veronica The Children's Hospital, Westmead
Williams, Professor Jim Director, Research School of Physical Sciences and Engineering, ANU
Willis, Professor Christine University of Bristol, UK
Wong, Professor Henry Dept. of Chemistry, Hong Kong
Xu, Dr Yibin Discipline of Biochemistry and Molecular Biology, James Cook University
Yablonsky, Professor Gregory Dept of Chemical Engineering, Washington University in St Louis, USA
Zard, Professor Samir Dept D'enseignement et de Recherche de Chimie Ecole Polytechnique, Palaiseau Cedex, France



Conference Presentations

Biological Chemistry

Protein Structure and Function

29th Lorne Conference on Protein Structure and Function, Lorne, Victoria, 8–12 February. The following posters were presented:
A Y Park, P Prosselkov, G Pintacuda, M A Keniry, P D Carr, D L Ollis, G Otting and N E Dixon: *Stabilization of the proofreading exonuclease subunit of E coli DNA polymerase III by backbone cyclization*

G Pintacuda, M A Keniry, T Huber, A Y Park, N E Dixon and G Otting: *Fast methods for NMR in structural biology*

P M Schaeffer, K Loscha, A J Oakley, E Liepinsh, B Bancia, M C J Wilce, G Otting and N E Dixon: *Primase-helicase interaction in the Escherichia coli replisome*

3rd East Coast *Bacillus* Meeting, Newcastle, New South Wales, 27 August. The following invited lectures were presented:
S Jergic: *Subunit interactions in DNA polymerase III*

K V Loscha: *Primase-helicase interactions*

P M Schaeffer: *Introduction to the E coli replisome*

ComBio2004, Perth, Western Australia, 26–30 September. The following invited lectures were presented:
K Loscha, A J Oakley, P M Schaeffer, E Liepinsh, M C J Wilce, G Otting and N E Dixon: *Structure and function of the DnaB binding domain of Escherichia coli primase*

S J Watt, N K Williams, P Prosselkov, G Otting, N E Dixon, M M Sheil and J L Beck: *Comparison of ^{1}H–^{2}H exchange kinetics of linear and cyclized DnaB-N (helicase) using mass spectrometry*

The following posters were presented:
M J Headlam, K Ozawa, D Mouradov, T Huber, S J Watt, J L Beck, K J Rodgers, R T Dean, G Otting and N E Dixon: *Translational incorporation of dihydroxyphenylalanine into proteins*

K Ozawa, S Jergic, M J Headlam, P M Schaeffer, G Otting and N E Dixon: *In vitro cell-free protein synthesis for NMR studies of protein–ligand interactions*

A Y Park, G Pintacuda, M A Keniry, P D Carr, P Prosselkov, D L Ollis, G Otting and N E Dixon: *Structure and function of cyclized versions of the proofreading exonuclease subunit of E coli DNA polymerase III*

A Robinson, P S-C Wu, S J Harrop, P M Schaeffer, N E Dixon, M R Gillings, A J Holmes, K M H Nevalainen, G Otting, H W Stokes, P M G Curmi and B C Mabbutt: *New proteins from the mobile genome: structural definitions of function*

Nuclear Magnetic Resonance

29th Lorne Conference on Protein Structure and Function, Lorne, Victoria, 8–12 February The following posters were presented:
A Y Park, P Prosselkov, G Pintacuda, M A Keniry, P D Carr, D L Ollis, G Otting and N E Dixon: *Stabilization of the proofreading exonuclease subunit of E coli DNA polymerase III by backbone cyclization*

G Pintacuda, M A Keniry, T Huber, A Y Park, N E Dixon and G Otting: *Fast methods for NMR in structural biology*

ComBio2004, Perth, Western Australia, 26–30 September. The following poster was presented:
A Y Park, G Pintacuda, M A Keniry, P D Carr, P Prosselkov, D L Ollis, G Otting and N E Dixon: *Structure and function of cyclized versions of the proofreading exonuclease subunit of E coli DNA polymerase III*

2nd Workshop on Biomolecular NMR, University of Wollongong, New South Wales, 6–10 December

M A Keniry presented a lecture entitled: *Coherence selection: phase cycling and gradient pulses*, and participated at the Australian NMR Workshop

Structural Biology

29th Lorne Conference on Protein Structure and Function, Lorne, Victoria, 8–12 February The following poster was presented:
P M Schaeffer, K Loscha, A J Oakley, E Liepinsh, B Bancia, M C J Wilce, G Otting and N E Dixon: *Primase-helicase interaction in the Escherichia coli replisome*

ComBio2004, Perth, Western Australia, 26–30 September

The following lectures were presented:
K Loscha, A J Oakley, P M Schaeffer, E Liepinsh, M C J Wilce, G Otting and N E Dixon: *Structure and function of the DnaB binding domain of Escherichia coli primase*

A J Oakley, R Bourgault, J D Bewley and M C J Wilce: Endo-beta-*mannanase from ripening tomatoes: structure and mechanism*

Biomolecular NMR

ANZMAG 2004, Barossa Valley, South Australia, 15–19 February

G Otting presented the invited lecture: G Otting, G Pintacuda, S Bennett and N E Dixon: *Paramagnetic tagging for protein NMR*

P Wu was selected for oral presentation of his poster: P Wu and G Otting: *Measurement and Φ angle dependence of CSA/DD cross-correlation effects between H^{α} and H^{N}*

The following poster was also presented:
G Pintacuda, G Otting, M A Keniry, T Huber, A Y Park and N E Dixon: *Fast structure-based assignment of ^{15}N-HSQC spectra of paramagnetic proteins*

28th Annual Scientific Meeting of the Australian Society for Biophysics, Fremantle, Western Australia, 29 September–2 October

G Otting presented the invited lecture: G Otting, G Pintacuda, T Huber, M A Keniry, A Y Park, N E Dixon, A Moshref, A Leonchiks, A Sharipo and A Kaikkonen: *Paramagnetic labelling for protein NMR studies*

2nd Workshop on Biomolecular NMR, University of Wollongong, New South Wales, 6–10 December

G Otting initiated and organized the workshop, including scientific programme, course material and student admission, and gave two of the lectures entitled *Data Processing and 3D NMR*

Inorganic Chemistry

Coordination Chemistry and Spectro-electro Chemistry

9th AICCM Symposium of the Painting Special Interest Group, Hobart, Tasmania, 18–20 March The following lecture was presented:
Maria Kubik: *Fibre-optic analysis of artists' materials used by the "Angry Penguins"*

Synthetic Organometallic and Coordination Chemistry

Second Australia and New Zealand Symposium on Organometallic Chemistry (OZOM2), University of Adelaide, 11–14 January. The following lectures were presented:
R D Dewhurst, A F Hill, A D Rae, M K Smith, and A C Willis: *A simple synthesis of heterobimetallic C_3 complexes*

M Schultz, A F Hill, A D Rae, and A C Willis: *Alkyne coupling reactions of Ru(0)*

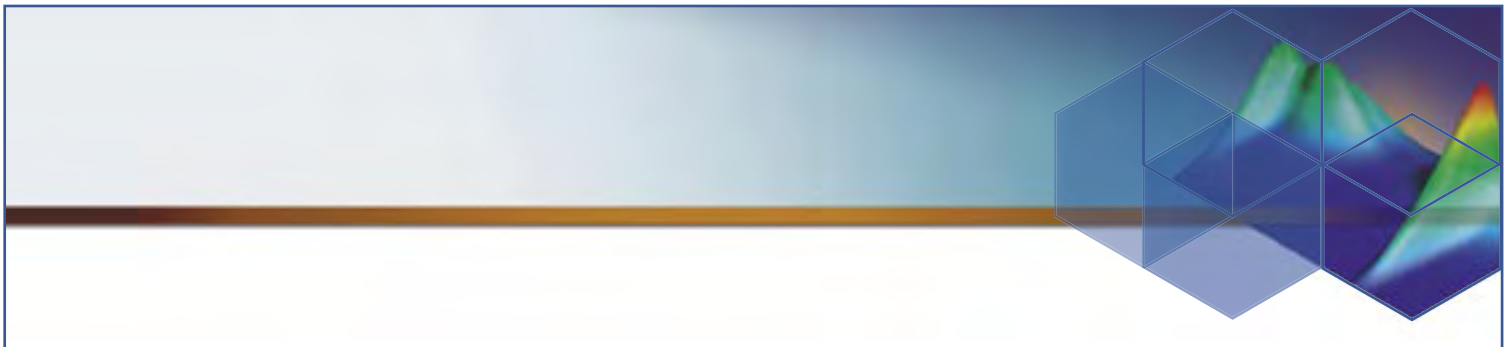
A F Hill and M K Smith: *Ruthenium(II) complexes of 2-mercapto-methylimidazole*

The following posters were presented:
L M Caldwell, A F Hill, A G Hulkes, M K Smith, A J P White, D J Williams, and A C Willis: *Organometallic chemistry of alkynyl selenolates, alkynyl selenoethers and isoselenocyanates*

R J Abernethy, A F Hill, and M K Smith: *"Soft" sulfur-donor borate transition metal complexes*

6th Reactive OrganoMetallic Symposium (ROMS-6), University of Sydney, 28 May. The following lectures were presented:
R J Abernethy: *Synthesis and reactivity of unusual alkoxy(pyrazolyl)borato complexes of ruthenium*

I R Crossley: *New developments in the main group chemistry of perflourovinyl and alkynyl reagents*



M K Smith: *Novel (2-mercaptomethimazolyl)borate complexes of a range of group 4, 5 and 14 metals*

Gordon Conference on Organometallic Chemistry, Newport RI, USA, 11–15 July. The following lectures were presented:
R D Dewhurst, A F Hill, A D Rae, M K Smith, and A C Willis: *Simple convergent routes to heterobimetallic C_3 complexes,* **for which R D Dewhurst was awarded a National Institute of Physical Sciences Travel Assistance Grant**

M Schultz, A D Rae, A C Willis, and A F Hill: Alkyne coupling reactions of zero-valent ruthenium

International Conference on Coordination Chemistry (ICCC 36), Mérida, Yucatán, México, 18–23 July. The following poster was presented:
L M Caldwell, P V Bernhardt, T B Chaston, P Chin, and D R Richardson: *Cytotoxic iron chelators: iron complexes of di-2-pyridyl keton isonicotonyl hydrazone (HPKIH) analogues*, **for which L M Caldwell was awarded a National Institute of Physical Sciences Travel Assistance Grant**

International Conference on Organometallic Chemistry (ICOMC 21), Vancouver, Canada, 25–30 July. The following lecture was presented:
M Schultz, A D Rae, A C Willis, and A F Hill: *Alkyne coupling reactions of Ru(0)*

The following posters were presented:
L M Caldwell, A F Hill, and A C Willis: *Group 6 selenoaroyl complexes: isoselenocyanates as single atom selenium transfer reagents,* **for which L M Caldwell was awarded a National Institute of Physical Sciences Travel Assistance Grant**

R D Dewhurst, A F Hill, A D Rae, M K Smith, and A C Willis: *Simple convergent routes to heterobimetallic C_3 complexes*, **for which R D Dewhurst was awarded a National Institute of Physical Sciences Travel Assistance Grant**

New Developments in Metal Alkynyl Chemistry, Research School of Chemistry, ANU, 12 November. A F Hill chaired the *Synthetic Methods* session The following lecture was presented:
R D Dewhurst, A F Hill, and A C Willis: *Investigating catalytic demercuration of bis(tricarbido) [Hg(CCCWML$_n$)$_2$] complexes*

The following posters were presented:
M J Bartlett, A F Hill, and M K Smith: *Bimetallics spanned by C_4, C_4H and C_4H_2 wires*

R D Dewhurst, A F Hill, and A C Willis: *The C_3 ligand: odd-numbered carbon bridges linking W with Rh, Ir and Hg*

The 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, New Zealand, 5–8 December. The following lectures were presented:
I R Crossley, A F Hill, E R Humphrey, and A C Willis: *Metallaboratranes: the synthesis and chemistry of a series of group 9 and 10 compounds exhibiting 'dative' metal-boron bonding*

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

R J Abernethy, I R Crossley, A F Hill, E R Humphrey, M K Smith, N Tshabang, and A C Willis: *Methimazolyl-derived tripodal ligands–(only) if the cap fits*

The following posters were presented:
R J Abernethy, A F Hill, and A C Willis: *Solvent-mediated reactions of ruthenium complexes with poly(pyrazolyl) borates*, **which was awarded second prize for a student contribution**

R J Abernethy, A F Hill, and A C Willis: *Synthesis and reactivity of molybdenum-allyl scorpionate complexes: $[H_2B(mt)_2]^-$ vs $[H_2B(pz)_2]^-$*

L M Caldwell, A F Hill, and A C Willis: *Synthesis and reactivity of group 6 selenoaroyl complexes*

R D Dewhurst, A F Hill, and A C Willis: *The C_3 ligand: odd-numbered carbon bridges linking W with Rh, Ir and Hg*

M J Bartlett, A F Hill, and M K Smith: *Bimetallics spanned by C_4, C_4H and C_4H_2 wires*

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

N Tshabang, A F Hill, M K Smith, and A C Willis: *Heterobimetallic complexes of poly(methimazolyl)borate ligands,* **for which N Tshabang was 'Highly Commended' for a student contribution**

Inorganic Stereochemistry and Asymmetric Synthesis

Second Australia and New Zealand Symposium on Organometallic Chemistry (OZOM2), University of Adelaide, 11–14 January. The following lectures were presented:

E H Krenske, K A Porter, and S B Wild: *Phosphine-stabilised arsenium salts as precursors for the asymmetric synthesis of tertiary arsines*, **for which E H Krenske was awarded a prize for the best student lecture**

R J Warr and S B Wild: *Inorganic asymmetric synthesis of two-bladed propeller octahedral metal complexes*

The following poster was presented:
X Zhou, A C Willis, and S B Wild: *Burrows' compounds revisited*

The 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, New Zealand, 5-8 December

S B Wild gave a plenary lecture entitled: *Chiral phosphines and arsines: resolutions and asymmetric syntheses*

The following lectures were presented:
N L Kilah and S B Wild: *Deracemisation of chiral arsines and phosphines via asymmetric transformation*

H J Kitto and S B Wild: *Polytertiary phosphine helicates*

A D Rae, R J Warr, S B Wild, and A C Willis: *Inorganic asymmetric synthesis of two-bladed propeller octahedral metal complexes*

Solid State Inorganic Chemistry

The Sixth Conference of the Asian Crystallographic Association (AsCA'04), Hong Kong, 27–30 June. The following lectures were presented:
Y Liu, R L Withers, F J Brink, L Norén, and V Ting: *Cubic perovskite-related phases in the ternary SrO-CuO-Nb_2O_5*

A D Rae: *Matching structure to cell distortion in twinned crystals*

V Ting, Y Liu, R L Withers, and L Norén: *Structural studies of the A_2InNbO_6 1:1 and $A_3CoNb_2O_9$ 1:2 ordered perovskites ($A = Ca^{2+}$, Sr^{2+}, Ba^{2+})*

The following poster was presented:
W Somphon, K J Haller, and A D Rae: *The order disorder transition at 150 K of polymeric $Ag(bipy)NO_3$*

The Australian Conference on Microscopy and Microanalysis (ACMM 18), Geelong, 1–6 February

R L Withers gave a keynote lecture: *A TEM and rigid unit mode (RUM) study of some inherently flexible framework structures*

The following lectures were presented:
F J Brink, L Norén, and R L Withers: *Electron diffraction evidence for continuously variable, composition-dependent, oxygen/fluorine ordering in niobium oxyfluorides*

V Ting, Y Liu, R L Withers, and L Norén: *A TEM study of the space group symmetries and structures of the A_2InNbO_6 1:1 and $A_3CoNb_2O_9$ 1:2 ordered perovskites ($A = Ca^{2+}$, Sr^{2+}, Ba^{2+})*

22nd European Crystallographic Meeting, Budapest, Hungary , 26–31 August. The following poster was presented:
A D Rae and A Linden: *Using symmetrized structure components to improve the refinement of an occupancy modulated structure*

Organic Chemistry

Synthesis and Mechanism

Colloquium for Humboldt Fellows and Awardees in Australia and New Zealand, Auckland, New Zealand, 20–22 February. The following workshop contributions were presented:
M G Banwell, *Natural products-inspired chemical synthesis studies*

M G Banwell and J Renner: *Towards practical total syntheses of the spinosyns – potent and environmentally benign insecticides*

The 3rd Chinese-Australian Organic Chemistry Symposium, Sydney, New South Wales, 25–26 February

