

## Key to Symbols Used to Identify Research Workers

The following symbols have been used to indicate the status of individuals who were not regular members of the RSC during 2003.

*	Not a member of the Australian National University
†	Former member of the Research School of Chemistry
‡	Summer Research Scholar
‡‡	Former Summer Research Scholar
≠	Visiting Fellow
≠≠	Former Visiting Fellow
+1	Faculty of Science (Chemistry)
+2	Faculty of Science (Biochemistry and Molecular Biology)
#1	IAS (John Curtin School of Medical Research)
#2	IAS (Research School of Physical Sciences and Engineering)
#3	IAS (Research School of Earth Sciences)
#4	IAS (Research School of Biological Sciences)

Journal title abbreviations used as found in Dodd, J.S., Ed. *The ACS Style Guide*, 2<sup>nd</sup> ed.; American Chemical Society: Washington DC, 1997.

## Protein Synthesis and Evolution

Elvin, C.M.\* , Liyou, N.E.\* , Pearson, R.\* , Kemp, D.H.\* , Dixon, N.E. **Molecular cloning and expression of the dihydrofolate reductase (*DHFR*) gene from adult buffalo fly (*Haematobia irritans exigua*): effects of antifolates.** *Insect Mol. Biol.* (2003), 12(2), 173–183.

Oakley, A.J.\* , Prosselkov, P., Wijffels, G.\* , Beck, J.L.† , Wilce, M.C.J.\* , Dixon, N.E. **Flexibility revealed by the 1.85 Å crystal structure of the β sliding-clamp subunit of *Escherichia coli* DNA polymerase III.** *Acta Cryst.* (2003), D59(7), 1192–1199.

## Nuclear Magnetic Resonance

Blake, C.J., Cook, V.C.† , Keniry, M.A., Kitto, H.J., Rae, A.D., Swiegers, G.F.† , Willis, A.C., Zank, J., Wild, S.B. **Diastereoselectivity and molecular recognition in the self-assembly of double-stranded dinuclear metal complexes of the type  $[M_2\{(R^*,S^*)\text{-tetraphos}\}_2](PF_6)_2$  (M = Ag and Au).** *Inorg. Chem.*(2003), 42(26), 8709–8715.

Keniry, M.A. **A comparison of the association of spermine with duplex and quadruplex DNA by NMR.** *FEBS Lett.* (2003), 542(1–3), 153–158.

## Protein Crystallography and Engineering

Murphy, J.M., Ford, S.C.<sup>#1</sup> , Wiedemann, U.M.<sup>#1</sup> , Carr, P.D., Ollis, D.L., Young, I.G.<sup>#1</sup> **A novel functional epitope formed by domains 1 and 4 of the human common β-subunit is involved in receptor activation by granulocyte macrophage colony-stimulating factor and interleukin 5.** *J. Biol. Chem.* (2003), 278(12), 10572–10577.

Xu, Y.† , Carr, P.D., Clancy, P.\* , Garcia-Dominguez, M.≠ , Forchhammer, K.\* , Florencio F.\* , Tandeau de Marsac, N.\* , Vasudevan, S.G.\* , Ollis, D.L. **The structures of the PII proteins from**

## Publications

the cyanobacteria *Synechococcus* sp. PCC7942 and *Synechocystis* sp. PCC 6803. *Acta Cryst.* (2003), D59, 2183–2190.

Yang, H., Carr, P.D., Yu McLoughlin, S., Liu, J.W., Horne, I. \*, Qiu, X. \*, Jeffries, C.M.J., Russell, R.J. \*, Oakeshott, J.G. \*, Ollis, D.L. **Evolution of an organophosphate-degrading enzyme: a comparison of natural and directed evolution.** *Protein Eng.* (2003), 16(2), 135–145.

### Structural Biology and Biophysics By Nmr

Liepinsh, E. \*, Bányai, L. \*, Pintacuda, G. \*, Trexler, M. \*, Patthy, L. \*, Otting, G. **NMR structure of the netrin-like domain (NTR) of human type I procollagen C-proteinase enhancer defines structural consensus of NTR domains and assesses potential proteinase inhibitory activity and ligand binding.** *J. Biol. Chem.* (2003), 278(28), 25982–25989.

Liepinsh, E. \*, Barbals, R. \*, Dahl, E. \*, Sharipo, A. \*, Staub, E. \*, Otting, G. **The death-domain fold of the ASC PYRIN domain, presenting a basis for PYRIN/PYRIN recognition.** *J. Mol. Biol.* (2003), 332(5), 1155–1163.

Liepinsh, E. \*, Génereux, C. \*, Dehareng, D. \*, Joris, B. \*, Otting, G. **NMR structure of *Citrobacter freundii* AmpD, comparison with bacteriophage T7 lysozyme and homology with PGRP domains.** *J. Mol. Biol.* (2003), 327(4), 833–842.

