# **Conference Presentations**

# **Biological Chemistry**

#### Protein Structure and Function

**29th Lorne Conference on Protein Structure and Function**, Lorne, Victoria, 8–12 February. The following posters were presented:

<u>A Y Park</u>, P Prosselkov, G Pintacuda, M A Keniry, P D Carr, D L Ollis, G Otting and N E Dixon: *Stabilization* of the proofreading exonuclease subunit of E coli DNA polymerase III by backbone cyclization

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

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

**3rd East Coast** *Bacillus* **Meeting**, Newcastle, New South Wales, 27 August. The following invited lectures were presented:

S Jergic: Subunit interactions in DNA polymerase III

K V Loscha: Primase-helicase interactions

P M Schaeffer: Introduction to the E coli replisome

**ComBio2004**, Perth, Western Australia, 26–30 September. The following invited lectures were presented:

<u>K Loscha</u>, A J Oakley, P M Schaeffer, E Liepinsh, M C J Wilce, G Otting and N E Dixon: *Structure and function of the DnaB binding domain of Escherichia coli primase* 

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

The following posters were presented:

<u>M J Headlam</u>, K Ozawa, D Mouradov, T Huber, S J Watt, J L Beck, K J Rodgers, R T Dean, G Otting and N E Dixon: *Translational incorporation of dihydroxyphenylalanine into proteins*  <u>K Ozawa</u>, S Jergic, M J Headlam, P M Schaeffer, G Otting and N E Dixon: *In vitro cell-free protein synthesis for NMR studies of protein–ligand interactions* 

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

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

#### Nuclear Magnetic Resonance

**29th Lorne Conference on Protein Structure and Function**, Lorne, Victoria, 8–12 February The following posters were presented:

<u>A Y Park</u>, P Prosselkov, G Pintacuda, M A Keniry, P D Carr, D L Ollis, G Otting and N E Dixon: *Stabilization* of the proofreading exonuclease subunit of E coli DNA polymerase III by backbone cyclization

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

**ComBio2004**, Perth, Western Australia, 26–30 September. The following poster was presented:

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

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

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

# Structural Biology

**29th Lorne Conference on Protein Structure and Function**, Lorne, Victoria, 8–12 February The following poster was presented:

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

**ComBio2004**, Perth, Western Australia, 26–30 September

The following lectures were presented:

<u>K Loscha</u>, A J Oakley, P M Schaeffer, E Liepinsh, M C J Wilce, G Otting and N E Dixon: *Structure and function of the DnaB binding domain of Escherichia coli primase* 

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

#### **Biomolecular NMR**

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

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

P Wu was selected for oral presentation of his poster: P Wu and G Otting: *Measurement and*  $\Phi$  angle dependence of CSA/DD cross-correlation effects between H<sup>a</sup> and H<sup>N</sup>

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

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

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

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

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

# **Inorganic Chemistry**

## Coordination Chemistry and Spectro-electro Chemistry

**9th AICCM Symposium of the Painting Special Interest Group**, Hobart, Tasmania, 18–20 March The following lecture was presented:

Maria Kubik: Fibre-optic analysis of artists' materials used by the "Angry Penguins"

## Synthetic Organometallic and Coordination Chemistry

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

<u>R D Dewhurst.</u> A F Hill, A D Rae, M K Smith, and A C Willis: A simple synthesis of heterobimetallic  $C_3$  complexes

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

A F Hill and <u>M K Smith</u>: Ruthenium(II) complexes of 2-mercapto-methylimidazole

The following posters were presented:

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

R J Abernethy, A F Hill, and <u>M K Smith</u>: "Soft" sulfurdonor borate transition metal complexes

6th Reactive OrganoMetallic Symposium (ROMS-6), University of Sydney, 28 May. The following lectures were presented:

<u>R J Abernethy</u>: Synthesis and reactivity of unusual alkoxy(pyrazolyl)borato complexes of ruthenium

<u>I R Crossley</u>: New developments in the main group chemistry of perflourovinyl and alkynyl reagents

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

Gordon Conference on Organometallic Chemistry, Newport RI, USA, 11–15 July. The following lectures were presented:

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

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

International Conference on Coordination Chemistry (ICCC 36), Mérida, Yucatán, México, 18–23 July. The following poster was presented:

<u>L M Caldwell</u>, P V Bernhardt, T B Chaston, P Chin, and D R Richardson: *Cytotoxic iron chelators: iron complexes of di-2-pyridyl keton isonicotonyl hydrazone (HPKIH) analogues*, for which L M Caldwell was awarded a National Institute of Physical Sciences Travel Assistance Grant

International Conference on Organometallic Chemistry (ICOMC 21), Vancouver, Canada, 25–30 July. The following lecture was presented:

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

The following posters were presented:

<u>L M Caldwell</u>, A F Hill, and A C Willis: Group 6 selenoaroyl complexes: isoselenocyanates as single atom selenium transfer reagents, for which L M Caldwell was awarded a National Institute of Physical Sciences Travel Assistance Grant

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

**New Developments in Metal Alkynyl Chemistry**, Research School of Chemistry, ANU, 12 November. A F Hill chaired the *Synthetic Methods* session The following lecture was presented:

<u>R D Dewhurst</u>, A F Hill, and A C Willis: *Investigating* catalytic demercuration of bis(tricarbido) [Hg(CCCWML\_,),] complexes The following posters were presented:

<u>M J Bartlett</u>, A F Hill, and M K Smith: *Bimetallics* spanned by  $C_a$ ,  $C_aH$  and  $C_aH_2$ , wires

<u>R D Dewhurst</u>, A F Hill, and A C Willis: The  $C_3$  ligand: odd-numbered carbon bridges linking W with Rh, Ir and Hq

The 2004 NZIC Inorganic and Organometallic Specialist Group Conference, Portage, New Zealand, 5–8 December. The following lectures were presented:

<u>I R Crossley</u>, A F Hill, E R Humphrey, and A C Willis: *Metallaboratranes: the synthesis and chemistry of a series of group 9 and 10 compounds exhibiting 'dative' metal-boron bonding* 

<u>R D Dewhurst</u>, A F Hill, and A C Willis: *Investigating* catalytic demercuration of bis(tricarbido) [Hg(CCCWML,),] complexes

R J Abernethy, I R Crossley, A F Hill, E R Humphrey, <u>M K Smith</u>, N Tshabang, and A C Willis: *Methimazolylderived tripodal ligands–(only) if the cap fits* 

The following posters were presented:

<u>R J Abernethy</u>, A F Hill, and A C Willis: *Solvent-mediated reactions of ruthenium complexes with poly(pyrazolyl) borates*, which was awarded second prize for a student contribution

<u>R J Abernethy</u>, A F Hill, and A C Willis: *Synthesis* and reactivity of molybdenum-allyl scorpionate complexes: [H<sub>2</sub>B(mt)<sub>2</sub>]<sup>-</sup> vs [H<sub>2</sub>B(pz)<sub>2</sub>]<sup>-</sup>

<u>L M Caldwell</u>, A F Hill, and A C Willis: Synthesis and reactivity of group 6 selenoaroyl complexes

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

M J Bartlett, <u>A F Hill</u>, and M K Smith: *Bimetallics* spanned by  $C_{a}$ ,  $C_{a}H$  and  $C_{a}H_{a}$  wires

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

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

# Inorganic Stereochemistry and Asymmetric Synthesis

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

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

<u>R J Warr</u> and S B Wild: Inorganic asymmetric synthesis of two-bladed propeller octahedral metal complexes

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

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

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

The following lectures were presented:

<u>N L Kilah</u> and S B Wild: Deracemisation of chiral arsines and phosphines via asymmetric transformation

<u>H J Kitto</u> and S B Wild: *Polytertiary phosphine helicates* 

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

#### Solid State Inorganic Chemistry

The Sixth Conference of the Asian Crystallographic Association (AsCA'04), Hong Kong, 27–30 June. The following lectures were presented:

<u>Y Liu</u>, R L Withers, F J Brink, L Norén, and V Ting: Cubic perovskite-related phases in the ternary SrO- $CuO-Nb_2O_5$ 

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

<u>V Ting</u>, Y Liu, R L Withers, and L Norén: *Structural* studies of the  $A_2 InNbO_6$  1:1 and  $A_3 CoNb_2O_9$  1:2 ordered perovskites ( $A = Ca^{2+}, Sr^{2+}, Ba^{2+}$ )

The following poster was presented: <u>W Somphon</u>, KJ Haller, and A D Rae: *The order disorder transition at 150 K of polymeric Ag(bipy)NO*<sub>2</sub>