M G Banwell presented the invited lecture: *The total synthesis of biologically active natural products*

20th Royal Australian Chemical Institute Organic Chemistry Conference, Cairns, Queensland, 4–8 July was attended by M G Banwell, M Bonnet, S Gross, O J Kokas, J Renner and P C Stanislawski

M G Banwell presented the 2004 Birch Medal Lecture

P Stanislawski presented the contributed lecture: *Towards the total synthesis of the erythrinan and homoerythrinan alkaloids*

The following posters were also presented:
M G Banwell, B D Kelly and J Renner: *Towards practical total syntheses of the spinosyns – potent and environmentally benign insecticides*

M G Banwell and O J Kokas: *Towards the total synthesis of (–)-brunsvigine*

M G Banwell, M J Coster and S Gross: *Studies directed towards the total synthesis of the marine alkaloid haliclonacyclamine A*

IUPAC ICOS-15, 15th International Conference on Organic Synthesis, Nagoya, Japan, 1–6 August. The following poster was presented:
M G Banwell and D T J Loong: *Chemoenzymatic approaches to total syntheses of cladospolides B, C and D*

15th Southern Highlands Conference on Heterocyclic Chemistry, Moss Vale, New South Wales, 5–7 September. The following poster was presented:
M G Banwell and D W Lupton: *New methods for the construction of Aspidosperma alkaloids*

Biotransformations and Synthesis, Queens University of Belfast, Belfast, Northern Ireland, 24 September

M G Banwell presented the plenary lecture: *Bugs for drugs: exploiting whole-cell biotransformations in the total synthesis of natural products and other biologically active compounds*

Royal Australian Chemical Institute NSW Organic Chemistry Group 25th Annual One-day Symposium, University of New South Wales, 30 November was attended by M G Banwell, M Bonnet, L Fearnside, M Friend, J C Jury, D T J Loong, D W Lupton and A T Phillis

D W Lupton presented the invited lecture: *A total synthesis of the alkaloid aspidospermidine* **for which he was awarded a prize for one of the best student talks**

The following posters were also presented:
M G Banwell and A T Phillis: *Approaches to functionalised gibbane skeleta using novel rearrangements of gem-dihalocyclopropanes*

M G Banwell and D T J Loong: *Chemoenzymatic approaches to the total synthesis of cladospolides B, C and D*

Biochemical Reactions and Molecular Recognition

38th International Wood Composites Symposium, Seattle, USA, 5–8 April

A Philbrook presented the opening invited lecture: *Demonstration of co-polymerisation in melamine-urea-formaldehyde reactions using ^{15}N NMR correlation spectroscopy*

9th International Symposium on Free Radicals, Porto-Vecchio, France, 6–11 June. The following posters were presented:
C J Easton and A Wright: *Evaluation of thiols as reagents to repair radical damage in peptides and proteins*

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

20th Royal Australian Chemical Institute Organic Chemistry Conference and 29th International Symposium on Macrocyclic Chemistry, Cairns, Queensland, 4–8 July were attended by L Barr, M M Cieslinski, R Dawson, C J Easton, I H W Li, A Philbrook, Y C Tsai, Z I Watts, and A Wright. The following lectures were presented:
M M Cieslinski, C J Easton, H Onagi, and S F Lincoln: *Cyclodextrins and stilbenes as components of molecular devices*

C J Easton, G P Savage, and G W Simpson: *Overcoming limitations in nitrile oxide cycloaddition chemistry*

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

A Wright and C J Easton: *Fighting an uphill battle: hydrogen atom transfer between thiols and amino acids*

The following posters were presented:
R Dawson, C J Easton, T Herlt, and S F Lincoln: *Stilbene and cyclodextrins as the basis of molecular shuttles*, **for which R Dawson was awarded the best poster prize**

I H W Li, B J W Barratt, C J Easton and J S Simpson: *α-Glycyl radical stability and PAM enzyme inhibition*

L Barr, C J Easton, A G Meyer and S F Lincoln: *Cyclodextrins as molecular reactors to reverse the regioselectivity of nitrile oxide cycloadditions*

A Philbrook, C J Blake, N Dunlop, C J Easton and M Keniry: *Demonstration of co-polymerisation in melamine-urea-formaldehyde reactions using ^{15}N NMR correlation spectroscopy*

Y C Tsai and C J Easton, *Oxidatively cleavable amino acid residues in peptides*

3rd Heron Island Conference on Reactive Intermediates and Unusual Molecules, Heron Island, Queensland, 17–23 July

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

17th IUPAC Conference on Physical Organic Chemistry, Shanghai, China, 15–20 August

C J Easton presented the plenary lecture: *Cyclodextrins as the basis of catalysts, molecular reactors and machines and microelectronic devices*

Orica Emerging Science Symposium, Melbourne, 12 November

A Philbrook presented the invited lecture: *Melamine replacements in MUF resins*

1st Pacific Symposium on Radical Chemistry, Kanazawa, Japan, 14–16 November

C J Easton presented the invited lecture: *Inhibition of PAM to regulate hormone production*

Adelaide Organic Chemistry Symposium, Adelaide, 6 December

C J Easton presented the plenary lecture: *Cyclodextrins as the basis of catalysts, molecular reactors and machines and microelectronic devices*

Organic Synthesis

20th Royal Australian Chemical Institute Organic Conference, Cairns, Queensland, 4–9 July

L N Mander gave an invited lecture: *Synthesis of the Galbulimima alkaloids*

IUPAC ICOS-15, 15th International Conference on Organic Synthesis, Nagoya, Japan, 1–6 August The following poster was presented:

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

Organic Synthesis, Methodology and Host-guest Chemistry

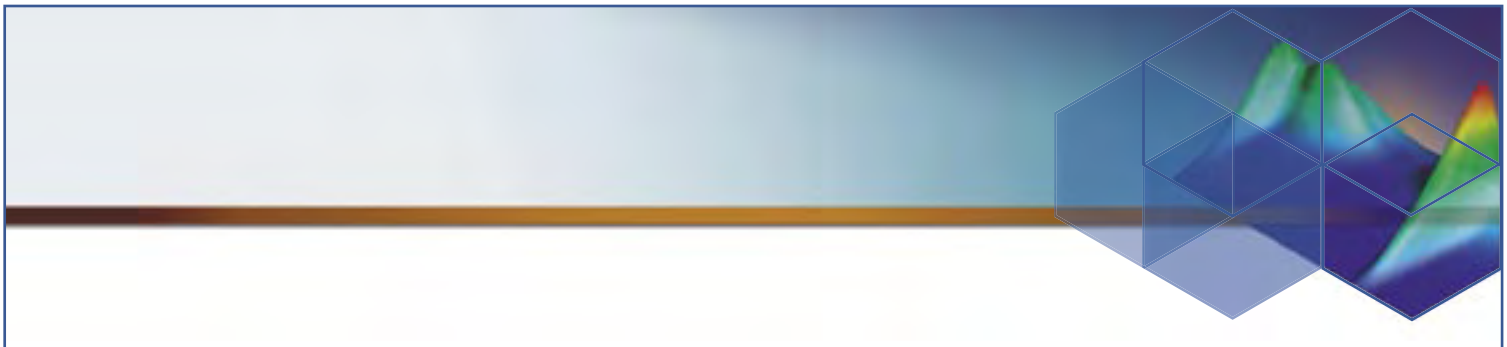
The 3rd Chinese–Australian Organic Chemistry Symposium, Sydney, New South Wales, 25–26 February

M S Sherburn presented the invited lecture: *Radicals and pericyclics as key steps in synthesis*

20th Royal Australian Chemical Institute Organic Chemistry Conference and 29th International Symposium on Macrocyclic Chemistry, Cairns, Queensland, 4–8 July was attended by M S Sherburn, E S Barrett, S K Goodwin, N Kanizaj, L C H Kwan, N A Miller, E L Pearson, A D Payne, A J Scott, L A Sharp, D J Sinclair, R Tripoli and C I Turner. The following lectures were presented:
E S Barrett and M S Sherburn: *Superbowls and next generation container molecules*

L A Sharp and M S Sherburn: *The intramolecular radical carboxyarylation reaction: scope and application to natural product synthesis*, **for which L A Sharp won a prize for best student presentation**

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



D J Sinclair and M S Sherburn: *Extending the chemistry of cavitands*

The following posters were also presented:
N Kanizaj and M S Sherburn: *Cooperative action of double cavity molecules? Synthesis and binding studies*

L Kwan and M S Sherburn: *Investigations into enantioselective catalysis of the intramolecular Diels–Alder reaction*

S K Goodwin, A D Payne and M S Sherburn: *Polycyclic molecules from acyclic precursors using the Diels–Alder reaction*

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

A J Scott and M S Sherburn: *Total synthesis of (–)-podophyllotoxin*, **for which A J Scott won a prize for best student poster**

R Tripoli and M S Sherburn: *A radical mechanism for the intramolecular Diels-Alder reaction?*

C I Turner and M S Sherburn: *A radical new approach to the total synthesis of (+)-podophyllotoxin*

IUPAC ICOS-15, 15th International Conference on Organic Synthesis, Nagoya, Japan, 1–6 August

N A Miller and M S Sherburn: *Synthesis and reactions of substituted dendralenes,* **for which N A Miller was awarded a prize for best poster**

15th Southern Highlands Conference on Heterocyclic Chemistry, Moss Vale, New South Wales, 5–7 September was attended by M S Sherburn, E S Barrett and C I Turner

E S Barrett was a postgraduate scholarship awardee and presented the invited lecture: *Synthesis and applications of cavitands to host-guest chemistry*

The following posters were also presented:
A J Scott and M S Sherburn: *Total synthesis of (–)-podophyllotoxin*

A J Reynolds, C I Turner and M S Sherburn: *A radical new approach to the total synthesis of (+)-podophyllotoxin*

C I Turner and M S Sherburn: *The intramolecular Diels–Alder reaction on steroids*

One-day Synthesis Symposium in Honour of Emeritus Professor Lew Mander, Canberra, 8 September was attended by M S Sherburn, E S Barrett, T N Cayzer, S K Goodwin, N Kanizaj, L C H Kwan, W Lording, N A Miller, E L Pearson, A D Payne, K Rands-Trevor, L A Sharp, D J Sinclair, R Tripoli and C I Turner

M S Sherburn presented the invited lecture: *From polyenes to polycycles*

1st Pacific Symposium on Free Radical Chemistry, Kanazawa, Japan, 15–16 November

M S Sherburn presented the invited lecture: *Total synthesis through radical carboxyarylation*

Royal Australian Chemical Institute NSW Organic Chemistry Group 25th Annual One-day Symposium, University of New South Wales, 30 November was attended by M S Sherburn, E S Barrett, S K Goodwin, N Kanizaj, L C H Kwan, W Lording, N A Miller, E L Pearson, A D Payne, D J Sinclair and C I Turner

L C H Kwan presented the invited lecture: *Towards an efficient construction of steroids using a domino IMDA reaction* **for which he was awarded a prize for one of the best student talks**

The following posters were presented:
N A Miller and M S Sherburn, *Synthesis and reactions of substituted dendralenes* **for which N A Miller was awarded a prize for one of the best student poster presentations**

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

Physical and Theoretical Chemistry

Theoretical Chemical Physics

RACI Conference on Physical Chemistry, Hobart, 1–5 February

M A Collins presented the Division Medal Lecture: *Chemical Reaction Mechanisms*

American Chemical Society Meeting, Anaheim, 1–4 April. The following lecture was presented:
M A Collins: *Nonadiabatic dynamics on interpolated diabatic potentials*

Faraday Discussion on Non-adiabatic Effects in Chemical Dynamics, Oxford, 5–7 April. The following poster was presented:
C R Evenhuis and M A Collins: *Growing diabatic potential energy surfaces*

1st Asian Pacific Conference on Theoretical and Computational Chemistry, Okazaki, 12–15 May. The following lecture was presented:
M A Collins: *Dynamics on interpolated adiabatic and diabatic potentials*

Dalian Institute of Chemical Physics Conference, Dalian, China, July 21–23. The following lecture was presented:
M A Collins: *Dynamics on interpolated adiabatic and diabatic potentials*

Computational Quantum Chemistry Polymer Chemistry

Royal Australian Chemical Institute Conference on Physical Chemistry (CPC2004), Hobart, 1–5 February

M L Coote presented the lecture: *What causes retardation in RAFT polymerization? A quantum-chemical approach*

1st Asian Pacific Conference on Theoretical and Computational Chemistry (APACTC), Okazaki, Japan, 12–15 May

M L Coote presented the invited lecture: *Ab Initio molecular orbital studies of RAFT polymerisation*

Orica Emerging Science Symposium, Melbourne, 12 November

M L Coote presented the invited lecture: *Modelling Polymer Formation*

1st Pacific Symposium on Radical Chemistry (PSRC-1), Kanazawa, Japan, 15–16 November

M L Coote presented the invited lecture: *Ab Initio studies of RAFT polymerisation*

Liquid State Chemical Physics

International Workshop on Dynamics in Viscous Liquids, Munich, Germany, 14–17 March

D J Evans: *The fluctuation theorem*

3rd International Conference Computational Modelling and Simulation of Materials Sicily, 30 May–4 June

D J Evans: *The fluctuation theorem*

CECAM Conference, Lyon, France, 19–22 July

D J Evans presented the invited lecture: *The fluctuation theorem*

Workshop – Stochastic and Deterministic Dynamics Equilibrium and Nonequilibrium Vienna, Austria, 25–28 August

D J Evans presented the invited lecture: *The fluctuation theorem*

Pacific Rim Conference on Nanotechnology Broome, 7–11 September

D J Evans presented the invited lecture: *The fluctuation theorem: Theory and experiment*

12th Biennial Computational Techniques Conference Melbourne, 27–29 September

D J Evans presented the invited lecture: *Fluctuation theorem: Simulation, theory and experiment*

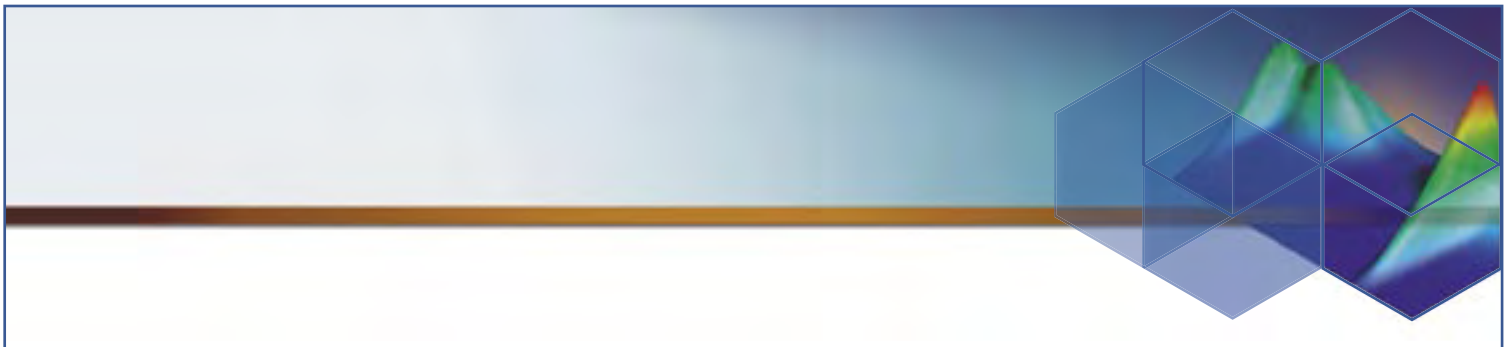
Laser and Optical Spectroscopy

Australasian Conference on Physical Chemistry (CPC04), Hobart, Tasmania, 1–5 February

B Prince, S , P Smith, R Pace and E Krausz: *Spectral Identification of P680*

The following posters were presented:
L Debono, B Prince, S Peterson, P Smith, R Pace and E Krausz: *Optical and EPR spectroscopy of cytochrome B_{559} in Photosystem II*

J L Hughes, B J Prince, H Riesen, P Smith, R Pace and E Krausz: *Persistent spectral hole-burning in active Photosystem II*



N Cox, P Smith, R Pace, G Fisher, B Prince and E Krausz: *An FTIR study on the oxygen evolving complex of Photosystem II*

Photosynthesis and Post-Genomic Era International Meeting, Trois Rivieres, Canada, 25–29 August. The following posters were presented:
E Krausz, J L Hughes, P J Smith, R J Pace, S Peterson Årsköld: *Assignment of the low-temperature fluorescence in oxygen-evolving Photosystem II*

