

## National and International Links

### Collaborative Research Projects

#### Biochemical Reactions and Molecular Recognition

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

Chemistry of scymnol by Professor C.J. EASTON, Ms M. GEBARA-COGLAN and Ms X. NGUYEN, with Mr J. Broadbent, McFarlane Laboratories Pty Ltd, Melbourne; and Dr G.W. Simpson, CSIRO Molecular Science, Melbourne.

Chlorine chemistry by Professor C.J. EASTON and Mr P.G. DUMANSKI, with Mr R. Faulkner, Australian Vinyls Pty Ltd, Melbourne; and Dr G.W. Simpson, CSIRO Molecular Science, Melbourne.

Cycloaddition reactions of nitrile oxides by Professor C.J. EASTON, Ms C.K.Y. LEE and Mr G.J. VUCKOVIC, with Drs G.P. Savage and G.W. Simpson, Dunlena Pty Ltd and CSIRO Molecular Science, Melbourne.

Free radical reactions of peptides and proteins by Professor C.J. EASTON, Ms R. BARBIELLINI, Mr B.J.W. BARRATT, Ms L.Y.F. CHOW, Ms N. LORIMER, Mr S.B. McNABB, Mr A.J. MORTIMER, Dr J.S. SIMPSON, Mr Z. WATTS, and Dr A. WRIGHT, with Dr M.J. Davies, Heart Research Institute, Sydney; Dr R. O'Hair, University of Melbourne; Dr D. Grice, Griffith University; and Professor A. Rauk, University of Calgary, Canada.

Lipid chemistry by Professor C.J. EASTON and Mr J.B. KELLY, with Professors A. Ferrante and A. Poulos, Adelaide Medical Centre for Women and Children.

Lipid modified coordinating ligands by Professor C.J. EASTON and Dr P.A. COGLAN, with Dr J. Altin, Division of Biochemistry and Molecular Biology, ANU; and Lipotek Pty Ltd, Canberra.

Supramolecular chemistry of cyclodextrins by Professor C.J. EASTON, Ms L. BARR, Ms M. CIESLINSKI, Ms N. LORIMER, Mr H. ONAGI and Dr J.S. SIMPSON, with Professor S.F. Lincoln, Ms J.S. Lock and Mr B.L. May, University of Adelaide.

The development of new generation anti-infective agents by Professors M.G. BANWELL and C.J. EASTON, Drs S.A. BENNETT, M.R. NAIRN, J.K. ROBINSON, D.J. SINCLAIR, M.K. SMITH, and L. XIA, with Dr P.J. O'Hanlon, GlaxoSmithKline, Harlow, UK.

Towards improved melamine-urea-formaldehyde resins by Professor C.J. EASTON and Ms A. PHILBROOK, with Mr G. Ryan and Dr N. Dunlop, Orica Adhesives and Resins, Melbourne, through the UniChe program.

#### Bioinorganic and Medicinal Chemistry

Determination of activation parameters for the reaction between coenzyme B<sub>12</sub> and cyanide by Dr N.E. BRASCH and Mr A.G. CREGAN with Professor R. van Eldik and Dr M.S.A. Hamza, University of Erlangen-Nuremberg, Germany.

Re-investigation of the reaction between methylcobalamin and cyanide by Dr N.E. BRASCH, Messrs S.J. BRODIE and A.G. CREGAN with Professor R. van Eldik, University of Erlangen-Nuremberg, Germany.

### Computational Quantum Chemistry

Multireference G2 and G3 theories by Professor L. RADOM, with Professor M.S. Gordon, Iowa State University, USA.

Radical addition reactions by Professor L. RADOM with Professor H. Fischer, University of Zurich, Switzerland.

Thermochemistry of metal oxides and hydroxides by Professor L. RADOM and Dr M.B. SULLIVAN, with Dr B.J. Smith, Walter and Eliza Hall Institute, Melbourne; Professor J.M.L. Martin, Weizmann Institute, Israel; and Dr L.A. Curtiss, Argonne National Laboratories, USA.

Acidities of alkali metal hydroxides by Professor L. RADOM, Dr M.B. SULLIVAN, Dr A.P. SCOTT and Mr T. BÜSGEN, with Professor S.R. Kass, University of Minnesota, USA.