Liepinsh, E. \*, Leonchiks, A. \*, Sharipo, A. \*, Guignard, L. \*, Otting, G. **Solution structure of the R3H domain from human Subp-2.** *J. Mol. Biol.* (2003), 326(1), 217–223.

Pintacuda, G. \*, Hohenthanner, K. \*, Otting, G., Müller, N. \* **Angular dependence of dipole-dipole-Curie-spin cross-correlation effects in high-spin and low-spin paramagnetic myoglobin.** *J. Biomol. NMR* (2003), 27(2), 115–132.

Usami, S. \*, Takahashi, K. \*, Yuge, I. \*, Ohtsuka, A. \*, Namba, A. \*, Abe, S. \*, Fransen, E. \*, Patthy, L. \*, Otting, G., Van Camp, G. \* **Mutations in the *COCH* gene are a frequent cause of autosomal dominant progressive cochleo-vestibular dysfunction, but not of Meniere's disease.** *Eur. J. Hum. Genet.* (2003), 11(10), 744–748.

### Bioinorganic and Medicinal Chemistry

Bernardo, P.H.<sup>+1</sup>, Brasch, N., Chai, C.L.L.<sup>+1</sup>, Waring, P.<sup>+1</sup> **A novel redox mechanism for the glutathione-dependent reversible uptake of a fungal toxin in cells.** *J. Biol. Chem.* (2003), 278, 46549–46555.

Brodie, S.J., Cregan, A.G., van Eldik, R. \*, Brasch, N.E. **The reaction between methylcobalamin and cyanide revisited.** *Inorg. Chim. Acta* (2003), 348, 221–224.

Hamza, M.S.A. \*, Cregan, A.G., Brasch, N.E., van Eldik, R. \* **Mechanistic insight from activation parameters for the reaction between co-enzyme B<sub>12</sub> and cyanide: further evidence that heterolytic Co–C bond cleavage is solvent-assisted.** *Dalton Trans.* (2003), 596–602.

#### Patent:

Brasch, N.E., Xia, L. **A method of synthesis of thiol-containing cobalamin compounds.** United States utility patent application 10/430,468, 13 May 2003.

### Coordination Chemistry and Spectro-Electro Chemistry

Heath, G.A., Edwards, A.J., Sterns, M.<sup>+1</sup>, Bailey, G.<sup>\*</sup>, Otieno–Alego, V.<sup>#</sup> **‘Crystals from an aged Merlin.’ Corrosion deposits found in the engines of the historic Avro–Lancaster bomber, G-for-George.** In *Conservation Science 2002. Papers from the Conference held in Edinburgh, Scotland 22–24 May 2002*, Eds J.H. Townsend, K. Eremin, A. Adriaens, Archetype Publications Ltd: London (2003), pp 227–235.

Hurst, S.K.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Morrall, J.P.<sup>+1</sup>, Cifuentes, M.P.<sup>+1</sup>, Samoc, M.<sup>#2</sup>, Luther–Davies, B.<sup>#2</sup>, Heath, G.A., Willis, A.C. **Organometallic complexes for nonlinear optics. Part 31. Cubic hyperpolarizabilities of ferrocenyl-linked gold and ruthenium complexes.** *J. Organomet. Chem.* (2003), 670(1–2), 56–65.

Knottenbelt, S.Z.<sup>#</sup>, McGrady, J.E.<sup>#</sup>, Heath, G.A. **The interplay between steric repulsions and metal-metal bonding in  $[\text{Ru}_2(\mu\text{-Cl})_3(\text{PR}_3)_6]^{z+}$ , R = H, Me, Et, z = 1, 2, 3: a hybrid QM/MM study.** *Dalton Trans.* (2003), (2), 227–232.

Morrall, J.P.<sup>+1</sup>, Powell, C.E.<sup>+1</sup>, Stranger, R.<sup>+1</sup>, Cifuentes, M.P.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Heath, G.A. **Organometallic complexes for nonlinear optics. Part 32. Synthesis, optical spectroscopy and theoretical studies of some osmium alkynyl complexes.** *J. Organomet. Chem.* (2003), 670(1–2), 248–255.

Powell, C.E.<sup>+1</sup>, Cifuentes, M.P.<sup>+1</sup>, Morrall, J.P.<sup>+1</sup>, Stranger, R.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Samoc, M.<sup>#2</sup>, Luther–Davies, B.<sup>#2</sup>, Heath, G.A. **Organometallic complexes for nonlinear optics. 30. Electrochromic linear and nonlinear optical properties of alkynylbis(diphosphine)ruthenium complexes.** *J. Am. Chem. Soc.* (2003), 125(2), 602–610.

### Synthetic Organometallic and Coordination Chemistry

Caldwell, L.M., Edwards, A.J., Hill, A.F., Neumann, H., Schultz, M. **Rhodium-induced fragmentation and rearrangement of 4,7,10-trithiatrideca-2,11-diyne.** *Organometallics* (2003), 22(12), 2531–2534.