J L Hughes, E Krausz, P J Smith R J Pace, H Riesen: *Probing the lowest energy chlorophyll a states of Photosystem II via selective spectroscopy: New insights on P680*

P J Smith, J L Hughes, B J Prince, E Krausz, S Peterson Årsköld, R J Pace: *S1 to S2 state turnover studies on Photosystem II core samples from higher plants*

N Cox, P J Smith, W Hillier, G Fischer, E Krausz, R J Pace, *FTIR studies on PS II core complexes from higher plants: First Identification of multiline and g4 1 features in S2/S1 turnover*

S Peterson Årsköld, P J Smith, J R Shen, R J Pace, E Krausz: *Key cofactors of Photosystem II cores from four organisms identified by 1 7-K*

13th International Congress on Photosynthesis, Montreal, Canada, August 29 – 3 September

J L Hughes, E Krausz, P J Smith, R J Pace, H Riesen: *The lowest-energy excited-state of P680 in oxygen-evolving Photosystem II extends to 700 nm*

The following posters were presented:
E Krausz, J L Hughes, P J Smith, R J Pace, S Peterson Årsköld: *The reaction centre of PSII in oxygen-evolving preparations*

S Peterson Årsköld, J Ström, J F Allen and E Krausz: *Low-temperature absorption and magnetic circular dichroism of the four haems of the chloroplast cytochrome b_6f complex*

P J Smith, J L Hughes, B Prince, E Krausz, R J Pace, S Peterson Årsköld: T*urnover studies using visible and far red light on PSII core samples from higher plants*

R J Pace, N Cox, P J Smith, W Hillier, G Fischer, E Krausz: *FTIR studies on PS II core complexes from higher plants: First identification of multiline and g4 1 features in S2-S1 turnover*

Fifth Student Conference on Physical Chemistry, Wagga Wagga, 27–30 September

L Debono: *The role of cytochrome b_{559} in photosystem II studied by MCD spectroscopy*

Computational Quantum Chemistry

Theory and Applications of Computational Chemistry, Gyeongju, Korea, 15–20 February

L Radom presented the invited lecture: *Stabilities and reactivities of free radicals*

Asian Pacific Symposium on Theoretical and Computational Chemistry, Okazaki, Japan, 12–15 May

L Radom presented the plenary lecture: *The mechanism of action of coenzyme B_{12}*

MM2004, Sydney, Australia, 30 June –3 July

L Radom presented the invited lecture: *The mechanism of B_{12}-mediated reactions*

Symposium in Honor of Professor H F Schaefer III, 228th National Meeting of the American Chemical Society, Philadelphia, USA, 22–26 August

L Radom presented the invited lecture: *Thermochemistry of calcium-containing molecules: An examination of the performance of high-level theoretical procedures*

One-day Synthesis Symposium in Honour of Emeritus Professor Lew Mander, Canberra, 8 September

L Radom presented the invited lecture: *Adventures in B_{12} chemistry: A theoretical mechanistic study*

Disordered Materials

European Crystallography Meeting, Budapest, Hungary

Welberry T R and R L Withers: *The importance of multisite correlations in disordered structures*

Australian Synchrotron Research Program User's Meeting, Australian National University

D J Goossens, T R Welberry and A P Heerdegen: *Measuring diffuse scattering*

Australian and New Zealand Institute of Physics 28rd Annual Condensed Matter Physics Meeting, Charles Sturt University, Wagga Wagga

D J Goossens, T R Welberry and A P Heerdegen: *Measuring diffuse scattering*

Asian Crystallography Association Meeting, Hong Kong, June

T R Welberry, D J Goossens, W I F David, M J Gutmann, M J Bull and A P Heerdegen: *Diffuse neutron scattering in benzil, $C_{14}D_{10}O_2$, using the time-of-flight Laue technique*

Solid State Molecular Science

Australian Synchrotron Research Program, Users Meeting, Canberra, ACT, Australia, 5–6 February. The following presentation was given:
M J Henderson: *Energy dispersive reflectometry*

Inter-Academy Forum, Academy of Science, Canberra, Australia, 23 March. The following presentation was given:
J W White: *Recent information on the UK's Research Assessment Exercise*

8th International Conference on Surface X-ray and Neutron Scattering, Bad Honnef, Germany, 28 June–2 July

M J Henderson presented the contributed talk: *High speed X-ray reflectometry*

Nanoethics Workshop, Australian National University, Canberra, Australia, 22 July

J W White gave the presentation: *Nanotechnology – ethical problems?*

Future Materials Workshop, Australian National University, Canberra, Australia, 24 August

J W White gave the presentation: *Material Science and the Research School of Chemistry*

Antarctic Science Symposium, Academy of Science, Canberra, Australia, 12 November

J W White gave the presentation: *Australia's Antarctic Research and National Research Priorities*

AINSE Neutron Symposium, Lucas Heights, Sydney, Australia, 14 December

J W White gave the presentation: *Mimicking biomineralisation*

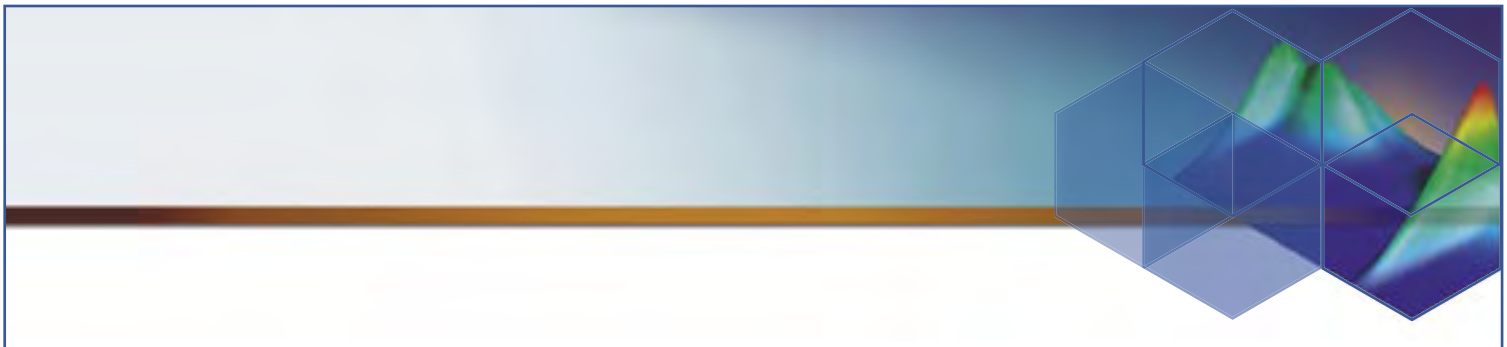
R W Rickards – Visiting Fellow (Post-retirement)

25th Anniversary Conference of the Science Teachers' Association of Western Australia, Curtin University, Muresk, WA, 28–30 May

R W Rickards gave the keynote address: *Organic science: Why I did chemistry*

Royal Australian Chemical Institute, Natural Products Group Annual Symposium, Southern Cross University, Lismore, NSW, 1 October The following lecture was presented:

W-P Yin, T-Z Zhao, C Zhao, C Liao, S C Trowell, R W Rickards: *Discovery of natural products where others have already looked*



Plenary and Invited Lectures

Professor M G Banwell

Some aspects of pyrrole chemistry: teaching an old dog new tricks? the Department of Chemistry, National University of Singapore 28 May

Exploitation of metabolites from whole-cell biotransformations in the total synthesis of biologically active natural products, the Department of Chemistry, University of Exeter, 28 September

He also presented the following named lectures:
The 2004 Nanjing University of Science and Technology International Exchange and Co-operation Lecture Series, Nanjing University of Science and Technology, Nanjing, China 1-2 June

The 2004 Boehringer–Ingelheim Lecture of the Ohio State University, *Chemoenzymatic methods for the synthesis of natural products*, the Department of Chemistry, Ohio State University, Columbus, Ohio, USA, 10 June; and at Boehringer–Ingelheim Pharmaceuticals Inc., Ridgefield, Connecticut, USA, 11 June

The 2004 Novartis Chemistry Lecture, Novartis Pharma, Basel, Switzerland, 22 September, and at the Novartis Horsham Research Centre, Horsham, UK, 27 September

Professor C J Easton

Gave an invited lecture on *Cyclodextrin based molecular reactors, machines and microelectronic devices* at the University of New South Wales, 21 September

Gave an invited lecture on *A free radical approach to developing enzyme inhibitors to regulate hormone levels* at Kobe Pharmaceutical University, Japan, on 12 November

Professor D J Evans

The fluctuation theorem, Moyal Medal Lecture, 22 October

Professor P M W Gill

§ *Hartree-Fock-Wigner models for electron correlation*, Computational Chemistry Working Party Meeting Imperial College, UK, 30 March

§ *Hartree-Fock-Wigner models for electron correlation,* Center for Computational Quantum Chemistry, University of Athens, USA, 7 April

§ *Hartree-Fock-Wigner models for electron correlation*, Department of Chemistry, University of Sussex, UK, 14 May

§ *A new type of functional for density functional theory*, Deutsche Forschungsgemeinschaft SPP 1145 Workshop Bonn, Germany, 24 May

§ *Hartree-Fock-Wigner models for electron correlation*, Department of Chemistry, University of Cambridge, UK, 2 June

§ *Optimal atomic charges sometimes look silly*, International Society of Quantum Biology and Pharmacology meeting Como, Italy, 6 June

Hartree-Fock-Wigner models for electron correlation, Department of Chemistry, University of Southern California, USA, 3 December

Describing electron correlation in position and momentum spaces, EPSRC "Mathematical challenges in quantum chemistry" Workshop, Warwick, UK, 13 December

§ Denotes invited lectures presented prior to commencement at RSC

Professor L N Mander

Presented two invited lectures: *Enabling Strategies for the Assembly of Complex Polycyclic Natural Products* at the University of Canterbury, NZ, May 10; and at the University of NSW, October 27

The Cornforth Lecture, to the University of Sydney Chemical Society, October 13; and the 2004 Wilson Baker Lecture at the University of Bristol, UK, November 2

Dr P A Reynolds

The Structure of Explosives, Orica Emerging Science Symposium 2004, Melbourne, Australia, 12 November

Dr M S Sherburn

Using free radicals to fight cancer, why pacman should be chiral, and other short stories, the Institute for Molecular Bioscience, University of Queensland, 16 April

Short synthetic approaches to natural product frameworks, CSIRO Molecular Science, Melbourne, 30 September; and at the School of Chemistry, University of Melbourne, 1 October

Professor J W White

Invited after-dinner speaker: NanoScience – an Exciting Quest, Some Emerging Trends in Chemistry, Molecular Level Conference, RMIT, Melbourne, Australia, 12 March

Service to External Organisations

Professor M G Banwell: Chair, Editorial Advisory Committee, *Australian Journal of Chemistry*; Consultant, Genencor International Inc, Palo Alto; Consultant, Biota Holdings Ltd, Melbourne; Consultant, Cryptopharma Pty Ltd, Melbourne; Member, Editorial Boards, *Indian Journal of Chemistry (Section B), Synlett*; Member, Board of Consulting Editors, *Tetrahedron*, *Tetrahedron Letters*; Asia-Pacific Representative, Advisory Committee to the International Society for Heterocyclic Chemistry; Member, Advisory Board, Special Centre for Green Chemistry, Monash University; Reader, ARC grant applications

Professor M A Collins: Committee member, Physical Chemistry Division, Royal Australian Chemical Institute (RACI)

Dr M L Coote: Member of the IUPAC task group on the *Kinetics of RAFT Polymerization* (organized by the IUPAC Macromolecular Division)

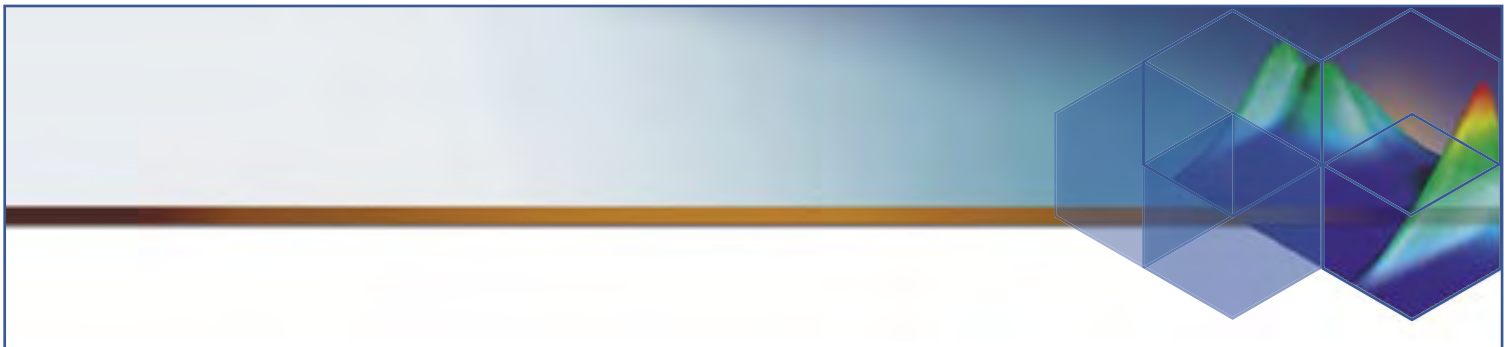
Dr N E Dixon: Visiting Lecturer, School of Chemistry, University of Sydney; Assessor, NH&MRC grant applications

Professor C J Easton: Chair, Organic Chemistry Division, RACI; Chair, RACI Fellowships Committee (ACT Branch); Member, External Academic Advisory Board (Chemistry), Deakin University; Specialist Advisor, Tertiary Education Commission, New Zealand; Member, Editorial Board, *ARKIVOC*; Member, Referee Panel, *Chemical Communications*; Member, Editorial Advisory Board, *Current Organic Synthesis*; *Mini Reviews in Organic Chemistry; Letters in Organic Chemistry*; Member, Board, Asian and Oceanian Cyclodextrin League; Member, Scientific Committee, Ninth International Society for Free Radical Research Conference, 2004; Chair, Organising Committee, 20th Royal Australian Chemical Institute Organic Conference; Member, Organising Committee, 29th International Symposium on Macrocyclic Chemistry; Chair, Organising Committee, Symposium on Free Radicals in Chemistry and Biology, Pacifichem 2005; Member, Management Committee, UnIChe Program; Member, Advisory Board, Chirogen Pty Ltd; Chair, Organising Committee, 10th International Symposium on Free Radicals; Consulting Fellow, World Innovation Fund

Professor D J Evans: Australian Academy of Science; Member, Merit Allocation Committee, Australian Partnership in Advanced Computing (APAC); Member, Organising Committee, Liblice Conferences on Statistical Mechanics of Liquids; Member, Editorial Advisory Board, *Chemical Physics*; Member, Editorial Boards, *Molecular Simulation*, *Molecular Physics*; Assessor/Reader, ARC grant applications

Professor P M W Gill: International panel member for the Deutsche Forschungsgemeinschaft

Dr G A Heath: Member, Raman Microscope Steering Committee, University of Canberra; Member, IR Beamline Advisory Panel, Australian Synchrotron Research Program; Advisor, Chemical Criminalistics



Section, Australian Federal Police, Weston; Advisor, Conservation Department, National Gallery of Australia; Advisor, Cary Spectrometer Division, Varian Analytical Instruments, Melbourne; Advisor, National Museum of Australia

Professor A F Hill: Member, Referee Panel, *Chemical Communications*; Editor, *Advances in Organometallic Chemistry* (Academic Press); Member, Editorial Advisory Board, *Organometallics*; Member, International Editorial Advisory Board, *Dalton Transactions*; Assessor, ARC grant applications (international reader)

Professor E R Krausz: Committee Member, RACI Physical Chemistry; Assessor, DOE, NSF and ARC grant applications

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

Professor D L Ollis: Assessor, ARC and NH&MRC applications

Professor G Otting: Member, Editorial Board, *Journal of Biomolecular NMR*; Assessor, ARC, NH&MRC and ETH grant applications

Dr A J Oakley: Assessor, NH&MRC grant applications; Tutorial developer, Theoretical and Computational Biophysics Group, University of Illinois at Urbana, Champaign, IL, USA

Professor L Radom: Vice-president and President-elect, World Association of Theoretically Oriented Chemists; Co-organiser, John Pople Memorial Symposium, San Diego, March 2005; Member, Editorial Advisory Boards, *Advances in Quantum Chemistry*; *European Journal of Mass Spectrometry*; *International Journal of Quantum Chemistry*; *Journal of Computational Chemistry*; *Journal of Molecular Structure: Theochem; Journal of Physical Organic Chemistry*