Reactions catalysed by vitamin B<sub>12</sub> by Professor L. RADOM, with Professor B.T. Golding, University of Newcastle upon Tyne, UK; Dr D.M. Smith, Institut für Organische Chemie, Munich, Germany; and Dr S.D. Wetmore, Mount Allison University, Canada.

Oxidative damage to proteins by Professor L. RADOM, Professor C.J. EASTON, Mr G.P.F. WOOD, Dr M.L. COOTE and Dr R. JACOB, with 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.

Structures and stabilities of weak complexes by Professor L. RADOM and Dr A.P. SCOTT, with Professor A. Legon, University of Exeter, UK.

Cleavage of alkoxy radicals by Professor L. RADOM and Dr D.J. HENRY, with Professor A. Rauk, University of Calgary, Canada; Professor R.J. Boyd, Dalhousie University, Halifax, Canada; and Professor S.L. Boyd, Mount St Vincent University, Canada.

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

### Disordered Materials

Diffuse scattering from benzil, C<sub>14</sub>H<sub>10</sub>O<sub>2</sub> by Professor T.R. WELBERRY with Professor W.I.F. David, ISIS, Rutherford Appleton Laboratory, Oxfordshire, UK.

Disorder in 1:1 adducts of hexamethylenetetramine with azelaic acid by Professor T.R. WELBERRY, with K.J. Schenk, Institut de Cristallographie, Université de Lausanne, Switzerland.

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

## National and International Links

High-pressure X-ray scattering of oxides with a nano-scaled 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.

### Inorganic Stereochemistry and Asymmetric Synthesis

Microbial phosphonate uptake and metabolism: enlisting microorganisms to deliver antimicrobials effectively by Professor S.B. WILD, with Dr G.L. Mendz, School of Biochemistry and Molecular Genetics, University of New South Wales, Sydney (ARC Discovery grant).

### Laser and Optical Spectroscopy

Parallel accumulation of Chemiluminescence for Analytical applications by Professor E. KRAUSZ, Dr Trevor Smith, University of Melbourne; and Associate Professor Neil Barnett, Deakin University.

Spectroscopy of PSII protein assemblies by Professor E. KRAUSZ and Dr S. PETERSON, with Dr R. Pace Department of Chemistry, ANU; Dr M. Seibert, NREL, Golden Colorado.

Spectroscopy of The Thermophilic PSII extracted from *Synechococcus Vulcanus* by Dr S. PETERSON, Professor E. KRAUSZ, with Dr R. Pace Department of Chemistry, ANU; Dr J.-R. Shen, Riken Institute, Hyogo, Japan

Spectroscopy of Chromium(III) Hole-burning materials by Professor E. KRAUSZ, with Dr H. Riesen, ADF.

Up-conversion and spectroscopy in rare earth systems by Professor E. KRAUSZ, with Dr M. Riley, University of Queensland; and Dr S. Lüthi, Gemfire, Stanford.

### Liquid State Chemical Physics

Applications of general temperature expressions by Professor D.J. EVANS and Mr O.G. JEPPS, with Dr G.S.D. Ayton, University of Utah, USA; and Dr L. Lue, University of Manchester Institute of Science and Technology, UK.

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, Mr E. MITTAG, Drs E.M. SEVICK and G.M. WANG, with Dr D.J. Searles, Griffith University, Brisbane.

Non-equilibrium hard sphere simulations by Dr J. PETRAVIC, with Dr O.G. Jepps, Department of Chemical Engineering, University of Queensland.

Shear viscosity of a simple fluid over a wide range of strain rates by Professor D.J. EVANS, with Dr I. Borzsák, Hungarian Academy of Sciences, Budapest; and Professor P.T. Cummings, University of Tennessee, USA.

Transport and entropy by Professor D.J. EVANS and Dr J. PETRAVIC, with Professor D.J. Isbister, University of New South Wales at ADFA, Canberra.

Transport coefficients of polar liquids and electrolytes by Professor D.J. EVANS and Dr J. PETRAVIC, with Dr B. Rousseau, Université Paris-Sud, France.

Transport properties of ionic liquids by Dr J. PETRAVIC, with Dr J. Delhommelle, Équipe de Chimie et Biochimie Théoriques, Université Henri Poincaré, Vandœuvre-lès-Nancy, France.

