

NATIONAL AND INTERNATIONAL LINKS

Collaborative Research Projects with Universities, CSIRO and Other Institutions

BIOLOGICAL CHEMISTRY

Protein Structure and Function – N E Dixon

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Nuclear Magnetic Resonance – M A Keniry

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

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

Structural Biology – A J Oakley

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

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

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

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

Protein Crystallography and Engineering – D L Ollis

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

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

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

Biomolecular NMR – G Otting

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

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

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

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

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

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

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

INORGANIC CHEMISTRY

Synthetic Organometallic and Coordination Chemistry – A F Hill

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

Inorganic Stereochemistry and Asymmetric Synthesis – S B Wild

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

Solid State Inorganic Chemistry – R L Withers

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

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

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

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

ORGANIC CHEMISTRY

Synthesis and Mechanism – M G Banwell

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

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

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

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

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

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

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

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

Biochemical Reactions and Molecular Recognition – C J Easton

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

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

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

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

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

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

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

Organic Synthesis – L N Mander

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

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

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

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

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

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

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

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

PHYSICAL AND THEORETICAL CHEMISTRY

Theoretical Chemical Physics – M A Collins

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

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

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

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

Computational Quantum Chemistry, Polymer Chemistry – M L Coote

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

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

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

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

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

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

Liquid State Chemical Physics – D J Evans

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

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

Theoretical Quantum Chemistry – P M W Gill

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

Laser and Optical Spectroscopy – E Krausz

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

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

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

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

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

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

Polymers and Soft Condensed Matter – E M Sevick

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

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

Disordered Materials – T R Welberry

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

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

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

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

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

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

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

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

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

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

Solid State Molecular Science – J W White

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

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

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

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

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

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

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

Molecular Electrochemistry – R D Webster

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

Academic Visitors

The Birch Lecturer

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

The David Craig Lecturer

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

Visiting Fellows

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

Beck, Dr Jennifer, University of Wollongong

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

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

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

Gibaud, Professor Alain, Université du Maine, France

Gilbert, Dr Elliot, Neutron Scattering Group, ANSTO

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

Hanley, Professor Howard, NIST, Colorado, USA

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

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

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

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

Larese, Professor John, University of Tennessee, USA

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

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

Namazian, Dr Mansoor, Yazd University, Iran

Neylon, Dr Cameron, University of Southampton, UK

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

Rennie, Dr Adrian, Uppsala University, Sweden.



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

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

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

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

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

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

Taylor, Dr Andrew, ISIS, Rutherford Laboratory, UK

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

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

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

Research Seminar Speakers

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

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

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

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

Bernhardt, Dr Paul, University of Queensland

Blair, Professor Ian, University of Pennsylvania, USA

Borden, Professor Weston, University of Washington, USA

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

Buckingham, Professor David, University of Cambridge, UK

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

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

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

Cisneros, Dr Gerardo, SGI (Silicon Graphics)

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

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

Cowden, Dr Cameron, Merck Research Laboratories, UK

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

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

Furneaux, Dr Richard, Crown Research Institute, NZ

Gelb, Dr William, Microcal Northampton, MA, USA

Ghiggino, Dr Ken, University of Melbourne

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

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

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

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

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

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

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

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

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

Karuso, Assoc. Professor Peter, Macquarie University

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

Kobayashi, Dr Rika, ANUSF/APAC National Facility

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

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

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

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

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

McKenzie, Dr Ross, University of Queensland

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

Möller, Dr Angela, University of Köln, Germany

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

Morokuma, Professor Keiji, Emory University, Atlanta, USA

Mueller, Professor Axel, University of Bayreuth, Germany

Nair, Dr Vijay, University of Trivandrum, India

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

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

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

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

Smith, David, Rudjer Boskovic Institute, Zagreb, Croatia

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

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

Conference Presentations

Biological Chemistry

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The following poster was also presented:

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

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

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

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

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

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

The following posters were also presented:

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

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

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

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

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

M D Mulcair: *Polarity determination in replication termination*

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

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

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

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

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

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

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

The following poster was also presented:

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

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

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

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

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

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

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

The following posters were presented:

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

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

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

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

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

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

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

Inorganic Chemistry

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The following posters were presented:

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

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

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

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

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

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

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

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

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

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

The following posters were presented:

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

W Somphon, K J Haller and A D Rae: *An order-disorder phase transition in [Ag(bipy)NO₃]*

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

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

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

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

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

Y Liu, R L Withers, V Ting, J D Fitz Gerald and L Norén: *Stacking faults in typical Ba₃M₁Nb₂O₉ (M = Mn and Co) perovskites and their impact on electrical properties*

V Ting, Y Liu and R L Withers: *Temperature-dependent neutron powder diffraction studies of the A₃CoNb₂O₉ (A = Ba²⁺, Sr²⁺ and Ca²⁺) perovskite*

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

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

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

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

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

The following posters were presented:

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

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

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

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

Organic Chemistry

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

The following posters were presented:

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

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

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

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

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

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

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

The following poster was also presented:

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

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

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

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

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

The following poster was presented:

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

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

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

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

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

The following posters were presented:

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

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

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

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

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

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

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

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

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

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

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

The following poster was also presented:

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

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

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

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

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

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

The following posters were presented:

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

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

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

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

Physical and Theoretical Chemistry

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

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



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

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

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

The following talks were also presented:

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

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

D J Goossens, T R Welberry and A P Heerdegen: *Modelling dynamic disorder in 3,3'-dimethoxybenzil, C₁₆H₁₄O₄*

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

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

K F Wilson, D J Goossens and M James: *Magnetic properties of Gd_{1-x}Sr_xCoO_{3-δ} (x = 0.67, 0.90 and 0.95)*

A poster was also presented:

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

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

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

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

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

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

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

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

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

M J Henderson: *Protein-silicate surfaces*

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

A Perriman: *Protein denaturation at interfaces*

P A Reynolds: *High internal phase emulsion structure*

J W White: *General discussion – new horizons*

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

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

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

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

D J Goossens, T R Welberry and A P Heerdegen: *Molecular Flexibility in 3,3'-dimethoxybenzil, C₁₆H₁₄O₄*

T R Welberry, D J Goossens, and M J Gutmann: *Neutron diffuse scattering and Monte Carlo study of the relaxor ferroelectric PbZn_{1/3}Nb_{2/3}O₃ (PZN)*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

J W White: *Suitcase science*

J W White: *Stem cell research*

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

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

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

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

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

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

Poster presentations:

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

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

J Kilmartin, M Riley, S Luthi and E Krausz: *Ni²⁺ doped CsCdBr₃ as a Novel Molecular Switch*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

D J Goossens, A P Heerdegen and T R Welberry: *Modelling disorder in 3,3'-dimethoxybenzil, C₁₆H₁₄O₄*

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

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

A poster was also presented:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Poster presentations:

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

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

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

D J Goossens, A G Beasley, A P Heerdegen, T R Welberry and P L Lee: *Diffuse X-ray scattering from Ibuprofen, C₁₃H₁₈O₂*

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

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

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

BioNano, Queensland, December

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

Pacificchem 2005, Honolulu, USA, 15–20 December

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

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

Plenary and Invited Lectures

Professor M G Banwell

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

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

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

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

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

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

He also presented the following named lectures:

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

2004 Novartis Chemistry Lectures (carried over into 2005):

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

Professor M A Collins

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

Dr M L Coote

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

Professor N E Dixon

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

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

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

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

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

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

Professor C J Easton

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

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

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

Professor D J Evans

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

Professor P M W Gill

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

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

Professor A F Hill

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

Professor E Krausz

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

Spectroscopy and photosynthesis, University Bonn, Germany, 27 October

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

Ms M Kubik

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

Dr P Mahon

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

Professor G Otting

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

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

Associate Professor E M Sevick

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

Associate Professor M S Sherburn

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

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

Professor J W White

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

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

Stem cell ethics, University House, ANU, September

Service to External Organisations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

External Lectures and Courses

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

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

Outreach Activities

Conference Organisation

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

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

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

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



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

Australian Academy of Science (AAS)

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

Australian Institute of Nuclear Science and Engineering (AINSE)