Cook, D.J.<sup>\*</sup>, Hill, A.F. **Metallathiirenes. 4. Thioaroyl complexes of molybdenum(II) and tungsten(II).** *Organometallics* (2003), 22(17), 3502–3512.

Eisenrager, F.<sup>\*</sup>, Gothlich, A.<sup>\*</sup>, Gruber, I.<sup>\*</sup>, Heiss, H.<sup>\*</sup>, Kiener, C.A.<sup>\*</sup>, Kruger, C.<sup>\*</sup>, Notheis, J.U.<sup>\*</sup>, Rominger, F.<sup>\*</sup>, Scherhag, G.<sup>\*</sup>, Schultz, M., Straub, B.F.<sup>\*</sup>, Volland, M.A.O.<sup>\*</sup>, Hofmann, P.<sup>\*</sup> **Sterically crowded diphosphinomethane ligands: molecular structures, UV-photoelectron spectroscopy and a convenient general synthesis of  $\text{tBu}_2\text{PCH}_2\text{P}^t\text{Bu}_2$  and related species.** *New J. Chem.* (2003), 27(3), 540–550.

Foreman, M.R.St.-J.<sup>\*</sup>, Hill, A.F., Owen, G.R.<sup>\*</sup>, White, A.J.P.<sup>\*</sup>, Williams, D.J.<sup>\*</sup> **Polyazoly chelate chemistry. 12. An unusual mode of coordination for the hydrotris(methimazoly)borato ligand.** *Organometallics* (2003), 22(22), 4446–4450.

Foreman, M.R.St.-J.<sup>\*</sup>, Hill, A.F., Tshabang, N., White, A.J.P.<sup>\*</sup>, Williams, D.J.<sup>\*</sup> **Metallathiirenes. 5. Bis- and tris(methimazoly)borato thiocarbamoyl complexes of molybdenum(II).** *Organometallics* (2003), 22(26), 5593–5596.

Foreman, M.R.St.-J.<sup>\*</sup>, Hill, A.F., White, A.J.P.<sup>\*</sup>, Williams, D.J.<sup>\*</sup> **Hydrotris-(methimazoly)borato alkylidyne complexes of tungsten.** *Organometallics* (2003), 22(19), 3831–3840.

## Publications

### Inorganic Stereochemistry and Asymmetric Synthesis

Blake, C.J., Cook, V.C.<sup>†</sup>, Keniry, M.A., Kitto, H.J., Rae, A.D., Swiegers, G.F.<sup>†</sup>, Willis, A.C., Zank, J., Wild, S.B. **Diastereoselectivity and molecular recognition in the self-assembly of double-stranded dinuclear metal complexes of the type  $\{M_2\{(R^*,S^*)\text{-tetraphos}\}_2\} (PF_6)_2$  (M = Ag and Au).** *Inorg. Chem.* (2003), 42(26), 8709–8715.

Delfs C.D., Kitto H.J., Stranger, R.<sup>†</sup>, Swiegers G.F.<sup>†</sup>, Wild S.B., Willis A.C., Wilson G.J.\* **Photoluminescence properties of four-coordinate gold(I)-phosphine complexes of the types  $[Au(\text{diphos})_2]PF_6$  and  $[Au_2(\text{tetraphos})_2](PF_6)_2$ .** *Inorg. Chem.* (2003), 42(14), 4469–4478.

### Solid State Inorganic Chemistry

Amini, M.M.\* , Foladi, S.\* , Aghabozorg, H.\* , Rae, A.D., Ng, S.W.\* **Crystal structures of bis[aquachlorotriphenyltin(IV)] dihydrate .1,4,7,10,13,16-hexacyclooctadecane - bis[aquachlorotriphenyltin(IV)] .1,4,7,10,13,16-hexacyclooctadecane (3/1) and bis[aquatrifluoroacetatotriphenyltin(IV)] dihydrate .1,4,7,10,13,16-hexacyclooctadecane-bis(aquatrifluoroacetatotriphenyltin(IV)) .1,4,7,10,13,16-hexacyclooctadecane (3/1) co-crystals at  $-105^\circ\text{C}$ .** *Chinese J. Struct. Chem.* (2003), 22, 77–83.

Blake, C.J., Cook, V.C.<sup>†</sup>, Keniry, M.A., Kitto, H.J., Rae, A.D., Swiegers, G.F.<sup>†</sup>, Willis, A.C., Zank, J., Wild, S.B. **Diastereoselectivity and molecular recognition in the self-assembly of double-stranded dinuclear metal complexes of the type  $\{M_2\{(R^*,S^*)\text{-tetraphos}\}_2\} (PF_6)_2$  (M = Ag and Au).** *Inorg. Chem.* (2003), 42(26), 8709–8715.