### Nuclear Magnetic Resonance

Defining the structure of a protein 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. Supported by a travel grant from the International Union Against Cancer.

### Organic Synthesis

Biosynthetic, structural and metabolic studies on gibberellins by Professor L.N. MANDER, with Dr M. Talon, Department of Citriculture, IVIA, E-46113, Moncada, Valencia, Spain; and Dr J. Zeevaart, MSU-DOE Plant Research Laboratory, Michigan State University, USA.

Biosynthetic, structural and metabolic studies on gibberellins by Professor L.N. MANDER, with Dr P. Hedden and Professor J. MacMillan, Long Ashton Research Station, Bristol, UK.

Biosynthetic, structural and metabolic studies on gibberellins by Professor L.N. MANDER and Mr B. TWITCHIN, with Dr V.M. Sponsel, Division of Life Sciences, University of Texas, San Antonio, Texas, USA.

Biosynthetic, structural and metabolic studies on gibberellins by Professor L.N. MANDER and Mr B. TWITCHIN, with Professor O. Junttila, Department of Plant Physiology and Microbiology, University of Tromsø, Norway.

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.

Biosynthetic, structural and metabolic studies on gibberellins by Professor L.N. MANDER and Mr B. TWITCHIN, with 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 H. Yamane, Biotechnology Research Center, University of Tokyo, 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.

Structural and biosynthetic studies on antheridiogens from fern gametophytes by Professor L.N. MANDER, with Dr J. Nester, Department of Biological Sciences, Sam Houston State University, Texas, USA.

## National and International Links

Structural studies on biologically active extractives from olives by Professor L.N. MANDER and Mr A.J. HERLT, with Drs P. Antolovitch, P. Prenzler, K. Robards, and D. Ryan, Charles Sturt University, Wagga Wagga.

Structural studies on biologically active extractives from Indonesian plant species by Professor L.N. MANDER and Mr A.J. HERLT, with Drs R. Rumampuk and P. Tarigan, Kimia Pascasarjana Laboratory, Padjadjaran University, Bandung, Indonesia.

Studies on fruit development by Professor L.N. MANDER and Mr B. TWITCHIN, with Dr P.S. Blake, Horticulture Research International, East Malling, UK.

Studies on gibberellin receptors by Professor L.N. MANDER, Dr E.J. BECK and Mr J.R. CROW, with Dr P.M. Chandler, CSIRO Division of Plant Industry, Canberra.

Studies on growth inhibition 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.

Studies on the genetics of *Pisum* by Professor L.N. MANDER and Mr B. TWITCHIN, with Dr J.J. Ross, Department of Plant Science, University of Tasmania, Hobart.

### Organometallic and Coordination Chemistry

Synthesis of methimazolyl phosphines and arsines by Professor A. F. HILL, with Professor J. D. Woollins, Department of Chemistry, University of St Andrews, Scotland, U. K.

Imidazolylidene complexes of rhodium(I) and iridium(I) by Professor A. F. HILL, with Dr Thomas Welton, Department of Chemistry, Imperial College of Science, Technology and Medicine, London, U. K.

### Protein Crystallography and Engineering

Structural studies of the IL-5 receptor by Dr D.L. OLLIS, Mr J.M. MURPHY and Dr P.D. CARR, with Professor I.G. Young, JCSMR, ANU.

Structural studies of the P<sub>II</sub> and GlnK proteins by Drs D.L. OLLIS and P.D. CARR, with Drs S.G. Vasudevan and Y. Xu, James Cook University, Queensland.

Structure function studies with esterases by Dr D.L. OLLIS, with Dr J. Oakshot, CSIRO Department of Entomology, Canberra.

### Protein Synthesis and Evolution

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

Crystallisation of the DnaB helicase and DnaB•DnaC complex by Drs N.E. DIXON, P.M. SCHAEFFER, Ms K.V. LOSCHA, and Mr M. MULCAIR, with Drs A. Oakley and M.C.J. Wilce, University of Western Australia.

Expression, isolation and crystallisation of the *Bacillus subtilis* DnaC helicase and DnaI proteins by Dr N.E. DIXON and Ms K.V. LOSCHA with Professor R.G. Wake, Drs D.B. Langley and J.M. Guss, School of Molecular and Microbial Biosciences, University of Sydney.