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

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

The following lectures were presented:

<u>F J Brink</u>, L Norén, and R L Withers: *Electron* diffraction evidence for continuously variable, composition-dependent, oxygen/fluorine ordering in niobium oxyfluorides

<u>V Ting</u>, Y Liu, R L Withers, and L Norén: *A TEM study* of the space group symmetries and structures of the  $A_2 lnNbO_6$  1:1 and  $A_3 CoNb_2O_9$  1:2 ordered perovskites ( $A = Ca^{2+}, Sr^{2+}, Ba^{2+}$ )

**22nd European Crystallographic Meeting**, Budapest, Hungary , 26–31 August. The following poster was presented:

<u>A D Rae</u> and A Linden: Using symmetrized structure components to improve the refinement of an occupancy modulated structure

# **Organic Chemistry**

#### Synthesis and Mechanism

Colloquium for Humboldt Fellows and Awardees in Australia and New Zealand, Auckland, New Zealand, 20–22 February. The following workshop contributions were presented:

M G Banwell, Natural products-inspired chemical synthesis studies

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

The 3rd Chinese-Australian Organic Chemistry Symposium, Sydney, New South Wales, 25–26 February M G Banwell presented the invited lecture: *The total synthesis of biologically active natural products* 

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

M G Banwell presented the 2004 Birch Medal Lecture

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

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

M G Banwell and <u>O J Kokas</u>: Towards the total synthesis of (–)-brunsvigine

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

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

M G Banwell and <u>D T J Loong</u>: Chemoenzymatic approaches to total syntheses of cladospolides B, C and D

15th Southern Highlands Conference on Heterocyclic Chemistry, Moss Vale, New South Wales, 5–7 September. The following poster was presented:

M G Banwell and <u>D W Lupton</u>: New methods for the construction of Aspidosperma alkaloids

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

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

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

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

The following posters were also presented:

M G Banwell and <u>A T Phillis</u>: Approaches to functionalised gibbane skeleta using novel rearrangements of gem-dihalocyclopropanes

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

#### Biochemical Reactions and Molecular Recognition

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

A Philbrook presented the opening invited lecture: Demonstration of co-polymerisation in melamineurea-formaldehyde reactions using <sup>15</sup>N NMR correlation spectroscopy

**9th International Symposium on Free Radicals**, Porto-Vecchio, France, 6–11 June. The following posters were presented:

<u>C J Easton</u> and A Wright: *Evaluation of thiols as* reagents to repair radical damage in peptides and proteins

<u>Z I Watts</u> and C J Easton: Regioselective radical chlorination of amino acids and peptides

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

<u>M M Cieslinski</u>, C J Easton, H Onagi, and S F Lincoln: *Cyclodextrins and stilbenes as components of molecular devices* 



C J Easton, <u>G P Savage</u>, and G W Simpson: Overcoming limitations in nitrile oxide cycloaddition chemistry

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

<u>A Wright</u> and C J Easton: Fighting an uphill battle: hydrogen atom transfer between thiols and amino acids

The following posters were presented:

<u>R Dawson</u>, C J Easton, T Herlt, and S F Lincoln: *Stilbene and cyclodextrins as the basis of molecular shuttles*, for which R Dawson was awarded the best poster prize

<u>I H W Li</u>, B J W Barratt, C J Easton and J S Simpson: *a*-*Glycyl radical stability and PAM enzyme inhibition* 

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

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

<u>Y C Tsai</u> and C J Easton, Oxidatively cleavable amino acid residues in peptides

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

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

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

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

**Orica Emerging Science Symposium**, Melbourne, 12 November

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

1st Pacific Symposium on Radical Chemistry, Kanazawa, Japan, 14–16 November C J Easton presented the invited lecture: *Inhibition* of *PAM to regulate hormone production* 

Adelaide Organic Chemistry Symposium, Adelaide, 6 December

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

#### Organic Synthesis

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

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

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

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

## Organic Synthesis, Methodology and Host-guest Chemistry

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

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

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

<u>E S Barrett</u> and M S Sherburn: *Superbowls and next generation container molecules* 

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

<u>N A Miller</u> and M S Sherburn: *Synthesis and reactions of substituted dendralenes* 

<u>D J Sinclair</u> and M S Sherburn: *Extending the chemistry of cavitands* 

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The following posters were presented:

<u>N A Miller</u> and M S Sherburn, *Synthesis and* reactions of substituted dendralenes for which N A Miller was awarded a prize for one of the best student poster presentations

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

# **Physical and Theoretical Chemistry**

#### Theoretical Chemical Physics

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

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

American Chemical Society Meeting, Anaheim, 1–4 April. The following lecture was presented: M A Collins: *Nonadiabatic dynamics on interpolated diabatic potentials*  Faraday Discussion on Non-adiabatic Effects in Chemical Dynamics, Oxford, 5–7 April. The following poster was presented:

C R Evenhuis and M A Collins: *Growing diabatic potential energy surfaces* 

**1st Asian Pacific Conference on Theoretical and Computational Chemistry**, Okazaki, 12–15 May. The following lecture was presented:

M A Collins: Dynamics on interpolated adiabatic and diabatic potentials

Dalian Institute of Chemical Physics Conference, Dalian, China, July 21–23. The following lecture was presented:

M A Collins: Dynamics on interpolated adiabatic and diabatic potentials

#### Computational Quantum Chemistry Polymer Chemistry

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

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

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

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

**Orica Emerging Science Symposium,** Melbourne, 12 November

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

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

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

# Liquid State Chemical Physics

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

D J Evans: The fluctuation theorem

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

D J Evans: The fluctuation theorem

CECAM Conference, Lyon, France, 19-22 July

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

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

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

Pacific Rim Conference on Nanotechnology Broome, 7–11 September

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

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

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

#### Laser and Optical Spectroscopy

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

B Prince, S , P Smith, R Pace and <u>E Krausz</u>: Spectral Identification of P680

The following posters were presented:

<u>L Debono</u>, B Prince, S Peterson, P Smith, R Pace and E Krausz: Optical and EPR spectroscopy of cytochrome  $B_{559}$  in Photosystem II

<u>J L Hughes</u>, B J Prince, H Riesen, P Smith, R Pace and E Krausz: *Persistent spectral hole-burning in active Photosystem II*  <u>N Cox</u>, P Smith, R Pace, G Fisher, B Prince and E Krausz: *An FTIR study on the oxygen evolving complex of Photosystem II* 

Photosynthesis and Post-Genomic Era International Meeting, Trois Rivieres, Canada, 25–29 August. The following posters were presented:

<u>E Krausz</u>, J L Hughes, P J Smith, R J Pace, S Peterson Årsköld: Assignment of the low-temperature fluorescence in oxygen-evolving Photosystem II

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

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

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

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

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

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

The following posters were presented:

<u>E Krausz</u>, J L Hughes, P J Smith, R J Pace, S Peterson Årsköld: *The reaction centre of PSII in oxygenevolving preparations* 

<u>S Peterson Årsköld</u>, J Ström, J F Allen and E Krausz: Low-temperature absorption and magnetic circular dichroism of the four haems of the chloroplast cytochrome b<sub>e</sub>f complex

<u>P J Smith</u>, J L Hughes, B Prince, E Krausz, R J Pace, S Peterson Årsköld: Turnover studies using visible and far red light on PSII core samples from higher plants

<u>R J Pace</u>, N Cox, P J Smith, W Hillier, G Fischer, E Krausz: *FTIR studies on PS II core complexes from higher plants: First identification of multiline and g4 1 features in S2-S1 turnover*  Fifth Student Conference on Physical Chemistry, Wagga Wagga, 27–30 September

L Debono: The role of cytochrome b<sub>559</sub> in photosystem Il studied by MCD spectroscopy

#### Computational Quantum Chemistry

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

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

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

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

MM2004, Sydney, Australia, 30 June -3 July

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

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

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

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

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

#### **Disordered Materials**

European Crystallography Meeting, Budapest, Hungary

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

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

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

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



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

Asian Crystallography Association Meeting, Hong Kong, June

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

## Solid State Molecular Science

Australian Synchrotron Research Program, Users Meeting, Canberra, ACT, Australia, 5–6 February. The following presentation was given:

M J Henderson: Energy dispersive reflectometry

Inter-Academy Forum, Academy of Science, Canberra, Australia, 23 March. The following presentation was given:

J W White: Recent information on the UK's Research Assessment Exercise

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

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

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

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

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

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

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

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

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

J W White gave the presentation: *Mimicking biomineralisation* 

# R W Rickards – Visiting Fellow (Post-retirement)

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

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

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

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