Dr M S Sherburn: President-elect, ACT Branch, Royal Australian Chemical Institute; Secretary, ACT Branch, Royal Australian Chemical Institute; Treasurer, 20th Royal Australian Chemical Institute Organic Chemistry Conference and 29th International Symposium on Macrocyclic Chemistry, Cairns, Queensland, 4–8 July; Treasurer, Organic Division, Royal Australian Chemical Institute

Professor T R Welberry: Co-editor, *Journal of Applied Crystallography*; Guest Editor, Special Issue of *Zeitschrift für Kristallographie* on 'Diffuse Scattering'; Member, National Committee for Crystallography of the Australian Academy of Science; Member, Single Crystal Instrument Advisory Team, Australian Nuclear Science and Technology Organisation; Alternate (for Professor J W White), Australian Synchrotron Research Program Policy and Review Board

Professor S B Wild: Consulting Editor, *Tetrahedron: Asymmetry*; Member, Editorial Advisory Board, Main Group Chemistry; Member, Selection Committee, Australian–German Research Cooperation Scheme; Guest Professor, PhD Program, University of Leipzig

Professor R L Withers: Member, Aperiodic Commission of the International Union of Crystallography; Member, Editorial Board, *Journal of Solid State Chemistry*; Member of Council, Society of Crystallographers in Australia and New Zealand (SCANZ); Australian Microscopy and Microanalysis Society (AMMS) Representative, Australian National Committee for Crystallography; Co-organiser, satellite workshop on *Structural Analysis of Aperiodic Crystals*, to be held in August 2005 in Florence preceding IUCr XX

Professor J W White: Member, Royal Australian Chemical Institute Steering Committee for review: *Future of Chemistry: Review of the Pathway to Chemists – from education to employment*; Member, RACI, Policy Committee; Member, RACI, Nominations Committee; Chair, National Committee for Crystallography, Australian Academy of Science; Chair, Advisory Committee on Replacement Research Reactor, Australian Academy of Science; Committee member, University of Chicago's Review of Chemistry Division, Argonne National Laboratory, USA; Chair, International Review Committee, Cooperative Research Centre for Polymer Blends; Member,

Emerging Science Panel, CSIRO; Program committee member for 8th International Conference on Surface X-ray and Neutron Scattering, Bad Honnef, Germany, 28 June - 2 July; Member, Prime Minister's Science, Engineering and Innovation Council Working Group on Antarctic Science; Chair, Scholarships Committee, Oxford-Australia Scholarship Fund; Vice-President, Australian Institute of Nuclear Science and Engineering; Chair, Management Committee of University-Industry Linkages in Chemistry (UnIChe); Member, Australian Synchrotron Research Program Policy and Review Board; Member of International Advisory Board, Centre of Excellence for Nanotechnology, University of Queensland; Member, Council of the Asian Crystallographic Association; Member, Board of Governors, Consortium for Advanced Radiation Sources, CARS, University of Chicago; Member, International Science Advisory Committee, Central Laboratory of the Research Councils, UK; Member, ISIS Scheduling Panel, Rutherford Appleton Laboratory, UK; Member, Beam Instruments Advisory Group, Australian Nuclear Science and Technology Organisation; Member, Council, Australian Academy of Science; Member, Council, Australian Institute of Nuclear Science and Engineering; Member, Neutron Scattering Specialist Committee, Australian Institute of Nuclear Science and Engineering; Member, Advisory Committee, School of Chemistry, University of Sydney; Member, Australian Academy of Science/Royal Society Exchange Program Committee; Chair, International Advisory Committee for Japanese Atomic Energy Research Institute/KEK J-PARC Project; Member, International Advisory Panel, Faculty of Science, National University of Singapore; Chair, Canberra Fellows Group, Australian Academy of Science; Member, Governing Board, Centre for Australian Cultural Studies; Member, Editorial Boards, *Advances in Physics*, *Current Opinion in Solid State and Materials Science*, *Journal of Materials Chemistry*, *Physical Chemistry Chemical Physics*; Assessor/Reader, ARC grant applications; Member, Institute for the Study of Christianity in an Age of Science and Technology; Founding member, International Society for Science and Religion

External Lectures and Courses

Dr N E Dixon

First-year special lecture in Molecular Biology and Genetics on *The Interface Between Chemistry and Biochemistry*, University of Sydney, 1 June

Professor C J Easton

Tasmanian Alkaloids Lecturer at the University of Tasmania, April-May

Outreach Activities

Australian Academy of Science (AAS)

Professor J W White is the AAS spokesperson on stem cell research and contributed to the national debate on the potential scientific value of embryonic stem cell research in Australia. He will be the convenor of a national conference on stem cell research to be held in May 2005. He also contributes to policy development for major national research facilities for the Academy of Science. Professor White was also the convenor of a symposium - *Science at the Shine Dome*, to celebrate the 50th anniversary of the Australian Academy of Science.

Australian Institute of Nuclear Science and Engineering (AINSE)

Professor J W White was Vice-President of AINSE in 2004 and, as part of strategic planning processes for the Institute, prepared a benchmarking report for AINSE science with Dr Rob Robinson (ANSTO).

CSIRO Student Research Scheme

The following year 12 students undertook research projects under the CSIRO student research scheme:

- Ms Grace Daley, Dickson College, with Drs N E Dixon/M J Headlam
- Mr Daniel Garcia, Marist College, with Professor S B Wild
- Mr Hans Gurleen, Canberra High School, with Mr J Hughes/Professor E Krausz
- Mr Francisco Silva, Marist College, with Drs N E Dixon/M J Headlam
- Mr Michael Taylor, Canberra Grammar School, with Professor S B Wild
- Mr Andrew Tuckwell, Canberra High School with Mr J Hughes/Professor E Krausz

Collaboration with RMIT University, Melbourne

As part of this collaboration between Professor M A Bennett and Professor S Bhargava (RMIT University), a PhD student, Kunihiko Kitadai, from the group of Professor Takahashi, Toho University, Japan, spent three weeks at the School carrying out experiments on gold-tertiary arsine complexes.

NMR Facility

On 17–19 March, the ANU's 800 MHz NMR Facility and Workshop, under the headship of Professor Gottfried Otting, was officially opened by Dr A Bax, NIH, USA. The particular features of this facility were presented at the Future Materials Workshop, ANU, on 24 August.

National Science Summer School

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

Royal Australian Chemical Institute (RACI)

Professor J W White is a member of the RACI Steering Committee for the forthcoming review: *Future of Chemistry: Review of the Pathway to Chemists – from education to employment.* He is also a long-standing member of the policy and nominations committees.

Symposia on Organometallic Chemistry

During November, Professor A F Hill, in collaboration with the Department of Chemistry, The Faculties, hosted a successful one-day symposium (**MC$_2$RO4**), bringing together chemists from Canberra, Adelaide, and Rennes, France, to highlight recent advances in alkynyl chemistry.

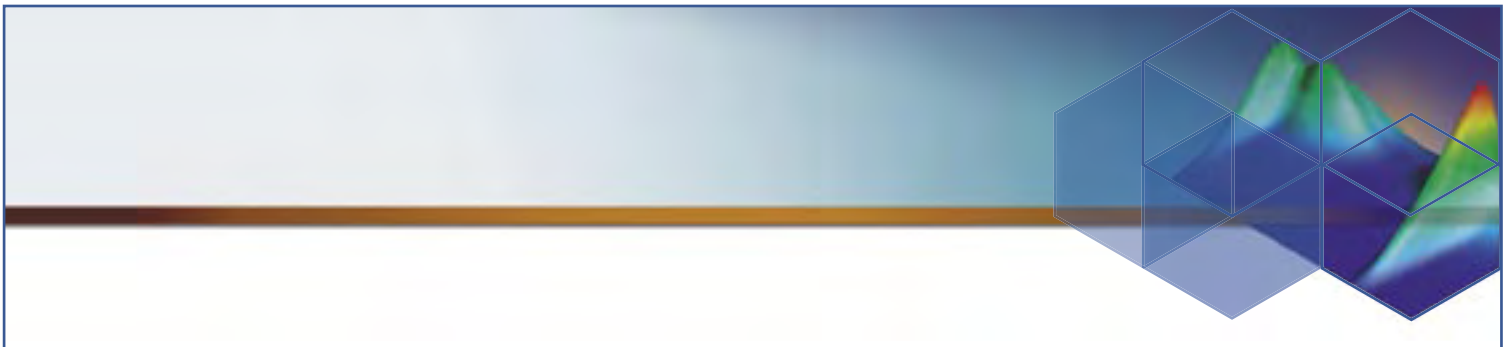
UnIChe (Universities, Industry, Chemistry)

The UnIChe project is an industry-linked chemistry outreach program from schools to PhDs. Funded by DEST, Orica Pty Ltd, and the Departments of Chemistry and Chemical Engineering at the Universities of Queensland, Melbourne, Newcastle, and the ANU, the project is coordinated by Dr P A Reynolds and chaired by Professor J W White. This project includes an undergraduate enrichment program for the ablest students to increase the flow of high quality chemistry graduates to industry; a school outreach program to raise awareness and value of the many interesting career options in chemistry; an industry relevant research PhD and Honours program; and a staff exchange program to strengthen the links between industry and university increasing the capacity of business to exploit and acquire university knowledge.

The undergraduate program continued with field trips for selected elite students from each of the four university departments. These included a Summer School (1-14 February) in both Canberra and Melbourne in which 35 students learnt about business and business practice in the classroom and followed this up in practice by visiting Orica industrial sites in Melbourne. This was augmented by two winter field trips in July and September to Newcastle for 40 students to see for themselves the 'ammonium nitrate trail' from synthesis by Incitec Ltd to the final end use in open-cut mining *via* the Orica explosives facilities.

Finally, UnIChe organised and financed two honours students and seven PhD students, selected on fundamental scientific merit, but also of interest to five of Orica's business areas. The students also presented their results to a joint Orica-University *Emerging Science* symposium with 48 participants, which was held in Melbourne on the 12 November to facilitate technology transfer to, and within the company.

UnIChe Summer School 2004



POST-GRADUATE CAREER DEVELOPMENT, EDUCATION AND TRAINING

The David Craig Lecture Series

The Craig Lecture was entitled *Nanoscale Molecular Architecture: Design and Self-assembly of Metallocyclic Polygons and Polyhedra via Coordination*. Other lectures in the series were: *Chemical Publishing: Perspectives of a JACS Editor, and Polyvalent Iodonium Chemistry*. The series was delivered by Professor Peter J Stang, Dean, College of Science, University of Utah; Distinguished Professor of Chemistry.

RSC Graduate Lectures

Dr Max Keniry 1D NMR techniques for Organic Chemists, August

PhD Degrees Awarded and Present Employment of Graduates

Dr Lorna Barr BSc *Strathclyde*
Modified Cyclodextrins as Catalysts and Molecular Reactors
Supervisor: Professor C J Easton
Currently: Postdoctoral Fellow, RSC

Dr Tory Nathan Cayzer BSc *Sydney*
Theoretical and Synthetic Investigations into the Intramolecular Diels-Alder Reaction
Supervisor: Dr M S Sherburn
Currently: Temporary Technical Officer, RSC, pending Church Ministry Traineeship in 2005/6

Dr James Richard Crow MChem *Sussex*
Studies Towards the Synthesis of Gibberellin Photoaffinity Probes
Supervisor: Professor L N Mander
Currently: Trainee Assistant Editor, Royal Society of Chemistry, Cambridge, UK

Dr Mariana Gebara-Coghlan BSc *Sydney* Hons *ANU*
Synthesis of the Triol Pharmacophore of Scmynol
Supervisor: Professor C J Easton
Currently: Therapeutic Goods Administration

Dr David Tien Jack Loong Btech (Chem Tech) *Massey*
Stereoselective Total Syntheses of the Macrolides (-)-Cladospolide A and (+)-Microcarpalide
Supervisor: Professor M G Banwell
Currently: Postdoctoral Fellow, School of Chemistry, University of Sydney

Dr Patrick David O'Connor BSc *Massey*
Synthesis of the Himandrine Skeleton
Supervisor: Professor L N Mander
Currently: Medicinal Chemist, BioFocus, UK; from 5/05 Postdoctoral Fellow, Ohio State University, Columbus, Ohio

Dr Andrew James Scott BSc *Sydney*
The Total Synthesis of (-)-Podophyllotoxin
Supervisor: Dr M S Sherburn
Currently: Postdoctoral Fellow, RSC

Dr Magne Olav Sydnes CandMag CandSc *Oslo*
Applications of gem*-Dihalocyclopropanes in Synthesis*
Supervisor: Professor M G Banwell
Currently: Research Fellow, Astra Zeneca Natural Product Discovery, Mt Gravatt Research Park, Brisbane

Dr Sean Yu McLoughlin BSc *James Cook*
Studies on the Phosphotriesterase from Agrobacterium Radiobacter *P230*
Supervisor: Professor D L Ollis
Currently: Postdoctoral Fellow, University of Colorado

MPhil Degrees Awarded

Mark James Abraham BSc *Tasmania*
Deconstructing Protein Threading Force Fields
Supervisor: Dr N E Dixon
Currently: PhD Scholar, JCSMR, ANU

Paul Gregory Dumanski BappSc *RMIT* Hons *Victoria UTech*
New Methods for Electrophilic Aromatic Halogenation
Supervisor: Professor C J Easton
Currently: Commonwealth Department of the Environment and Heritage

Ochitha Pumalie Karunaratne BAppSc *RMIT*
Microbially-Derived cis*-1,2-Dihydrocatechols as Starting Materials in Natural Products Synthesis: A Total Synthesis of the Stryryllactone (+)-Gonioldiol and Approaches to the Alkaloid (-)-Galanthamine*
Supervisor: Professor M G Banwell
Currently: CSIRO Molecular Science Laboratories, South Clayton, Victoria

Postdoctoral Fellows, Research Fellows and Fellows – Completions and Destinations

The School provides one of the very best environments for the education and research training of graduate students and postdoctoral fellows. Our interest in their welfare extends well beyond the time spent at the RSC, in part through a comprehensive alumni program. Although the School was founded only thirty-three years ago, many of our alumni now occupy senior positions in academia, government and industry, both in Australia and overseas.

Dr Joanne Bright accepted a position as senior research officer with the Department of Education, Science and Training, Canberra.

Dr Elizabeth R Humphrey returned to study at the University of Bristol to become a teacher.

Dr Natasha Hungerford accepted an appointment as a research scientist with the Chemical Synthesis Centre, University of Sydney.

Dr Thanh Phuoc Le accepted an appointment as lecturer, College of Science, Can Tho University, Vietnam.

Dr David T J Loong took up a postdoctoral fellowship at the University of Sydney.

Dr Peter Mahon accepted the position of Manager, Raman Microscopy Unit at the University of Canberra.

Dr Guido Pintacuda accepted a postdoctoral fellowship at Ecolé Normale Superieure de Lyon, France.

Dr Madeleine Schultz accepted an appointment as Research Fellow at the University of Queensland.

Dr Jamie S Simpson accepted a Marie Curie International Incoming Fellowship, Cambridge University, UK.

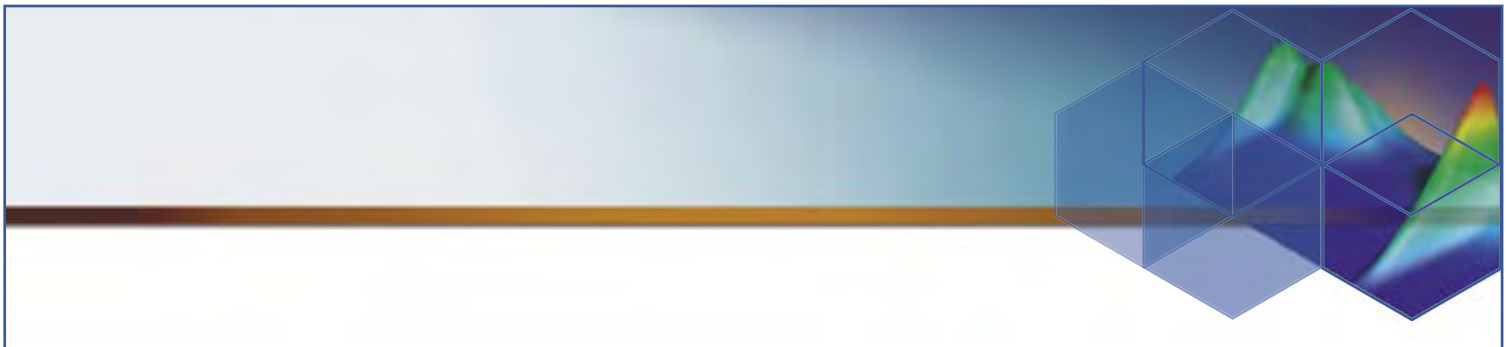
Dr Leon Wong accepted an appointment as Associate Lecturer in Chemistry, Charles Darwin University.