Brink, F.J., Norén, L., Goossens, D.J.<sup>†</sup>, Withers, R.L., Liu, Y., Xu, C.-N.\* **A combined diffraction (XRD, electron and neutron) and electrical study of  $Na_3MoO_3F_3$ .** *J. Solid State Chem.* (2003), 174(2), 450–458.

Brink, F.J., Norén, L., Withers, R.L. **Synthesis, electron diffraction, XRD and DSC study of the new elpasolite-related oxyfluoride,  $Tl_3MoO_3F_3$ .** *J. Solid State Chem.* (2003), 174(1), 44–51.

Brown, K.N.<sup>†</sup>, Geue, R.J.<sup>†</sup>, Hambley, T.W.\* , Hockless, D.C.R.<sup>†</sup>, Rae, A.D., Sargeson, A.M.<sup>‡</sup> **Specificity in template syntheses of hexaaza-macrobicyclic cages:  $[Pt(\text{Me}_5\text{-tricosatrieneN}_6)]^{4+}$  and  $[Pt(\text{Me}_5\text{-tricosaneN}_6)]^{4+}$ .** *Org. Biomol. Chem.* (2003), 1, 1598–1608.

Enjalbert, R.\* , Galy, J.\* , Castro, A.\* , Lidin, S.\* , Withers, R., Van Tendeloo, G.<sup>‡</sup> **Order and twinning in  $Sb_2W_{0.75}Mo_{0.25}O_6$ .** *Solid State Sci.* (2003), 5(5), 721–724.

Höche, T.\* , Esmailzadeh, S.\* , Withers, R.L., Schirmer, H.\* **Structural studies on the fresnoite type compound  $Ba_2VSi_2O_8$ .** *Z. Kristallogr.* (2003), 218, 788–794.

Liu, Y., Norén, L., Withers, R.L., Hadermann, J.\* , Van Tendeloo, G.<sup>‡</sup>, García-García, F.J.\* **The metastable  $Ni_{7\pm x}S_6$ , and mixed  $Ni_{6\pm x}(S_{1-y}Se_y)_5$ , phases.** *J. Solid State Chem.* (2003), 170(2), 351–360.

Liu, Y., Withers, R.L. **Rigid unit modes (RUMs) of distortion, local crystal chemistry and the inherent displacive flexibility of microporous  $AlPO_4\text{-11}$ .** *J. Solid State Chem.* (2003), 172(2), 431–437.

Liu, Y., Withers, R.L., Fitzgerald, J.<sup>#3</sup> **A TEM, XRD and crystal chemical investigation of oxygen/vacancy ordering in  $(Ba_{1-x}La_x)_2In_2O_{5+x}$ ,  $0 \leq x \leq 0.6$ .** *J. Solid State Chem.* (2003), 170(2), 247–254.

- Liu, Y., Withers, R.L., Norén, L. **An electron diffraction, XRD and lattice dynamical investigation of the average structure and rigid unit mode (RUM) modes of distortion of microporous  $\text{AlPO}_4\text{-5}$ .** *Solid State Sci.* (2003), 5(3), 427–434.
- Ng, S.W.<sup>\*</sup>, Rae, A.D. **The twinned and disordered structure of tetrakis(triphenyl phosphine)silver(I)bis(trifluoroacetato)triphenylstannate(IV).** *Z. Kristallogr.* (2003), 218, 581–584.
- Norén, L., Withers, R.L., Brink, F.J. **Te for two. Ordering phenomena in doped  $\text{Ni}_{1+x}\text{M}_y\text{Te}_2$  ( $\text{M} = \text{Ag, Cu, In}$ ).** *J. Alloys Compd.* (2003), 353(1–2), 133–142.
- Notaras, E.G.A.<sup>+1</sup>, Lucas, N.T.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Willis, A.C., Rae, A.D. **Mixed-metal cluster chemistry. 23. Synthesis and crystallographic and electrochemical studies of alkyne-coordinated group 6–iridium clusters linked by heterocyclic groups.** *Organometallics* (2003), 22, 3659–3670.
- Rae, A.D., Willis, A.C. **9,10 Phenanthroquinone, not your average structure.** *Z. Kristallogr.* (2003), 218, 221–230.
- Rahman, A.F.M.M.<sup>\*</sup>, Jackson, W.G.<sup>\*</sup>, Willis, A.C., Rae, A.D. **Synthesis and crystal and molecular structure of a hydrido tetraamine cobalt(III) complex.** *Chem. Commun.* (2003), 2748–2749.
- Sugiyarto, K.H.<sup>\*</sup>, McHale, W.-A.<sup>\*</sup>, Craig, D.C.<sup>\*</sup>, Rae, A.D., Scudder, M.L.<sup>\*</sup>, Goodwin, H.A.<sup>\*</sup> **Spin transition centres linked by the nitroprusside ion. The cooperative transition in bis(2,6-bis(pyrazol-3-yl)pyridine)iron(II) nitroprusside.** *Dalton Trans.* (2003), 2443–2448.
- Walker, G.W.<sup>†</sup>, Geue, R.J.<sup>†</sup>, Haller, K.J.<sup>‡</sup>, Rae, A.D., Sargeson, A.M.<sup>‡</sup> **New synthetic routes to hexa-aza cages using cobalt(III) tris(1,2-diamine) templates.** *Dalton Trans.* (2003), 279–281.
- Withers, R.L. **An analytical solution for the zero frequency hyperbolic RUM modes of distortion of  $\text{SiO}_2$ -tridymite.** *Solid State Sci.* (2003), 5(1), 115–123.
- Withers, R.L., James, M.<sup>\*</sup>, Goossens, D.J. **Atomic ordering in the doped rare earth cobaltates  $\text{Ln}_{0.33}\text{Sr}_{0.67}\text{CoO}_{3-d}$  ( $\text{Ln} = \text{Y}^{3+}, \text{Ho}^{3+}$  and  $\text{Dy}^{3+}$ ).** *J. Solid State Chem.* (2003), 174(1), 198–208.
- Withers, R.L., Welberry, T.R., Brink, F.J., Norén, L. **Oxygen/fluorine ordering, structured diffuse scattering and the local crystal chemistry of  $\text{K}_3\text{MoO}_3\text{F}_3$ .** *J. Solid State Chem.* (2003), 170(2), 211–220.
- Ying, L.<sup>\*</sup>, Hon, L.S.<sup>\*</sup>, White, T.<sup>\*</sup>, Withers, R., Hai, L.B.<sup>\*</sup> **Controlled nanophase development in photocatalytic titania.** *Materials Trans.* (2003), 44(7), 1328–1332.