Geminivirus DNA replication mechanisms by Dr N.E. DIXON, with Dr A. Rezaian, CSIRO Division of Plant Industry, Glen Osmond, SA.

*In vitro* protein synthesis by Drs N.E. DIXON, M.J. HEADLAM, K. OZAWA and Professor G. OTTING, with Drs E. Liepinsh, S. Pursglove and L. Guignard, Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm; 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 Mr S. HAMDAN, with Dr J.L. Beck, Mr A. Kapur, Mr R. Gupta, Mr S.J. Watt, and Professor M.M. Sheil, Department of Chemistry, University of Wollongong.

Properties of proteins circularized by intein-mediated reactions by Drs N.E. DIXON, P. PROSELKOV and Professor G. OTTING, with Dr N.K. Williams, Institute for Biomedical Research and 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.

Radiolabelled antibodies for cancer diagnosis and treatment by Dr N.E. DIXON, Ms N.M. DI BARTOLO and Professor A.M. SARGESON, with Dr S. Smith, Australian Nuclear Science and Technology Organization, Sydney.

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 a circularised protein by Drs N.E. DIXON and P. PROSELKOV, with Drs K. Alexandrov and A. Niculae, Department of Physical Biochemistry, Max-Planck-Institute for Molecular Physiology, Dortmund, Germany.

Structures and functions of *Escherichia coli* replisomal proteins, by Drs N.E. DIXON, P. PROSELKOV, P.M. SCHAEFFER, Ms K.V. LOSCHA, Ms A.-Y. PARK, and Professor G. OTTING, with Drs C.M. Elvin, K. Kongsuwan, and G. Wijffels, CSIRO Division of Livestock Industries, Brisbane; Drs A. Oakley and M.C. Wilce, University of Western Australia.

Structures of complexes of the proofreading exonuclease subunit of DNA polymerase III, by Drs N.E. DIXON, P.D. CARR, D.L. OLLIS, M.A. KENIRY, Professor G. OTTING, Mr S. HAMDAN and Ms A.-Y. PARK, with Dr E. Liepinsh, Department of Medical Biochemistry and Biophysics, Karolinska Institutet, 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 Biotecnología, Universidad Autónoma, Madrid, Spain.

## National and International Links

### Solid State Inorganic Chemistry

Structural instabilities induced by the the electronic band structure of  $\text{FeF}_2$  by Drs F. BRINK, L. NORÉN and R.L. WITHERS, with Dr T. Larsson, Outokumpo Copper R&D, Sweden.

Neutron diffraction studies of the incommensurately modulated  $\text{Ni}_{1+x}\text{In}_y\text{Te}_2$  system by Drs L. NORÉN and R.L. WITHERS, with Dr H. Rundlöf, Studsvik Neutron Research Laboratory, Sweden.

Constrained refinement techniques for problem crystal structure refinements involving pseudo symmetry, disorder and twinning by Professor A.D. RAE, with Drs K.J. Haller and W. Somphon, Suranaree University of Technology, Nakhon Ratchisima, Thailand.

A modulated structure approach to the refinement of commensurate superstructures by Professor A.D. RAE, with Dr S.W. Ng, University of Malaya, Kuala Lumpur, Malaysia.

Problem crystal structure refinements by Professor A.D. RAE, with Professor A.T. Baker, University of Technology, Sydney.

Problem crystal structure refinement involving zones of different symmetry by Professor A.D. RAE, with Dr A. Linden, University of Zurich, Switzerland.

Problem crystal structure refinement involving zones of different symmetry by Professor A.D. RAE, with Dr H.O. Sorensen, University of Copenhagen, Denmark.

Atomic ordering in the doped, rare earth, cobaltates  $\text{Ln}_{1-x}\text{Sr}_x\text{CoO}_{3-\square}$  by Dr R.L. WITHERS, with Drs D. Goosens and M. James, Australian Nuclear Science and Technology Organisation, Menai, NSW.

Modulated structures in the metastable  $\text{Ni}_{7\pm x}\text{S}_6$ , and mixed  $\text{Ni}_{6\pm x}(\text{S}_{1-y}\text{Se}_y)_{5r}$  systems by Drs Y. LIU, L. NORÉN and R.L. WITHERS, with Professor G. van Tendeloo and Mr J. Hadermann, University of Antwerp, Belgium; and Mr F.J. García-García, Stockholm University, Sweden.