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 = UnICche
Deutscher Akademischer Austausch Dienst e.V. = DAAD
RSC Tuition Fee Scholarship = RSCT

Abernethy, Robyn BSc *Massey* BSc Hons *ANU*	ANU PhD
Bancia, Bogdan Dipl *Cuza Iasi, Romania*	ANU PhD/RSCT
Baranyai, Krisztian J BSc MSc *Monash*	ANU PhD
Barr, Lorna BSc *Strathclyde*	ANU PhD/RSCT
Barratt, Brendon BSc *Deakin*	ANU PhD
Barrett, Elizabeth S BSc *Sydney*	APA
Beck, Daniel BSc *RMIT*	APA
Bowen, Saara K BSc *New England*	ANU PhD
Brink, Franciscus J BAppSc *SAust* MAppSc *LaTrobe*	
Caldwell, Lorraine M BSc *UQ*	GSS/RSC
Carberry, David M BSc BEng Hons *ANU*	ANU PhD
Cayzer, Tory N BSc *Sydney*	
Chand, Satish BSc *USP* MSc *Macquarie*	ANU PhD
Chow, Leonie BSc *Melbourne*	
Cieslinski, Marta M BSc *Adelaide*	GSS/RSC
Crow, James MChem *Sussex*	ANU PhD/IPRS
Dawson, Ryan E BSc *Adelaide*	ANU PhD
Debono, Lesley BSc *New South Wales*	ANU PhD
Deev, Vitali BSc *Canterbury NZ*	GSS/RSC
Dewhurst, Rian D BSc *Canterbury NZ*	ANU PhD
Duncan, Alexander H BSc *Macquarie*	
Evenhuis, Christian R BSc *Tasmania*	APA
Fairweather, Kelly A BSc *Auckland* Hons *ANU*	APA
Fearnside, Luisa BSc *Melbourne* BSc Hons *UQ*	APAI
Friend, Martin P BSc *Murdoch*	APAI
Goodwin, Shelley K BSc *Griffith*	ANU PhD
Harfoot, Gwion BSc MSc *Waikato NZ*	
Harvey, Michael J MSc *Waikato NZ*	ANU PhD
Hughes, Joseph L BSc *ANU*	GSS/RSC
Hutt, Oliver E BSc *Otago, NZ* Hons *ANU*	ANU PhD
Jackson, Colin J BSc *Otago NZ*	GSS/RSC
Jergic, Slobodan AssocSc *La Guardia Coll NY* BSc *Belgrade*	ANU PhD/IPRS
Jury, Jasmine C BSc *Massey*	ANU PhD
Kanizaj, Nicholas BSc PGDip *UQ*	ANU PhD

Karunaratne, Ochitha BAppSc *RMIT*	APA
Khurana, Jeevan BScAgr *Sydney*	CSIRO
Kilah, Nathan L BSc *UQ*	APA
Kitto, Heather J BSc *Canterbury NZ*	GSS/RSC
Kokas, Okanya J BBiotech *UQ*	ANU PhD
Krenske, Elizabeth H BSc *UQ*	APA/VC
Kubik, Maria E BA Qld BAppSc *Canberra*	GSS
Kwan, Ching H L BSc/BCA *Victoria U Wellington* MSc *LSE UK*	GSS
Li, Iris H W BSc *Auckland*	ANU PhD
Lin, Ching-Yeh BS App Chem *National Chiao Tung, Taiwan*	ANU PhD/RSCT
Lording, William J BAppSci *RMIT*	ANU PhD
Loscha, Karin V BSc Dipl *Göttingen*	ANU PhD/DAAD
Lupton, David W BSc *Adelaide*	GSS/VC
Miller, Natalie A BSc *Sydney*	ANU PhD
Mortimer, Adam J BSc *Wollongong*	
Mulcair, Mark BSc *Monash*	ANU PhD
O'Connor, Patrick D BSc *Massey*	GSS
O'Neill, Darragh BA Mod Comp Chem *Trinity College, Dublin*	ANU PhD/RSCT
Padmakshan, Dharshana BSc MSc BEd *Kannur*	ANU PhD/RSCT
Park, Ah Young BSc *Victoria U Wellington* Hons *ANU*	ANU PhD
Pearson, Emma L BSc *WA*	ANU PhD
Perriman, Adam W BSc *James Cook*	ANU PhD
Philbrook, Amy A BSc *Maine*	UnIChe
Phillis, Andrew T BSc MSc *Waikato NZ*	ANU PhD
Reid, James C BSc LLB *Victoria U Wellington*	GSS
Sandala, Gregory M BSc *Windsor*	ANU PhD/IPRS
Scott, Andrew J BSc *Sydney*	APA
Sharp, Lisa A BSc *Sydney*	APA
Smith, Michael H BSc *Melbourne* Hons *Sydney*	
Stanislawski, Pauline C BSc *Monash*	ANU PhD
Stevenson, Bradley J BSc *Lincoln NZ*	GSS/VC
Sydnes, Magne O CandMag CandSc *Oslo*	ANU PhD/RSCT
Taylor, Rebecca M BSc MSc *Waikato NZ*	ANU PhD
Ting, Valeska P BSciTech *Victoria U Wellington*	ANU PhD
Tsai, Yi-Chin C BSc *Canterbury NZ*	ANU PhD
Tshabang, Never BSc *Botswana* MSc *Sussex*	U Botswana
Warr, Rebecca J BSc *Canterbury NZ*	GSS
Watson, Morgan A BSc Biochem *Canterbury NZ*	GSS/RSC
Watts, Zachary I BApplSc *RMIT*	ANU PhD
Wells, Kerrina BSc *ANU*	ANU PhD
Wu, Peter BAppSc *QUT* BSc Hons *ANU*	APA/VC



Visiting Scholars

As part of the recruitment program the School hosts international and Australian scholars for visits of two to six months to undertake research projects with individual staff members. In most instances the projects formed part of course requirements and the scholars were supported financially by their home institution:

Blüchel, Christian Diss *Federal Institute of Tech, Zurich*	M G Banwell
Buchan, Alexander MChem *Aberdeen*	C J Easton
Dumontet, Michael Masters *ENS de Cachan*	M A Collins
Esser, Simon PhD *Institute of Biotechnology 2, Jülich*	M G Banwell
Fontaine, Jean-Gonzague Chem Studies *ECPM Strasbourg*	M G Banwell
Hau, Tran V PhD *Can Tho, Vietnam*	L N Mander
Ilgen, Florian Diplom-Vorprüfung Chem *LMU, Munich*	M G Banwell
Kitadai, Kunihiko PhD *Tohu, Chiba*	M A Bennett
Olson, Ryan PhD *Iowa State*	M A Collins
Patrick, Joanna PhD *Adelaide*	C J Easton
Phyland, James PhD *Melbourne*	M G Banwell
Polster, Uwe PhD *Leipzig*	S B Wild
Somphon, Weenawan PhD *Suranaree UTech*	A D Rae
Vararattanavech, Ardcharaporn PhD *Mahidol, Thailand*	A J Oakley
Varganov, Sergey PhD *Iowa State*	M A Collins

Honours Scholars

The following scholars undertook joint Honours projects with the School and the Chemistry Department, The Faculties:

Baker, Matthew *ANU*	E M Sevick/D J Evans/R M Pashley
Bartlett, Michael *Curtin UT*	A F Hill/M G Humphrey
Hawley, Adrian *Melbourne*	J W White/R J Pace
Rands-Trevor, Karen *UQ*	M S Sherburn/M J Piggott

Summer Scholar Program

Summer Research Scholarships, of eight to ten weeks duration from November to February 2005, were awarded to twenty-two undergraduate students from Australia and New Zealand. All were involved in research projects with individual staff members:

Barber, Jeffrey *UTS*	R L Withers
Beasley, Andrew *WA*	T R Welberry
Bradford, Tanya B *UQ*	M S Sherburn
Brittain, David R B *Adelaide*	C J Easton
Burns, Nicholas D *Otago*	N E Dixon/M Keniry
Chan, Raymond S L *Adelaide*	N E Dixon
Chen, Jack L Y *Auckland*	L N Mander
Dao, Chau B *UQ*	N E Dixon
De Livera Jennifer *ANU*	C J Easton
Dennis, Eric *Flinders*	M S Sherburn
Hawley, Adrian M Melbourne/*ANU*	J W White
Hodgson, Jennifer L *ANU*	M L Coote
Keys, Timothy G *Griffith*	A Oakley
Kong, Wing C (Billy) *Adelaide*	A Oakley
Lampe, Stefan *Macquarie*	M G Banwell
Man, Bradley *NSW*	G Otting
Nath, Artika P *Otago*	E R Krausz
Pinkerton, David M *ANU*	M G Banwell
Sheridan, Morgan B *ANU*	D L Ollis
Watts, Frances M *Sydney*	S B Wild/A F Hill
Yeatman, Holly R *Murdoch*	D L Ollis
Zayya, Almas I *Victoria U Wellington*	A F Hill/S B Wild

INTERACTIONS ACROSS THE UNIVERSITY

Undergraduate Lecture Courses Presented in The Faculties

The following are lecture courses were given by RSC staff to undergraduate and Honours classes in The Faculties:

Department of Chemistry, Faculty of Science

Chem A16 Chemical Characterisation – 4 lectures (Hill, coordinator)
Chem A16 Organic Chemistry – 4 lectures (Sherburn)
Chem A16 Biological Chemistry – Introduction to the Chemistry of Life – 4 lectures (Headlam, Prosselkov, Schaeffer, N Williams)
Chem A16 Organic Chemistry – Protein Structure and Function – 1 lecture (Headlam)
Chem A16 Organic Chemistry – 4 lectures (Sinclair)
Chem A16 Organic/Medicinal Chemistry – 4 lectures (Sinclair)
Chem A17 The Chemistry of Food – 4 lectures (Loong)
Chem A17 Structural Biology by NMR – 4 lectures (Otting)
Chem 3105 Quantum Chemistry – 9 lectures, 1 tutorial (Collins)
Chem 3106 Lanthanoid and Actinide Coordination Chemistry – 7 lectures (M Smith)

The following research students undertook demonstrating and marking in the Department of Chemistry:
Chem A14/A16 Demonstrating (Bartlett)
Chem A14/A16 Demonstrating (Dewhurst)
Chem A14/A16 Demonstrating (Jergic)
Chem A14/A16 Demonstrating (Kitto)
Chem A14/A16 Demonstrating (Krenske)
Chem A14/A16 Demonstrating (Warr)
Chem A15/A17 Demonstrating (Beck)
Chem A15/A17 Demonstrating (Warr)
ChemA15/A17 Demonstrating (Kilah)
Chem A15 Demonstrating and marking (Wu)

The following Honours student were jointly supervised by RSC staff and staff of the Chemistry Department:

Mr Michael Bartlett	Hill/Humphrey
Mr Adrian Hawley	White/Pace
Ms Karen Rands-Trevor	Sherburn/Piggott
Mr Matthew Baker	Pashley/Sevick/Evans

Department of Physics, Faculty of Science

Phys3032 - Solid State and Statistical Physics - 6 lectures, 1 tutorial, 3 practicals (Goossens)

Division of Biochemistry and Molecular Biology, Faculty of Science

Biol 2162 Molecular Biotechnology – 3 lectures (Dixon)
Biol 2171 Biochemistry – 2 lectures (Ollis)
Biol 3181 Protein Structure and Function – 4 lectures, 1 tutorial (Otting)

University Service

Professor M G Banwell IAS Representative, Admissions Committee; Chair, Working Group on Research Development at the ANU

Dr N E Dixon Member, Chemistry Library Advisory Committee (CHEMLAC); Member, Radiation Safety Committee; Liaison Officer, Institutional rDNA Committee; Member, Medical Sciences Board of Studies

Professor C J Easton Convenor, Graduate Studies in Chemistry; Member, Board of the Institute of Advanced Studies; Member, SHE Divisional Research Committee; Member, SHE Graduate Studies Committee; Member, Steering Committee, National Institute of Bioscience; Member, Department of Chemistry Review Committee

Professor D J Evans Member, ANU Council; Member, Academic Board; Chair and IAS representative, Consultative Committee, Chair, Centre for the Science and Engineering of Materials (CSEM); Chair, High Performance Computing Advisory Committee; Chair, Supercomputer Time Allocation Committee, ANU Supercomputer Facility (ANUSF); Member, Research Advisory Board, Research School of Astronomy and Astrophysics; Member, Board of the National Centre for Theoretical Physics; Chair, Centre for Complex Systems

Professor A F Hill Member, National Institute of Science Steering Committee; Member, Research Committee; Member, Forum of the Institute of Advanced Studies; Coordinator, National Youth Science Forum; RSC Course Coordinator, Chemistry A16/A17, The Faculties

Dr M A Keniry Head, University Nuclear Magnetic Resonance Centre; ex officio Member, University Nuclear Magnetic Resonance Centre Management Committee

Professor E R Krausz Member, Centre for Science and Engineering of Materials Committee; Adviser, Research Integrity; Coordinator, ANU Mentoring; Member ANU Radiation Safety Committee

Emeritus Professor L N Mander Chair, MSNMR Sub-committee of Major Equipment Committee

Professor D L Ollis Member, Board of Studies, Biochemistry and Molecular Biology Graduate Program

Professor G Otting Member, Research Advisory Board, John Curtin School of Medical Research

Professor A D Rae Member, Radiation Safety Subcommittee–Occupational Health and Safety Policy

Dr M S Sherburn Management Representative, ANU Occupational Health and Safety Policy Committee

Professor T R Welberry Member, RSAA/RSES Local Promotions Committee

Professor J W White Member, University Staff Consultative Committee; Member, Art Acquisitions Committee, Member Vice-Chancellor's "Engagement Committee"

Professor R L Withers Member, Board of Studies of the Graduate Program in Chemistry; Member, ANU Science, Health and Engineering (SHE) Post-graduate Research Scholarships Committee; Member, ANU Science, Health and Engineering (SHE) Divisional Education Committee

A list of School committees, representatives and office bearers is given in the Internal Management section

INTERNAL MANAGEMENT

Administrative Support Structure

The management of the School is coordinated through the Business Office and the Academic Secretary's Office. The senior administrative staff in 2004 comprised:

- the Laboratory Manager *(L Harland)*, who is responsible for non-academic functions in the School, including managerial, financial and budgetary, occupational health and safety, and the supervision and well-being of the technical support staff;
- the Business Officer *(L Scarr)*, who is responsible for the supervision of the School's administrative and security/cleaning staff, and assists the Laboratory Manager with the business management of the School;
- the Academic Secretary *(M A Holloway)*, who is responsible for matters pertaining to academic staff and students, particularly appointments, promotions, current rules, regulations and practices, and is the focus for outreach issues. The Academic Secretary acts as secretary to the Faculty Board and their committees, and provides advice and administrative assistance to the Dean;
- the Facilities Officer *(K Cooper)*, who is responsible for the maintenance, operation and safety of the building plant and services;
- the Laboratories and Safety Co-ordinator *(L L Welling)*, who is responsible for the maintenance and operation of laboratory facilities, and oversees the control of hazards in all of the School laboratories;
- the Purchasing Officer *(N Bayley)*, who is responsible for the supervision of the purchasing/stores staff and the procurement of goods and services for the School. The Purchasing Officer is responsible for the provision of the imprest store, which services the RSC and other areas of the ANU.

Technical Support and Research Services

The capacity of the School to undertake leading-edge research is underpinned by highly skilled technical staff, whose skills and expertise complement those of the academic staff.

Technical Support

The output of experimental groups in the RSC is supported by technical staff attached to individual groups. 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, but their expertise is also made available to other groups. The technical staff contribute to the research projects of their groups and this is acknowledged by co-authorship of publications. In addition, the technical staff assist the Laboratory Manager in implementing and monitoring safety policy within the groups.

ANU Microanalytical Services Unit

During 2005, the Unit completed a total of 1954 analyses on 1649 samples submitted by 200 individuals, most of which (79%) were CHN analyses. This year 45% of requests originated in the RSC. External organisations requesting analyses (30% of total requests) include the University College UNSW ADFA, James Cook (Townsville Campus), Melbourne, Newcastle, University of New South Wales, Queensland, Sydney, Sydney Grammar School, Deakin, Western Australia, Western Sydney and Wollongong. Significant requests continue to come from Commercial and Governmental sources

(18%). Commercial and Governmental clients included the Institute for Drug Technology, ANSTO, Access Pharmaceuticals, Children's Cancer Institute, CSIRO (Centre for Materials and Infrastructure Technology), Concorde Repatriation Hospital, Progen Industries, and the Victoria Museum.