## Synthesis and Mechanism

Banwell, M.G. **Trityl thionitrite.** *Encyclopedia of Reagents for Organic Synthesis [Online (eEROS)]*, eds. L. A. Paquette, D. Crich, P. L. Fuchs and P. Wipf, John Wiley & Sons Ltd., (2003), <http://www.mrw.interscience.wiley.com/eros/>.

Banwell, M.G., Bezos, A.<sup>#1</sup>, Chand, S., Dannhardt, G.<sup>\*</sup>, Kiefer, W.<sup>\*</sup>, Nowe, U.<sup>\*</sup>, Parish, C.R.<sup>#1</sup>, Savage, G.P.<sup>\*</sup>, Ulbrich, H.<sup>\*</sup> **Convergent synthesis and preliminary biological evaluations of the stilbenolignan ( $\pm$ )-aiphanol and various congeners.** *Org. Biomol. Chem.* (2003), 1(14), 2427–2429. Also included in the *Chemical Biology Virtual Journal* which can be accessed via [www.rsc.org/chembiol](http://www.rsc.org/chembiol).

## Publications

Banwell, M.G., Chun, C.<sup>‡</sup>, Edwards, A.J., Vögtle, M.M.<sup>†</sup> **Competitive intramolecular Diels–Alder reactions of bis- $\alpha,\beta$ -unsaturated ester derivatives of enzymatically derived and enantiopure *cis*-1,2-dihydrocatechols. Enantiodivergent synthesis of monochiral bicyclo[2.2.2]oct-2-enes.** *Aust. J. Chem.* (2003), 56(9), 861–869.

Banwell, M.G., Coster, M.J., Edwards, A.J., Karunaratne, O.P., Smith, J.A.<sup>†</sup>, Welling, L.L., Willis, A.C. **A total synthesis of the styryllactone (+)-goniodiol from naphthalene.** *Aust. J. Chem.* (2003), 56(6), 585–595.

Banwell, M.G., Coster, M.J., Edwards, A.J., Vögtle, M.<sup>†</sup> **CP-225,917 and CP-263,114 synthesis support studies: testing a radical cyclization strategy for installation of the side-chains.** *Aust. J. Chem.* (2003), 56(6), 577–583.

Banwell, M.G., Coster, M.J., Harvey, M.J., Moraes, J.<sup>‡</sup> **Selective cleavage of *N*-benzyl-protected secondary amines by triphosgene.** *J. Org. Chem.* (2003), 68(2), 613–616.

Banwell, M.G., Edwards, A.J., Essers, M., Jolliffe, K.A.<sup>†</sup> **Conversion of (–)-3-dehydroshikimic acid into derivatives of the (+)-enantiomer.** *J. Org. Chem.* (2003), 68(17), 6839–6841.

Banwell, M.G., Edwards, A.J., Harfoot, G.J., Jolliffe, K.A.<sup>†</sup>, McLeod, M.D.<sup>†</sup>, McRae, K.J.<sup>†</sup>, Stewart, S.G.<sup>†</sup>, Vögtle, M.<sup>†</sup> **Chemoenzymatic methods for the enantioselective preparation of sesquiterpenoid natural products from aromatic precursors.** *Pure Appl. Chem.* (2003), 75(2–3), 223–229.