### Solid State Molecular Science

Ion and solvent kinetics at the nickel hydroxide–liquid interface by Dr M.J. HENDERSON, with Professor A.R. Hillman and Ms H. French, University of Leicester, UK.

Bonding in transition metal complexes by Dr P.A. REYNOLDS, with Professor B.N. Figgis and Dr A.N. Sobolev, University of Western Australia.

The interface between complex fluids and solids by Dr P.A. REYNOLDS, Professor J.W. WHITE and Dr M.J. HENDERSON, with Dr S.A. Holt, Rutherford Appleton Laboratory, Oxford, UK; and Dr D. Tunaley, Orica Ltd, Australia.

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. Holt, 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 and Dr P.A. REYNOLDS, with Drs R. Goodridge and C. Such, Orica Ltd, Australia.

Structure of polymer latex solutions by Professor J.W. WHITE, with Professor R. Gilbert and Dr H. de Bruyn, University of Sydney.

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

Structure of porous glasses by Professor J.W. WHITE, with Dr C. Buckley, Curtin University, Western Australia.

Structure of templated silicate films by Professor J.W. WHITE, with Dr M. Trau, University of Queensland, Brisbane.

Surface activity of poly(*t*-butylacrylate) polymer films by Professor J.W. WHITE, Dr M.J. HENDERSON and Mr A. PERRIMAN, with Dr S.A. Holt, Rutherford Appleton Laboratory, Oxford, UK; and Dr G. Dennis, University of Western Sydney.

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.

The following collaborators visited the group during 2002 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); Mr R. Webster (University of New South Wales); Dr H. de Bruyn (Sydney University); Dr D. Martin (University of Queensland); Dr C. Buckley (Curtin University of Technology); Dr G. Dennis (UNSW); Dr A. Whittaker, University of Queensland; Dr G. War (University of Sydney); Dr J. Ruggles (University of Queensland); Dr K. Doolan (University of Western Sydney)

### Structural Biology and Biophysics by NMR

Application of a high-yield *in vitro* protein expression system by Professor G. OTTING, Drs N.E. DIXON and K. OZAWA, with Drs L. Guignard and S. Pursglove, Karolinska Institute, Stockholm, Sweden.



## National and International Links

Application of an intein-based system for protein cyclization by Professor G. OTTING, Drs N.E. DIXON, P. PROSELKOV, with Dr N.K. Williams, University of Sydney; Drs D.R. Littler and P.M.G. Curmi, University of New South Wales; Dr E. Liepinsh, Karolinska Institute, Stockholm, Sweden; Drs A. Sharipo and I. Line, University of Latvia, Riga, Latvia.

Determination of the three-dimensional structure of AmpD by Professor G. OTTING, with Drs E. Liepinsh and L. Guignard, Karolinska Institute, Stockholm, Sweden; and Drs B. Joris, C. Génèreux, and D. Dehareng, University of Liège, Belgium.

Determination of the three-dimensional structure of human CLP by Professor G. OTTING, with Drs E. Liepinsh and O. Rådmark, 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 the DAPIN domain by Professor G. OTTING, with Dr E. Liepinsh, Karolinska Institute, Stockholm, Sweden; Drs A. Sharipo and R. Babals, University of Latvia, Riga, Latvia; and Dr E. Staub, metaGen Pharmaceuticals, Berlin, Germany.

Determination of the three-dimensional structure of the PCOLCE NTR domain by Professor G. OTTING, with Drs G. Pintacuda and E. Liepinsh, Karolinska Institute, Stockholm, Sweden; and Professor L. Patthy, Hungarian Academy of Sciences, Budapest, Hungary.

Determination of the three-dimensional structure of the R3H domain by Professor G. OTTING, with Drs E. Liepinsh and L. Guignard, Karolinska Institute, Stockholm, Sweden; and Drs A. Sharipo and A. Leonchiks, University of Latvia, Riga, Latvia.

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.

Long-range angle restraints from dipole-CSR cross-correlation measurements by Professor G. OTTING, with Dr G. Pintacuda, Karolinska Institute, Stockholm; and Ms K. Hohenthanner and Professor N. Müller, University of Linz, Austria.