Ms Reet Bergman was 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 submission of samples can be found on the website. *(V L Withers*[⊕]*, A Melnitchenko)*

External earnings for 2003 were $49,874.07

http://rsc.anu.edu.au/facilities/micro.php

Computer Unit

The Computer Unit provides support for the diverse range of software and hardware used in the School. The School has 45 Unix workstations (Linux, SGI and Sun). These Unix computers are used for a variety of purposes including data-reduction, desktop use and a small amount of computation. 150 Apple Macintosh computers are used as the desktop systems for most staff and students. In addition, 80 PCs mainly running Microsoft Windows are used for controlling experimental and data collection equipment. Printing services are provided by twenty laser printers and 4 thermal wax colour printers.

The School main servers run Debian Linux. These servers provide external services including the School's e-mail and web services and internal services such as authentication and file-serving, plus the ability to run small to medium sized computational tasks. A separate server provides mirroring of all the Unix disks and most of the machines running OSX in the School. Archives and backups of the Schools computers are now done to hard-disk.

The major hardware acquisitions this year have been of Apple Macintosh Dual G5s, Imac G5s, Emacs, ibook G4s, G4 Laptops as well as several new small to medium Linux servers, several Linux workstations and ten new PCs running Microsoft Windows. The School's web page is administered by Chris Blake and can be found at http://rsc.anu.edu.au/index.php. *(P R Cohen, C D Delfs, R Faletic*[⊕]*, G A Lindsell)*

http://rsc.anu.edu.au/~rsccu/index.html

Single Crystal X-ray Diffraction Unit

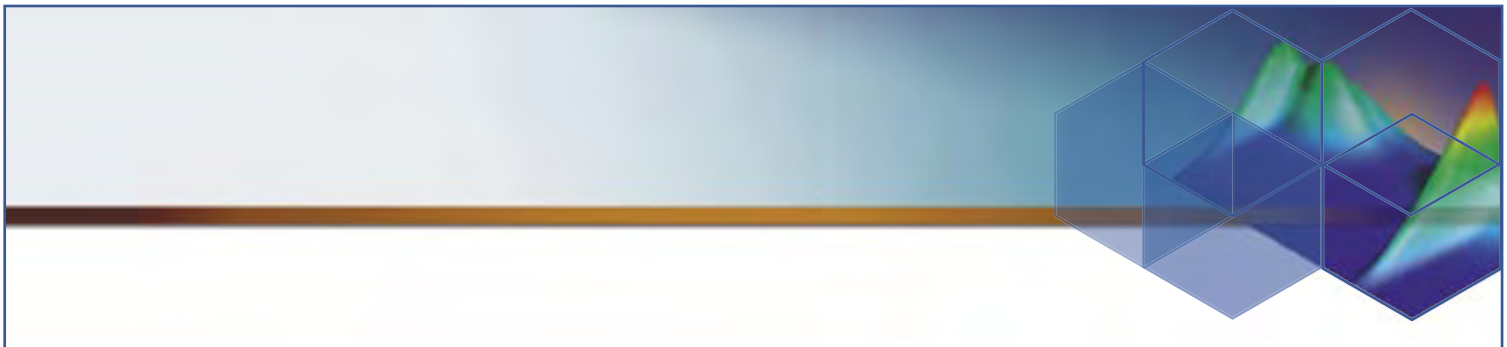
The unit performs crystal structure analyses on samples provided by various groups within the RSC. Some of the structures now being solved and refined have as many as 400 non-hydrogen atoms and so are similar in size to small proteins. X-ray diffraction data sets are collected on a Nonius Kappa-CCD area-detector diffractometer equipped with IFG capillary X-ray-focusing collimators and an Oxford Cryosystems crystal cooling device. Data sets were also collected for other members of the RSC to solve and refine. Several 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, 167 data sets were collected and 109 final reports produced for the year. External work was performed for University College UNSW ADFA, the South Australian Museum, Monash University and RMIT University. *(A J Edwards, A C Willis)*

Group	Data Sets Collected	Reports Completed
RSC	150	100
Others (ANU)	10	9
Others (External)	7	–
TOTAL	167	109

Mass Spectrometry Service

During 2004 the new Bruker Apex 3 HR FTICR Mass Spectrometer was finally commissioned after initial installation difficulties. In total, 5602 measurements were made throughout the year on the six different Mass Spectrometers. The Synthesis and Mechanism Group (1920) is still the heaviest user to date. The majority of samples were run for the RSC along with the Chemistry Department (450) being the other major outside users.



The total samples run through each Mass Spectrometer are as follows: VG Autospec (2916), VG Quattro 2 (1286), Micromass ZMD (908), HP Agilent GC/MS (351), Bruker FTICR (102), VG ZAB (39). *(J M Allen [Head], G Lockhart, A Jeyasingham⊕ [from mid 04])*

http://rsc.anu.edu.au/facilities/mass.php

University NMR Centre

In the past year, the first 800 MHz spectrometer to be delivered in Australia was installed at the ANU. This spectrometer is a joint facility of a consortium of Universities from the ACT and NSW. A cryoprobe, ordered with the spectrometer, will be delivered and installed by mid-2005. The 800 MHz spectrometer is housed in a purpose-built building adjacent to the ANU NMR Centre. The very-high field NMR spectrometer joins six other lower field instruments at the ANU NMR Centre. Consistent reliability of all the instrumentation during 2004 has enabled a high productivity for the NMR Centre.

During the year the University NMR Centre catered for 120 users from RSC, the Research School of Physical Sciences, Research School of Biological Sciences, John Curtin School of Medical Research, The Faculties, Charles Sturt University, University College UNSW ADFA, University of Sydney, University of NSW and the University of Wollongong. Applications include *in vivo* NMR, nucleotide and protein structure determination, analysis of natural products and synthetic intermediates, NMR of organometallic compounds and variable temperature NMR. *(M A Keniry, C J Blake, P T Culnane, P M Simmonds)*

http://bloch.anu.edu.au/

Research Services

Staff of the section provided expert advice on the design, manufacture, maintenance and refurbishment of equipment to the academic and research staff of the School, the ANU and the broader community. The primary focus of this section is the support of RSC research and teaching programs.

Carpentry and Paint Workshops

These workshops are well equipped with carpentry and joinery machinery and spray painting facilities, and provide outstanding custom furniture and fittings for the School's laboratories and offices, in addition to specialised scientific apparatus and specialised surface finishes to engineering materials of all workshop sections. Major projects in 2004 included work related to the installation of the 800 MHz NMR spectrometer. *(I J Clarke, R J O'Brien)*

Cryogenics Unit

This unit provides cryogens, liquid nitrogen and helium, to the School and the wider ANU community (Department of Chemistry, The Faculties, and RSES). *(P Devitt, R J O'Brien)*

Electrical Unit

This unit provides services in electrical wiring and modifications, new equipment verification and installation, maintenance of electrical research and plant equipment. The mandatory electrical safety checking of appliances throughout the School is co-ordinated by staff in this unit. *(F Vera [from 24/5/03], R J O'Brien)*

Electronics Unit

This unit is equipped with design, development, and construction facilities, including specialised services for computer-aided design and printed circuit board (PCB) manufacture. In addition, electronic repair services are provided for the research groups within the School and the instrumentation service units, such as the Mass Spectrometry Unit, in preference to using external service engineers. *(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, or safety. Throughout 2004 the unit continued to provide an impeccable service to research programs within the RSC and the wider ANU community, as well as undertaking work for external clients. *(P Siu, C J Tomkins)*

Mechanical Workshops

This main workshop is equipped with precision engineering capabilities for instrument development (*e.g.* precision milling, turning, and welding), mechanical maintenance and repair, and the design and manufacture of prototype apparatus in metal or plastic. In support of all laboratory research programmes, extensive maintenance, repair and fabrication services were provided by the workshop. Installation of services (gas, water, vacuum, equipment racks) associated with fume-cupboard and laboratory upgrades continued, together with support of the environmental program to convert instrument cooling systems reliant on mains water to recirculating chilled water systems. The workshop also continued to provide support to the wider ANU community, such as the Facilities and Services Division Zone-3 maintenance section.

The mechanical prototype workshop provides mechanical engineering services, prototypes of advanced scientific instrumentation, high vacuum, cryostat, and helium leak detection services to the School. *(P Devitt, R Filardo, M J Hill, K L Jackman, R J O'Brien)*

⊕ = part-time

School Committees, Representatives and Office Bearers

Faculty Board

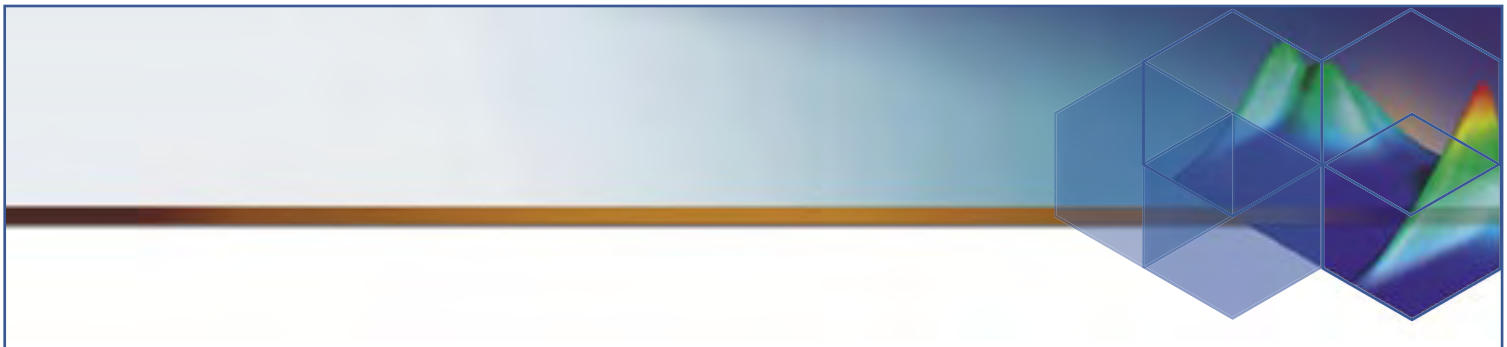
Professor D J Evans, Dean *(Chair) (ex officio)*
Professor C J Easton, Deputy Dean *(IF rep) (ex officio)*
Professor R A Withers, Associate Dean (Students) *(ex officio)*
Professor M G Banwell
Professor M A Collins
Professor P M W Gill *(from 31 August)*
Professor A F Hill *(Academic rep IF)*
Professor E R Krausz
Professor Emeritus L N Mander
Professor D L Ollis
Professor G Otting
Professor L Radom *(to 31 Oct)*
Professor A D Rae
Professor J W White
Professor T R Welberry
Professor S B Wild
Professor J W White
Dr M L Coote
Dr N E Dixon *(MS Board of Studies rep)*
Dr G A Heath
Dr M J Henderson *(Faculty rep)*
Dr M A Keniry
Dr A J Oakley
Dr E M Sevick
Dr M S Sherburn
Dr D Sinclair *(Faculty Rep; IF rep)*
Mr K Cooper
Ms L Harland

Academics-in-Charge

Crystal Structure Service:	Professor C J Easton
Mass Spectrometry:	Professor C J Easton
Microanalytical Unit:	Professor C J Easton
UNMRC:	Dr M A Keniry
EPR Facilities:	Dr R D Webster

Advisory Committee on Safety

Professor T R Welberry *(Chair)*
Professor M G Banwell
Mr K Cooper
Mr P A Gugger
Mrs P E Lilley
Mr H McGlinchey



Mr C J Tomkins
Mr L L Welling
Professor S B Wild
Mrs V Withers
Ms L Harland
Dr J-W Liu

ANU Radiation Safety Committee Officer and Licensee for Radiochemicals, AQIS and Institutional rDNA Committee Liaison Officer

Dr N E Dixon

ANU Marketing Committee

Ms Marilyn Holloway *(RSC rep)*

Board of Studies of the Graduate Program in Chemistry

Professor C J Easton *(Chair/Convenor)*
Professor M G Banwell
Professor R L Withers
Professor A F Hill

Chemistry Library Advisory Committee (CHEMLAC)

Professor M G Banwell *(Chair)*
Professor M A Collins
Professor A F Hill
Dr N E Dixon
Ms S Jackson
Mr P McNamara
Dr M Humphrey *(Chemistry, Faculty of Science)*
Mrs J Smith
Dr C Chai *(Chemistry, Faculty of Science)*

Crystallography Committee

Professor A F Hill *(Chair)*
Professor A D Rae
Dr A C Willis
Professor C J Easton
Dr M Humphrey *(Faculty Rep)*

Dean's and Crawford Prize Selection Committee

Professor T R Welberry *(Convenor)*
Professor S B Wild
Professor M G Banwell

Distinguished Visitors Selection Committee

Professor M G Banwell *(Chair)*
Professor S B Wild
Professor P M W Gill
Professor T R Welberry

IT Committee

Professor T R Welberry *(Chair to April)*
Professor M G Banwell *(Chair from May)*
Mr C J Blake
Ms P Cohen
Professor E R Krausz

Local Area Consultative Committee (LACC)

Mr K Cooper *(Chair)*
Dr P Carr
Dr M S Sherburn *(Academic Rep)*
Dr R Webster *(RO Rep)*
Ms P Cohen
Dr J Renner *(Postdoctoral Fellows Reps)*
Mr P Sui, Mr M J Hill *(Technical Officer Reps)*
Mr C Evenhuis, Ms H Kitto *(Grad Students Reps)*

Ex-officio Members:

Professor D J Evans, *Dean*
Ms M A Holloway, *Academic Secretary*
Ms L Harland, *Laboratory Manager*

National Science Teachers Summer School RSC Coordinators

Professor R W Rickards
Dr E M Sevick

Occupational Safety and Liaison Officers

Mrs R E Enge
Dr A Scott
Mrs L M Monaghan
Mrs S Riches
Dr G A Lindsell
Ms N Johnson
Mrs E O'Toole

Ombudspersons

Professor C J Easton
Ms M A Holloway
Dr E M Sevick
Professor R L Withers

Promotions Committee (Local Area)

Professor D J Evans *(Chair)*
Professor M G Banwell
Professor S B Wild
Professor E Krausz
Professor G Otting

External members:

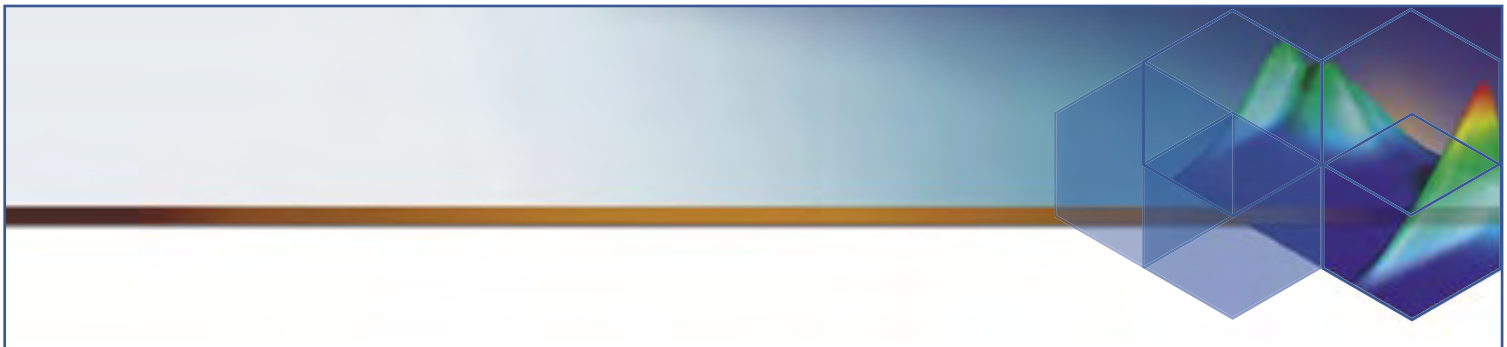
Adjunct Professor V James OAM, Formerly U Sydney
Professor A Byrne, Head, Dept of Physics, Faculty of Science
Secretary: Ms M A Holloway

Visitors Grants Committee

Professor T R Welberry *(Chair)*
Dr N E Dixon
Professor C J Easton

WWW Site Committee

Professor E R Krausz *(Chair)*
Ms P Cohen
Mr C J Blake *(Webmaster)*
Ms M A Holloway



FINANCE

Financial Summary

The School continued its success in obtaining funding through the Australian Research Council's competitive grants schemes, thus the financial strategy in 2004 again focused on consolidation and up-grading of resources required to support both new and on-going research. Several new items of equipment were purchased, and the ongoing programme of expenditure on small to medium items of research and IT equipment to replace old and obsolete items was continued.