Banwell, M.G., Edwards, A.J., Jolliffe, K.A.<sup>†</sup>, Smith, J.A.<sup>†</sup>, Hamel, E.<sup>\*</sup>, Verdier–Pinard, P.<sup>\*</sup> **Total synthesis of (±)-rhazinal, an alkaloidal spindle toxin from *Kopsia teoi*.** *Org. Biomol. Chem.* (2003), 1(2), 296–305. Also included in the *Chemical Biology Virtual Journal* which can be accessed via [www.rsc.org/chembiol](http://www.rsc.org/chembiol).

Banwell, M.G., Hockless, D.C.R.<sup>†</sup>, McLeod, M.D.<sup>†</sup> **Chemoenzymatic total syntheses of the sesquiterpene (–)-patchoulone.** *New J. Chem.* (2003), 27(1), 50–59.

Banwell, M.G., Kelly, B.D., Kokas, O.J.<sup>‡</sup>, Lupton, D.W. **Synthesis of indoles via palladium[0]-mediated Ullmann cross-coupling of *o*-halonitroarenes with  $\alpha$ -halo-enones or -enals.** *Org. Lett.* (2003), 5(14), 2497–2500.

Banwell, M.G., Ma, X., Asano, N.<sup>\*</sup>, Ikeda, K.<sup>\*</sup>, Lambert, J.N.<sup>\*</sup> **Chemoenzymatic syntheses of (–)-1-deoxymannojirimycin (DMJ) and its naturally occurring 6-*O*- $\alpha$ -L-rhamnopyranosyl glycoside.** *Org. Biomol. Chem.* (2003), 1(12), 2035–2037. Also included in the *Chemical Biology Virtual Journal* which can be accessed via [www.rsc.org/chembiol](http://www.rsc.org/chembiol).

Crasto, C.F.<sup>†</sup>, Forrest, A.K.<sup>\*</sup>, Karoli, T.<sup>†</sup>, March, D.R.<sup>†</sup>, Mensah, L.<sup>\*</sup>, O’Hanlon, P.J.<sup>\*</sup>, Nairn, M.R., Oldham, M.D.<sup>†</sup>, Yue, W.<sup>†</sup>, Banwell, M.G., Easton, C.J. **Synthesis and activity of analogues of the isoleucyl tRNA synthetase inhibitor SB-203207.** *Bioorg. Med. Chem.* (2003), 11(13), 2687–2694.

Heinrich, M.R.<sup>\*</sup>, Steglich, W.<sup>\*</sup>, Banwell, M.G., Kashman, Y.<sup>\*</sup> **Total synthesis of the marine alkaloid halitulins.** *Tetrahedron* (2003), 59(46), 9239–9247.

Hungerford, N.L., Armit, D.J.<sup>†</sup>, Banwell, M.G. **Syntheses of showdomycin and its anomer using *N*-(triisopropylsilyl)pyrrole as a synthetic equivalent for the maleimide C3-anion.** *Synthesis* (2003), (12), 1837–1843.

Taylor, R.M. **gem-Dihalocyclopropanes as building blocks in natural product synthesis.** *Aust. J. Chem.* (2003), 56(6), 631.

**Patents:**

Banwell, M.G., Liu, L.<sup>†</sup>, Parish, C.R.<sup>#1</sup>, Freeman, C.G.<sup>#1</sup> **Linked cyclitols and their polysulfated derivatives.** International Patent Number WO 03/004454 A1, (2003), 84 pp.

Banwell, M.G., Lupton, D.W. **A method of indole synthesis.** Australian Provisional Patent Application Number 2003902023 (filed 29 April 2003).

### Biochemical Reactions and Molecular Recognition

Brown, S.E.<sup>†</sup>, Easton, C.J., Kelly, J.B.<sup>†</sup> **Surface plasmon resonance to determine apparent stability constants for the binding of cyclodextrins to small immobilized guests.** *J. Inclusion Phenom. Macrocyclic Chem.* (2003), 46(3–4), 167–173.

Coghlan, D.R.\* , Easton, C.J., Tiekink, E.R.T.\* **Crystal structure of meso-dimethyl 2,3-dibenzamido-2,3-dimethylbutanedioate, C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>6</sub>.** *Z. Kristallogr. NCS* (2003), 218(3), 359–360.

Coghlan, D.R.\* , Easton, C.J., Tiekink, E.R.T.\* **Crystal structure of dl-dimethyl 2,3-dibenzamido-2,3-dimethylbutanedioate, C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>6</sub>.** *Z. Kristallogr. NCS* (2003), 218(3), 361–362.