Protein-labelling with paramagnetic ions by Professor G. OTTING, with Dr G. Pintacuda, Karolinska Institute, Stockholm.

Structure restraints from measurements of cross-correlated relaxation by Professor G. OTTING, with Professor G. Bodenhausen, Ecole Normale, Paris, France; Professor C. Griesinger, Max-Planck-Institute Göttingen, Germany; Professor I. Bertini, University of Florence, Italy; Professor R. Kaptein, University of Utrecht, Netherlands; and Dr J. Boyd, Oxford University, England.

### Synthesis and Mechanism

Biotransformations by Professor M.G. BANWELL, with Dr G.M. Whited, Genencor International Inc, Palo Alto, California, USA.

Combinatorial synthesis of potential anti-mitotic drugs by Professor M.G. BANWELL and Mr D.J. WONG, with Dr A.M. Bray, Chiron Technologies Pty Ltd, Clayton, Victoria.

The development of new generation anti-infective agents by Professors M.G. BANWELL and C.J. EASTON, Drs S.A. BENNETT, M.R. NAIRN, J.K. ROBINSON, D.J. SINCLAIR, M.K. SMITH and L. XIA, with Dr P.J. O'Hanlon, GlaxoSmithKline, Harlow, UK.

The development of novel carbohydrate-like drugs by Professor M.G. BANWELL, Drs J. RENNER and P. GUAN, with Drs R.H. Don and V. Ferro, Progen Industries Ltd, Brisbane.

The synthesis of sialic acid analogues by Professor M.G. BANWELL and Mr X.H. MA, with Dr J. Lambert, Biota Chemistry Laboratories, Department of Chemistry, Monash University.

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.

### Theoretical Chemical Physics

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

Hydrogen abstraction in  $H^+ + CH_4$  by Professor M.A. COLLINS, with Associate Professor D.H. Zhang, National University of Singapore.

Nonadiabatic dynamics and coupled potential energy surfaces by Professor M.A. COLLINS, with Professor D. Yarkony, Johns Hopkins University, USA.

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.

### Coordination and Spectro-electrochemistry

Characterisation of unwarranted combustion deposits in aero-engines by Drs G. A. HEATH, L. NOREN and Mr P.A. GUGGER, with Dr M. Sterns, Department of Chemistry, ANU; Mr G. Bailey, Australian War Memorial; Dr V. Otiengo-Alego, University of Canberra; and Mr A. Romeyn, Australian Transport Safety Bureau, Canberra.

Computational modelling of electrochemical responses by Dr P.J. MAHON, with Ms J.C. Myland and Professor K.B. Oldham, Trent University, Ontario, Canada.

Corrosion analysis and conservation treatments by Drs G.A. HEATH, P.J. MAHON and R.D. WEBSTER, with Professor D.C. Creagh and Dr V. Otiengo-Alego, University of Canberra.

Redox-modulation of the biological nitrogen-fixing 'FeMoco' cluster by Dr G. A. HEATH, with Dr S.P. Best, University of Melbourne; Dr L. L. Martin, Flinders University; and Professor C. J. Pickett, John Innes Centre, Norwich, UK.

## National and International Links

Spectro-electrochemical investigation of conjugated bis-porphyrin radical cations and anions by Dr G.A. HEATH with Dr D. P. Arnold, Queensland University of Technology, Brisbane.

Spectro-electrochemical investigation of redox-switched non-linear-optical materials by Dr G.A. HEATH, with Drs M.P. Cifuentes and M.G. Humphrey, Department of Chemistry, ANU; and Dr M.J. Samoc, RSPHYSSE, ANU.

### Queen Elizabeth II Fellows

DFT investigations of the insertion reactions of alkynes into M–C bonds by Dr E. WENGER, with Dr S.A. Macgregor, Heriot-Watt University, Edinburgh, UK.

Weathering and photostability of benzoylated wood by Dr R.D. WEBSTER and Dr S. SCHMID with Professor P.D. Evans, Department of Wood Science, University of British Columbia, Canada; and Professor N.L. Owen, Brigham Young University, USA.

Corrosion of copper in portable water systems by Dr R. D. WEBSTER, with Dr A. Lowe and Mr M. Stoll, Department of Engineering, ANU; and Dr V. Otiengo-Alego, University of Canberra.