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

CSIRO Student Research Scheme

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

International Conference on Neutron Scattering in the Asia Pacific Region

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

National Science Summer School

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



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

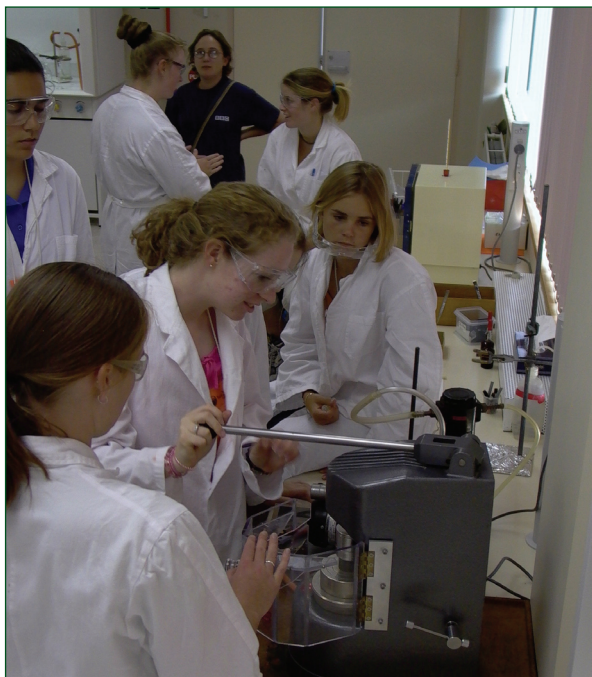
National Youth Science Forum

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



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

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



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

Royal Australian Chemical Institute (RACI)

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

UniChe (Universities, Industry, Chemistry)

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

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

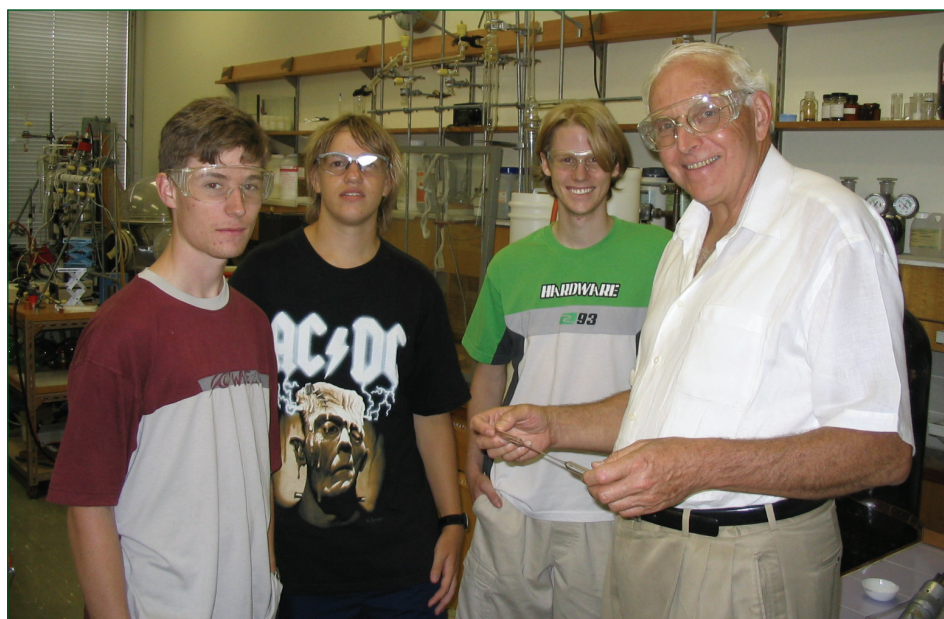
A high priority for the UniChe project is to attract more students to the enabling sciences and to increase the retention rate of students in chemistry. In order to achieve this, UniChe coordinators were appointed: Dr M J Ellison, ANU; Dr S Leitch, University of Newcastle; and Dr P Myatt, University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

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

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

A well attended lecture titled *UniChe – a Scheme bringing Australian School and University Students into touch with Chemical Industry* was given by Professor John White at the CONNECT 2005 conference organised by RACI in July in Sydney.

Finally, UniChe organised and financed eleven honours students, ten PhD students and sixteen Summer Scholars, selected on fundamental scientific merit, but who are also of interest to five of Orica's business areas.



Professor John White with students at the UniChe Summer School in February.