Crasto, C.F.<sup>†</sup>, Forrest, A.K.\* , Karoli, T.<sup>†</sup>, March, D.R.<sup>†</sup>, Mensah, L.\* , O'Hanlon, P.J.\* , Nairn, M.R., Oldham, M.D.<sup>†</sup>, Yue, W.<sup>†</sup>, Banwell, M.G., Easton, C.J. **Synthesis and activity of analogues of the isoleucyl tRNA synthetase inhibitor SB-203207.** *Bioorg. Med. Chem.* (2003), 11(13), 2687–2694.

Croft, A.K.<sup>†</sup>, Easton, C.J., Kociuba, K.<sup>†</sup>, Radom, L. **Strategic use of amino acid N-substituents to limit  $\alpha$ -carbon-centered radical formation and consequent loss of stereochemical integrity.** *Tetrahedron: Asymm.* (2003), 14(19), 2919–2926.

Croft, A.K.<sup>†</sup>, Easton, C.J., Radom, L. **Design of radical-resistant amino acid residues: a combined theoretical and experimental investigation.** *J. Am. Chem. Soc.* (2003), 125(14), 4119–4124.

Dumanski, P.G., Easton, C.J., Lincoln, S.F.<sup>‡</sup>, Simpson, J.S. **Effect of cyclodextrins on electrophilic aromatic bromination in aqueous solution.** *Aust. J. Chem.* (2003), 56(11), 1107–1111.

Easton, C.J., Edwards, A.J., McNabb, S.B.<sup>†</sup>, Merrett, M.C.<sup>†</sup>, O'Connell, J.L.<sup>†</sup>, Simpson, G.W.\* , Simpson, J.S., Willis, A.C. **Allylic halogenation of unsaturated amino acids.** *Org. Biomol. Chem.* (2003), 1(14), 2492–2498.

Easton, C.J., Hughes, C.M.M.\* , Tiekink, E.R.T.\* **Crystal structure of 3-(2,6-dichlorophenyl)-6,7-dihydro-4H-pyrano[3,4-d]isoxazol-4-one, C<sub>12</sub>H<sub>7</sub>Cl<sub>2</sub>NO<sub>3</sub>.** *Z. Kristallogr. NCS* (2003), 218(3), 363–364.

Easton, C.J., Hughes, C.M.M.\* , Tiekink, E.R.T.\* **Crystal structure of 3-(2,6-dichlorophenyl)-4,5-dihydro-7H-pyrano[4,3-d]isoxazol-7-one, C<sub>12</sub>H<sub>7</sub>Cl<sub>2</sub>NO<sub>3</sub>.** *Z. Kristallogr. NCS* (2003), 218(3), 365–366.

Harper, J.B.<sup>†</sup>, Easton, C.J., Lincoln, S.F.<sup>‡</sup> **A cyclodextrin-based molecular reactor to template the formation of indigoid dyes.** *Tetrahedron Lett.* (2003), 44(31), 5815–5818.

## Publications

Onagi, H., Blake, C.J., Easton, C.J., Lincoln, S.F.<sup>‡</sup> **Installation of a ratchet tooth and pawl to restrict rotation in a cyclodextrin rotaxane.** *Chem. Eur. J.* (2003), 9(24), 5978–5988.

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

Robinson, B.S.<sup>\*</sup>, Rathjen, D.A.<sup>\*</sup>, Trout, N.A.<sup>\*</sup>, Easton, C.J., Ferrante, A.<sup>\*</sup> **Inhibition of neutrophil leukotriene B<sub>4</sub> production by a novel synthetic N-3 polyunsaturated fatty acid analogue,  $\beta$ -oxa 21:3n-3.** *J. Immunol.* (2003), 171(9), 4773–4779.

West, L.C.<sup>\*</sup>, Wyness, O.<sup>\*</sup>, May, B.L.<sup>\*</sup>, Clements, P.<sup>\*</sup>, Lincoln, S.F.<sup>‡</sup>, Easton, C.J. **Diazacoronand linked  $\beta$ -cyclodextrin dimer complexes of Brilliant Yellow tetraanion and their sodium(I) analogues.** *Org. Biomol. Chem.* (2003), 1(5), 887–894.

### Patent:

Easton, C.J., Barratt, B.J.W., Simpson, J.S. **Enzyme inhibitors.** International Patent Application Number PCT/AU03/00905.

## Organic Synthesis

### 2002

Liu, J.P.<sup>†</sup>, Mander, L.N. **Attempt to build 13-hydroxy-9,15-cyclo GA skeletons.** *Chin. Chem. Lett.* (2002), 13(12), 1152–1153.

### 2003

Adamson, G.<sup>†</sup>, Mander, L.N. **Conversion of gibberellic acid into the B-ring *seco*-kaurenoid, longirabdolactone.** *Aust. J. Chem.* (2003), 56(8), 805–809.

Buttle, L.A.<sup>†</sup>, Morris, J.C.<sup>†</sup>, Mander, L.N. **Further investigations into the preparation and [4+2] cycloaddition reactions of vinyl norcaradiene derivatives.** *ARKIVOC* (2003), (8), 118–134.