In addition to recurrent income, the research contracts with biotechnology company Progen Industries Ltd and ORICA (Australia) Ltd continued throughout the year. The UnIChe Project, part of the DEST Higher Education Innovation Programme, was renewed for a further two years. 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 ($10,742,000) was supplemented by external income of $5,369,287.

Outside Grants and Contracts

** denotes a new grant in 2004

The recipients and sources of external grants are as follows:

Biochemical Reactions and Molecular Recognition

Professor C J Easton
Amino acid and peptide radicals in biochemistry and synthesis
Australian Research Council, Discovery-Project, January 2003–December 2005

Professor C J Easton
Platform technology for new pharmaceuticals
ACT Government, March 2003–March 2004

Professor C J Easton **
29th international symposium on macrocyclic chemistry and 20th Royal Australian Chemical Institute Organic Chemistry Conference
DEST, Innovation Access Program, February 2004–July 2004

Professor C J Easton and Dr M Casarotto
Synthetic compounds to specifically activate or inhibit ryanodine receptor calcium ion channels
Australian Research Council and Biotron Ltd, Linkage-Projects, January 2003–December 2005

Professor C J Easton and Professor S F Lincoln **
Supramolecular Assemblies as nanoscale devices to control chemical and physical processes
Australian Research Council, Discovery-Projects, January 2004–December 2008

Biomolecular NMR

Professor G Otting
New methods for structural biology in solution
Australian Research Council, Federation Fellowship, January 2002–December 2006

Professor G Otting
New methods for structural biology in solution
Australian Research Council, Discovery-Projects, January 2003–December 2007

Professor G Otting and Dr N E Dixon
Enabling technologies for structural genomes
Australian Research Council, Discovery-Projects, January 2003–December 2005

Computational Quantum Chemistry, Polymer Chemistry

Dr M L Coote
Hydrogen abstraction in chemical, biochemical and polymerisation processes
Australian Research Council, Postdoctoral Research Fellowship, June 2002–June 2005

Coordination Chemistry and Spectro-electrochemistry

Dr G A Heath **
The first development of multi-dimensional spectro-electrochemistry and its application to crucial transformations in inorganic systems
Australian Research Council, Discovery-Projects, January 2004–December 2006

Disordered Materials

Professor T R Welberry
*Development of methods and strategies for the measurement, interpretation and analysis of diffuse X-ray scattering from disordered materials**
Australian Research Council, Discovery-Projects, January 2003-December 2005

Professor T R Welberry **
An energy resolved study of diffuse neutron scattering from benzil the temperature dependence of diffuse neutron scattering from benzil
ANSTO, Access to Major Research Facilities Program, January 2004

Professor T R Welberry, Professor R L Withers, Professor A Pring and Dr N Ishizama
The effects of local strain on the crystal structure of solid solutions
Australian Research Council, Discovery-Projects, January 2003-December 2005

Dr D Goossens **
Structure and magnetic order in $Ln_{1-x}Sr_xCoO_3$(Ln = Y, Ho) using neutron powder diffraction
AINSE, Access to Facilities Program, March 2004

Dr D Goossens **
Study of the structural phase transition in d-benzil using neutron powder diffraction
AINSE, Access to Facilities Program, June 2004

Dr D Goossens **
Phonon softening at the structural transition in d-benzil $C_{14}D_{10}O_2$
ANSTO, Access to Major Research Facilities Program, October 2004

Electrochemistry

Dr R D Webster
In situ electrochemical NMR spectroscopy
Australian Research Council, Queen Elizabeth II Fellowship, June 2001–June 2006

Inorganic Stereochemistry and Asymmetric Synthesis

Professor S B Wild
Asymmetric synthesis of chiral phosphines, arsines and stibines
Australian Research Council, Discovery-Projects, January 2003-December 2005

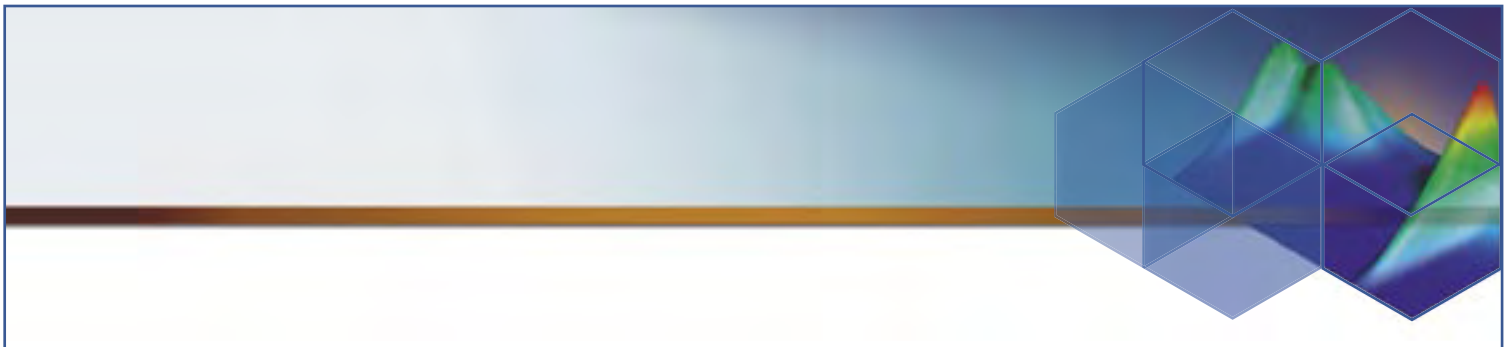
Liquid State Chemical Physics

Professor D J Evans and Dr E M Sevick
Experimental demonstrations of violations of the Second Law of Thermodynamics
Australian Research Council, Discovery-Projects, January 2003-December 2005

Professor D J Evans and Dr D J Bernhardt **
Fluid properties and chaotic dynamics in equilibrium and nonequilibrium states
Australian Research Council, Discovery-Projects, January 2004-December 2008

Organic Synthesis

Professor L N Mander
Preparation of photo-affinity molecular probes for the identification of gibberellin receptors
Australian Research Council, Discovery-Projects, January 2003-December 2005



Organic Synthesis, Methodology and Host-guest Chemistry

Dr M S Sherburn
New cascade routes to biologically important molecules
Australian Research Council, Discovery-Projects, January 2002-December 2004

Dr M S Sherburn and Professor M Paddon-Row
New horizons in Diel-Alder chemistry
Australian Research Council, Discovery-Projects, January 2003-December 2005

Polymers and Soft Condensed Matter

Dr E M Sevick and Professor D J Evans
Experimental demonstrations of violations of the Second Law of Thermodynamics
Australian Research Council, Discovery-Projects, January 2003-December 2005

Dr E M Sevick and Professor J S Williams and Professor B W Ninham **
Salt, sugar and sequence: The effect of molecular forces on polymer conformation
Australian Research Council, Discovery-Projects, January 2004-December 2006

Protein Crystallography and Engineering

Professor D L Ollis
Directed evolution used to probe protein structure and funcation: new enzymes for bio-remediation and industry
Australian Research Council, Discovery-Projects, January 2003-December 2005

Dr P D Carr **
Structural studies of the cytokine receptor complexes involved in IL-3, IL-5 and GM-CSF signalling
ANSTO, Access to Major Research Facilities Program, February 2004

Dr P D Carr **
Interactions of the epsilon subunit of E coli DNA polymerase III with nucleotides
ANSTO, Australian Synchrotron Research Program, February 2004

Dr P D Carr **
Cytokine receptor complexes involved in IL-3,IL-5 and GM-CSF sign
ANSTO, Australian Synchrotron Research Program, November 2004

Protein Structure and Function

Dr N E Dixon, Dr E Liepinsh and Dr J Carazo
Structures and functions of bacterial replisomal proteins
Australian Research Council, Discovery–Projects, January 2002–December 2004

Dr N E Dixon and Professor G Otting
Enabling technologies for structural genomes
Australian Research Council, Discovery-Projects, January 2003–December 2005

Dr N E Dixon and Dr G Coia **
New methods for directed molecular evolution of novel protein functions
Australian Research Council and Evogenix Pty Ltd, Linkage-Projects, March 2004–December 2005

Dr K Ozawa
Subunit contacts in the replicative DNA polymerase: A new paradigm for protein-protein interactions
Australian Research Council, Linkage-Postdoctoral Fellowship (CSIRO), October 2003-October 2006

Solid State Inorganic Chemistry

Dr R L Withers **
The crystal structure of some photocatalytic 1:1 and 1:2 B-site substituted complex perovskites
AINSE, Access to Facilities Program, June 2004

Professor R L Withers, Professor T R Welberry, Professor A Pring and Dr N Ishizama**
The effects of local strain on the crystal structure of solid solutions
Australian Research Council, Discovery-Projects, January 2003-December 2005

Solid State Molecular Science

Professor J W White **
The UnIChe project
DEST, Higher Education Innovation Program, January 2004–December 2005

Professor J W White **
Drying of dairy proteins – strategies for preserving functional properties during dehydration
Food Science Australia, January 2004–December 2006

Professor J W White **
Making film-stars: Nano-composite films for solar energy capture
DEST, Innovation Access Program, March 2004–May 2006

Professor J W White **
High internal phase emulsions – structure and rheology control
ORICA (Australia) Ltd, April 2004–March 2005

Professor J W White **
Designer surfactants for creation of emulsion properties
Australian Research Council and ORICA (Australia) Ltd, Linkage–Projects, 2004–2008

Professor J W White **
Protein structure at oil-water surfaces
AINSE, Access to Facilities Program, June 2004

Professor J W White **
Structure of titanium oxide films at solid surfaces
AINSE, Access to Facilities Program, August 2004

Professor J W White **
Mechanisms of the structure formation in templated growth of metal oxide films
ANSTO, Access to Major Research Facilities Program, August - December 2004

Professor J W White **
Interfacial structure of block copolymers at the air-water interface; kinetics of the absorption of lysozyme at the air-water interface; interfacial structure of block copolymers at the oil-water interface; cosurfactant stabilization of high internal phase emulsions
ANSTO, Access to Major Research Facilities Program, September - December 2004

Professor J W White and Dr S A Holt
The nanoscale structure of milk: Stability implications for milk products
Dairy Research and Development Program, January 2001–June 2004

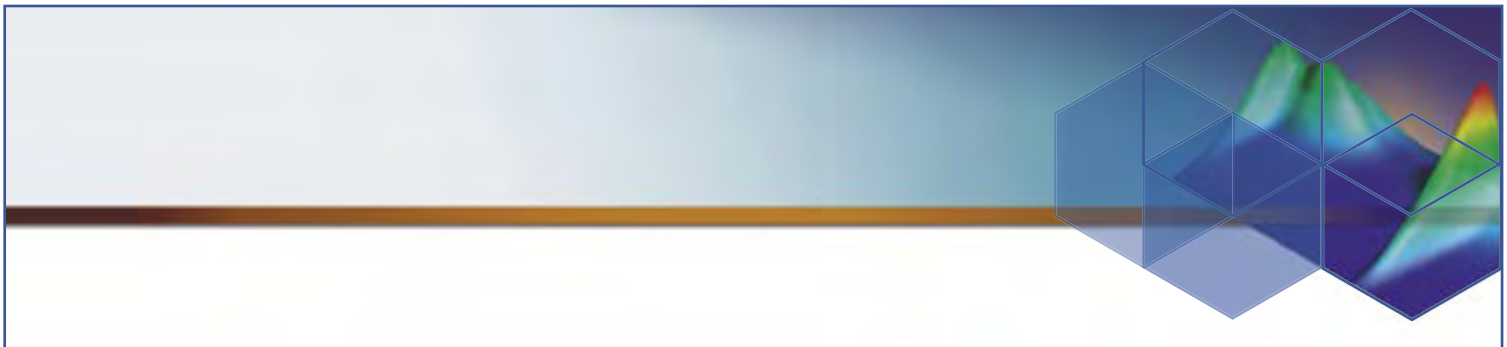
Professor J W White, Dr P A Reynolds, Dr R J Goodridge and Dr C Such
High internal phase emulsions – structure and rheology control
Australian Research Council and ORICA Australia Ltd, Linkage-Projects, January 2002–December 2004

Professor J W White and Dr M Henderson **
The aggregation behaviour of protein/sugar complexes
AINSE, Access to Facilities Program, August - October 2004

Professor V James **
A study of the diffraction patterns of hair with disease
ANSTO, Access to Major Research Facilities Program, January 2004

Mr A Perriman
Protein behaviour at interfaces
Australian Institute of Nuclear Science and Engineering Student Award, July 2003-June 2004

Dr P A Reynolds **
Aggregation in high internal phase emulsions
ANSTO, Access to Major Research Facilities Program, February 2004



Synthesis and Mechanism

Professor M G Banwell
Progen phase III synthesis and identification of novel, heparinoid mimetics and development of the heparanase enzyme as a diagnostic and therapeutic target
Progen Industries Ltd, October 2002–September 2005

Professor M G Banwell
Generation and exploitation of fermentation products in the chemical synthesis of biologically active compounds with therapeutic potential
Australian Research Council, Discovery–Projects, January 2002–December 2004

Professor M G Banwell and Mr M P Friend
Development of chemoenzymatic methods for the selective elaboration of polyfunctional therapeutic agents to oligomers with improved efficacy
Australian Research Council and Biota Holdings Ltd, Linkage–Projects, December 2003–December 2006

Professor M G Banwell and Ms L Fearnside **
Chemoenzmatic routes to novel dendritic architectures suitable for Pharmaceutical Applications,
Australian Research Council and Starpharma Ltd, Linkage–Projects, March 2004–December 2006

Professor M G Banwell and Associate Professor M J Garson **
Synthetic, Molecular and biological studies on novel marine metabolites isolated from Great Barrier Reef sponges
Australian Research Council, Discovery–Projects, January 2004–December 2006

Synthetic Organometallic and Coordination Chemistry

Professor A F Hill
Metallaboratranes: Soft scorpionates and masked metal bases
Australian Research Council, Discovery-Projects, January 2003–December 2005

Theoretical Chemical Physics

Professor M A Collins and Associate Professor M Zhang **
The energetics and dynamics of chemical reactions of polyatomic molecules involving multiple electronic states
Australian Research Council, Discovery–Projects, January 2004–December 2006

ENVIRONMENT POLICY

A summary of management practices that benefit the environment follows:

Energy and Resource Conservation

- diaphragm pumps are being used in several 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

Gender Issues

The following actions have been taken in the School in support of affirmative action:

The Rita Cornforth Fellowship

The Fellowship, named in honour of the distinguished Australian chemist, Rita Cornforth, was created specifically for young women with high academic potential, to allow them the resources and independence to become established in preparation for the uptake of a tenured position. It was established in 1996 and it carries special conditions designed to assist the successful candidate in establishing and furthering her research career. Dr Nicola Brash held the inaugural fellowship from 1998-2002. The second Fellowship was awarded to Dr Michelle Coote for a fixed-term of five years in October 2003. Dr Coote, as head of Computation Quantum Chemistry, Polymer Chemistry Group, has since won two ARC Discovery Grants, one jointly with Professor Bruce Wild.

Senior Women

The School continues with two independent research groups headed by women, Dr Michelle Coote (as above) and Dr Edith Sevick, on a standard appointment as Senior Fellow and head of the Polymers and Soft Condensed Matter Group.

Professor Veronica James OAM, formerly of the University of New South Wales, continued her three-year appointment as Adjunct Professor. She serves the School on promotions and selection committees and continues research collaborations with Professor John White.

Comment on Gender Equity Strategies

An informal program to meet gender equity objectives is continuously in progress in the Research School. Professor Elmars Krausz, formerly the representative on the ANU Equity and Diversity Consultative Group, continues to advise the Dean on such matters as required.

Student and Academic Staff Recruitment Profiles

In the RSC PhD program the number of females recruited annually since 1994 averaged 24% of total recruits to 2001. Since then, the average number of females recruited to the program has risen to 36%.

In the Summer Scholar program since 1990 the number of females offered scholarships annually averaged 36.7% to 2001. Since then, that average has risen slightly to 39%.

The following table shows, in a gender specific way, the data for applications and appointments to academic positions over a nine-year period; and the % of females in the PhD student population from 1996.

Academic	1996	1997	1998*	1999	2000	2001	2002	2003*	2004
Positions advertised	8	17	17	7	13	10	3	16	5
Total applications	167	153	126	77	109	49	73	151	28
No. appointments w/out advertisement							2	4	15
Total of all women applicants as %	37	18	26	22	16.5	26.5	17.8	29.67	33.3
Total appointments	6	12	12	6	15	12	8	25	19
Total of all women appointed as %	17	17	42	16	46.6	33.3	50	12	31.5
% of female PhD students	28	26.8	30.35	25	21.4	27.2	32.7	36.5	38.5

* = Rita Cornforth recruitment year

STAFF

Academic Staff

⊕ Part-time
\# Left during 2004

Professors

Banwell, Martin G BSc PhD *Wellington* FRACI, Hon FRSNZ, FAA
Collins, Michael A BSc PhD *Sydney*
Easton, Christopher J BSc *Flinders* PhD DSc *Adelaide* FRSC, FRACI, FAA
Evans, Denis J BSc *Sydney* PhD *ANU* FRACI, FAA
Gill, Peter M W MSc *Auckland* PhD *ANU*
Hill, Anthony F MSc (Hons) *Auckland* DrRerNat *Bayreuth* FRSC
Krausz, Elmars R BSc PhD *Sydney* FRACI
Mander, Lewis N (Emeritus) (Adjunct) MSc *Auckland* PhD *Sydney* FRACI, FAA, FRS
Ollis, David L BSc NSW PhD *Sydney*
Radom, Leo (Adjunct) MSc PhD *Sydney* DSc *ANU* FRACI, FAA (# 31/10/04)
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*

Adjunct Professors

Amos, Roger D BSc *Glasgow* PhD *York*
James, Veronica J BA BSc *Queensland*, BSc PhD *NSW* OAM
Radom, Leo MSc PhD *Sydney* DSc *ANU* FRACI, FAA (# 1/11/2004)

Senior Fellows

Dixon, Nicholas E BSc PhD *Queensland*
Heath, Graham A BSc PhD *Melbourne*
Sevick, Edith M BSE *Pittsburgh* PhD *Massachusetts*

Fellows

Keniry, Max A BSc PhD *Sydney* (RSC/UNMRC)
Oakley, Aaron J BSc *Tasmania* PhD *St Vincent's IMR Melbourne*
Sherburn, Michael S BSc PhD *Nottingham*

Rita Cornforth Fellow

Coote, Michelle L BSc PhD *NSW*

Research Fellows

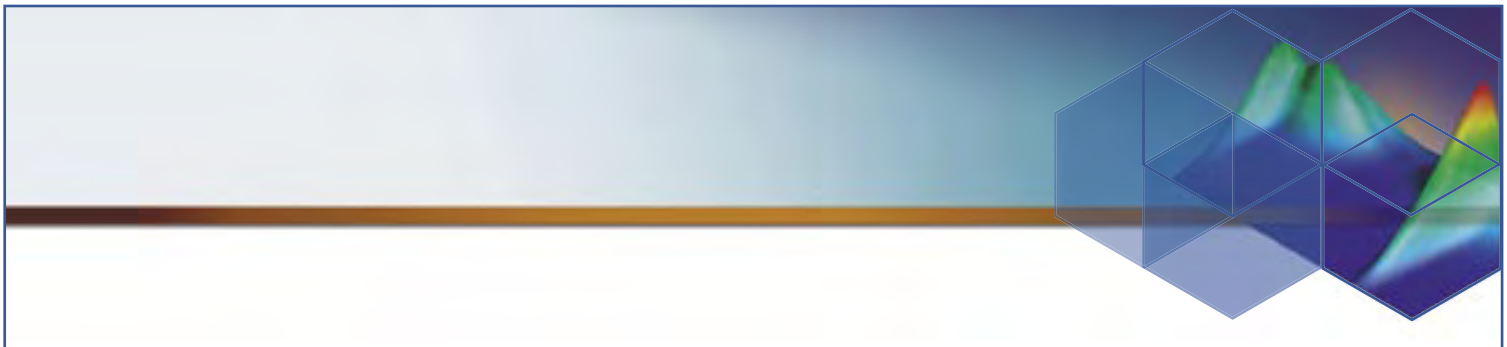
* denotes ARC grant funded

Goossens Darren J BAppSci *Ballarat* PhD *Monash* (* from 3/6/03)
Henderson, Mark J BSc PhD *WA*
Mahon, Peter J BSc PhD *Deakin* (# 8/7/04)
Prosselkov, Pavel MSc PhD *Woronezh, Russia*
Schaeffer, Patrick M DEA *Chem Louis Pasteur, Strasbourg* PhD *Basel* (* from 21/5/02)
Robinson, J Kenneth BA PhD *Oxford* (* from 8/9/03)
Schultz, Madeleine BSc LLB *ANU* PhD *UCLA Berkeley* (# 3/10/04)
Simpson, Jamie S BSc PhD *Queensland* (# 7/5/04)
Williams, Neil K BSc PhD *Sydney* (* from 16/6/03)
Zank, Johann DiplChem *DrRerNat Tech Munich* (* from 18/3/03)

Postdoctoral Fellows

* denotes ARC grant funded

Backes, Michael DiplChem DrRerNat *RWTH Aachen* (* from 5/7/04)
Barr, Lorna BSc *Strathclyde* PhD *ANU* (* from 15/7/04)
Barrett, Elizabeth S BSc *Sydney* PhD *ANU*
Bennett, Simon A BSc PhD *ANU* (* from 12/5/03)
Bright Joanne N BSc *Sydney* PhD *ANU* (# 23/7/04)
Crossley, Ian R MChem PhD *UMIST* (* from 8/1/04)



Del Signore, Giuseppe Laurea *La Sapienza Rome* DrRerNat *RWTH Aachen* (*from 25/3/04)
Gilbert, Andrew T B BSc *Massey* PhD *Cambridge*
Godsi, Oded BA MA *Tel-Aviv* PhD *Technion Israel* (* from 8/11/04)
Headlam Madeleine J BSc PhD *WA* (* from 18/11/02)
Humphrey, Elizabeth R BSc PhD *Bristol* (to 28/2/04)
Hungerford, Natasha L BSc PhD *Queensland* (* from 06/05/02) (# 07/02/04)
Izgorodina, Ekaterina I BSc MSc *Russian Academy of Science* DrRerNat *Münster*
Jackson Andrew J MChem DPhil *Oxford* (* from 6/11/03)
John, Michael DiplChem *Philipps Marburg* DrRerNat *Tech Munich* (* from 17/11/04)
Kim, Hye-Kyung BSc MSc *Yeungnam Korea* PhD *Chalmers* (* from 5/6/03)
Le, Thanh Phuoc BSc *Can Tho Vietnam* MSc *Amsterdam* PhD ANU (# 10/1/04)
Liu, Yun BSc MSc PhD *Xi'an Jiaotong, China* (* from 3/7/03)
Loong, David T J BTech *Massey* NZ PhD *ANU* (# 18/12/04)
McDonough Matthew J BSc PhD *WA* (* from 12/03/03)
Moyano, Gloria BSc PhD NatU *Colombia*
Payne, Alan D BSc PhD *WA* (* from 31/03/03)
Pintacuda, Guido BS MS *Pisa* PhD *Scuola Normale Superiore Pisa* (# 16/10/04)
Scott, Andrew J BSc *Sydney* PhD *ANU* (Orica grant funded from 22/4/04)
Sinclair, David J BSc PhD *NSW* (* from 24/2/03)
Smith, Matthew K BSc PhD *James Cook* (* from 7/4/03)
Su, Xun-Cheng MSc PhD *Nankai China* (* from 24/8/04)
Tripoli Regis J-P DEA Chem *Bordeaux* PhD *Strathclyde* (* from 15/7/03)
Turner Craig BSc *Massey* PhD *Sydney*
Williams Stephen R BAppSci PhD *RMIT* (* from 18/08/03)
Wong Leon S-M BSc PhD *Sydney* (# 4/2/04)
Wright, Adam BMedChem *Wollongong* PhD *Sydney* (* from 27/02/03)
Zhou Xiangting BSc *Hebei China* MSc *Zhengzhou/Hebei* PhD *NSW* (* from 18/03/03)

Research Staff Externally Funded

ARC Queen Elizabeth II Fellow

Webster, Richard D BSc *Auckland* Hons PhD *La Trobe*

ARC Linkage-Australian Postdoctoral Fellow (CSIRO)

Ozawa, Kiyoshi BEng *Yokohama*, MSc PhD *Tokyo*

ARC Postdoctoral Fellows

Coote, Michelle L BSc PhD *NSW*
Oakley, Aaron J BSc *Tasmania* PhD *St Vincent's IMR Melbourne*

Progen Industries Fellows

Bonnet Muriel Dipl *Bordeaux* PhD *ETH Zurich*
Kreipl, Andreas T DiplChem *Hamburg* DrRerNat *Munich*

Feodor Lynen Fellows (Alexander von Humbolt Stiftung Foundation)

Gross Steffen Dipl PhD Freie *Berlin*
Renner, Jens Dipl DrRerNat *Kaiserslautern*

UniChe Project

Reynolds, Philip A BA DPhil *Oxford* FRACI

Visiting Fellows (Post-retirement)

Beckwith, Emeritus Professor Athelstan LJ 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

Business Office

Harland, Lesley BSc MSc *E Anglia*	Laboratory Manager
Scarr, Lorraine	Business Officer
Bayley, Neil	Purchasing Officer
Monaghan, Lorna M	Administrative Assistant
O'Brien, Brendan J	Administrative Assistant
O'Toole, Elouise E	Administrative Assistant
Russell, Kurt	Requisitioning Clerk
Scarr, Barry	Administrative Assistant
Davies, Christine ⊕	Receptionist
Rawlings, Kim C⊕	Receptionist

Academic Secretary's Office

Holloway, Marilyn A	Academic Secretary
Slocum, Maureen	Academic Staff Administrator
Murray, Valerie J ⊕	Postgraduate Student Administrator
Riches, Susan ⊕	Administrative Assistant

Departmental Administrative Assistants

Enge, Rosemary E ⊕	Inorganic Chemistry
Johnson, Nikki #	Physical and Theoretical Chemistry
Roper, Carrie-Jo #	Physical and Theoretical Chemistry
Williams, Suzanne R	Physical and Theoretical Chemistry
Riches, Susan ⊕	Organic Chemistry
Wayte, Valerie ⊕	Physical Chemistry (UnlChe)

The Dean's Executive Assistant Baker, Michelle

Facilities Officer Cooper, Kevin DipBus AIM *ACT*

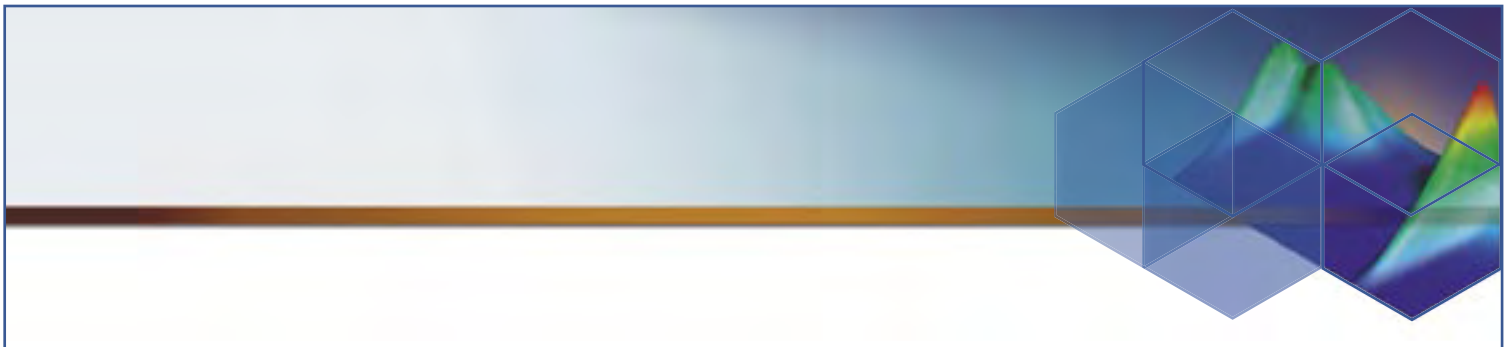
Laboratories and Safety Coordinator Welling, Lee L BSc(App) *Canberra CAE*

Engineer King, David J BE BSc *NSW*

Facility Coordinator, University NMR Centre Keniry, Max A BSc PhD *Sydney*

Technical and Research Services Staff

Allen, John M BSc *NZ*
Carr, Paul D BSc PhD *Keele*
Cayzer, Tory N BSc(Hons) *Sydney*, PhD *ANU*
Clarke, Ian J
Culnane, Pui T DipAppChem *Melbourne*
Devitt, Peter J
Edwards, Alison J BSc PhD *Melbourne*
Filardo, Raffaele J
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 AssocDip (Eng) *CIT*
Lee, Stephen B
Lilley, Penny E BSc(App) *Canberra CAE* ⊕
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*
Neumann, Horst
Noren, Lasse H BSc PhD *Uppsala*
O'Brien, Robert J
Owen, Elisabeth A BAppSc GradDipChem Grad DipAdmin *WAIT*
Padmakshan, Dharshana BSc MSc *Kannar (India)* #
qI, Ruhu BSc *Lanzhou* (*China*)
Scott, Anthony P BSc PhD *New England* #
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* ⊕

Laboratory Attendants

Jansen, Sally ⊕#
Hogan, Carol ⊕

Programmers

Blake, Christopher J BSc(Appl) *Canberra CAE* GradDip (Comp) *UC*
Cohen, Pam BA *ANU*, GradDip(CompSci) *Canberra CAE* ⊕
Delfs, Christopher D BSc PhD *WA*
Faletic, Rado ⊕
Lindsell, Graeme A BSc *NSW* PhD *ANU*

Chemistry Librarian (ANU Staff)

Smith, Joan E

Stores Staff

Easton, Norman
Galarza, Marcelo

Security Officers

McGlinchey, Hugh
Jamieson, Stephen
Ross, Ian T
Smith, Don M
Stuart, Ian

Cleaning Staff

Antunovic, Marica⊕
Lauc, Draga ⊕
Lockhart, Rosemary ⊕
Stavreska, Luba ⊕

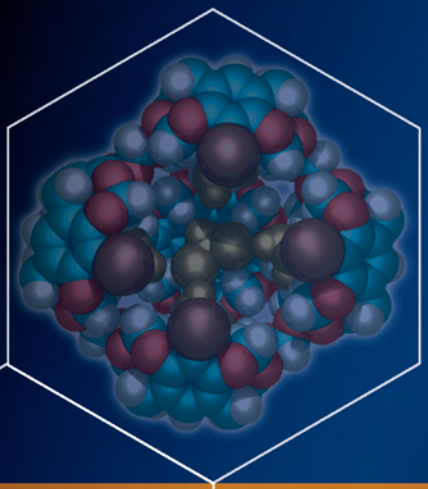
Tea Assistant

Van Kampen, Lena

STATISTICS

Total academic staff at 31 March 2004			**59**	**(12)**
Standard appointments	17.5	(1)		
Fixed term appointments *(excluding PDFs)*	13.5	(3)		
(School funded)	*5.5*	*(2)*		
(ARC grant funded)	*5*	*(1)*		
(UniChe grant funded)	*1*	*(0)*		
ARC Federation Fellow	*1*	*(0)*		
ARC QEII Fellow	*1*	*(0)*		
Total Postdoctoral Fellows	28	(9)		
(ARC PDFs)	*2*	*(1)*		
(School funded PDFs)	*9*	*(3)*		
(ARC grant funded PDFs)	*12*	*(3)*		
(Progen funded PDFs)	*2*	*(1)*		
(ARC/CSIRO Linkage funded PDF)	*1*	*(0)*		
(Feodor Lynen funded PDFs)	*2*	*(1)*		
Visiting Fellows during 2004			**23**	**(3)**
Postgraduate students at 31 March 2004 (including 2 part time; excluding 3 completing students – TTS)			**70**	**(27)**
PhD degrees awarded			**9**	**(2)**
MPhil degrees awarded			**3**	**(1)**
General staff at 31 March 2004 (equivalent full-time positions)			**65.8**	**(23.8)**
Technical/Research	35.1	(7.6)		
Administrative/Computing	19.9	(12.4)		
Other	10.8	(3.8)		

The number of females included in the totals is shown in brackets.



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