King, R.W.<sup>\*</sup>, Evans, L.T.<sup>\*</sup>, Mander, L.N., Moritz, T.<sup>\*</sup>, Pharis, R.P.<sup>†</sup>, Twitchin, B. **Synthesis of gibberellin GA<sub>6</sub> and its role in flowering of *Lolium temulentum*.** *Phytochemistry* (2003), 62(1), 77–82.

Leitch, S.K.<sup>†</sup>, Blake, P.S.<sup>\*</sup>, Mander, L.N. **Synthesis and structure determination of three new 12 $\beta$ -hydroxy C<sub>20</sub> gibberellins (GA<sub>127</sub>, GA<sub>128</sub> and GA<sub>129</sub>).** *ARKIVOC* (2003), (7), 145–160.

Mander, L.N. **Charles William Shoppee 1904–1994.** *Historical Records of Australian Science* (2003), 14(4), 509–528.

Mander, L.N. **Charles William Shoppee 1904–1994.** *Biographical Memoirs of Fellows of the Royal Society* (2003), 49, 495–507.

Mander, L.N. **Twenty years of gibberellin research.** *Nat. Prod. Rep.* (2003), 20(1), 49–69.

Mander, L.N., McLachlan, M.M.<sup>†</sup> **The total synthesis of the galbulimima alkaloid GB 13.** *J. Am. Chem. Soc.* (2003), 125(9), 2400–2401.



Mander, L.N., O'Sullivan, T.P.<sup>†</sup> **An exploration of the potential of [4+2] cycloadditions of  $\alpha$ -pyrones with indenones for the synthesis of the norditerpenoid tropone, harringtonolide.** *Synlett* (2003), (9), 1367–1369.

Mander, L.N., Thomson, R.J.<sup>†</sup> **Total synthesis of sordaricin.** *Org. Lett.* (2003), 5(8), 1321–1324.

Mander, L.N., Williams, C.M.<sup>†</sup> **Oxidative degradation of benzene rings.** *Tetrahedron* (2003), 59(8), 1105–1136.

Stokes, T.S.\* , Mander, L.N., Croker, S.J.\* , Twitchin, B., Hanke, D.E.\* **3 $\beta$ ,13-Dihydroxylated C<sub>20</sub> gibberellins from inflorescences of *Rumex acetosa* L.** *Phytochemistry* (2003), 62(2), 165–174.

Williams, C.M.<sup>†</sup>, Mander, L.N. **Bridgehead arylation: a direct route to advanced intermediates for the synthesis of C-20 diterpene alkaloids.** *Org. Lett.* (2003), 5(19), 3499–3502.

Williams, C.M.<sup>†</sup>, Mander, L.N., Bernhardt, P.V.<sup>†</sup> **1-Ethynyl-2-isopropoxy-3-methoxybenzene.** *Acta Cryst.* (2003), E59(4), o561–o563.

### Organic Synthesis, Methodology And Host-Guest Chemistry

Cayzer, T.N., Paddon-Row, M.N.\* , Sherburn, M.S. **Stereocontrol of the intramolecular Diels–Alder reaction by internal hydrogen bonding.** *Eur. J. Org. Chem.* (2003), (20), 4059–4068.

Reynolds, A.J.\* , Scott, A.J., Turner, C.I., Sherburn, M.S. **The intramolecular carboxyarylation approach to podophyllotoxin.** *J. Am. Chem. Soc.* (2003), 125(40), 12108–12109.

Scott, A. **Oxazolines as directing agents in the nucleophilic addition to naphthalenes.** *Aust. J. Chem.* (2003), 56(9), 953.

Turner, C.I., Williamson, R.M.\* , Turner, P.\* , Sherburn, M.S. **The domino intramolecular Diels–Alder approach to 16-oxasteroids.** *Chem. Commun.* (2003), (13), 1610–1611.

Wong, L.S.-M., Sherburn, M.S. **IMDA-radical cyclization approach to (+)-himbacine.** *Org. Lett.* (2003), 5(20), 3603–3606.

### Theoretical Chemical Physics

Brouard, M.\* , Burak, I.\* , Marinakis, S.\* , Minayev, D.\* , O'Keeffe, P.\* , Vallance, C.\* , Aoiz, F.J.\* , Bañares, L.\* , Castillo, J.F.<sup>‡</sup>, Zhang, D.H.<sup>‡</sup>, Xie, D.\* , Yang, M.\* , Lee, S.-Y.\* , Collins, M.A. **Cross section for the H + H<sub>2</sub>O abstraction reaction: experiment and theory.** *Phys. Rev. Lett.* (2003) 90, 093201–093204.

Brouard, M.\* , Burak, I.\* , Minayev, D.\* , O'Keeffe, P.\* , Vallance, C.\* , Aoiz, F.J.\* , Bañares, L.\* , Castillo, J.F.<sup>‡</sup>, Zhang, D.H.<sup>‡</sup>, Collins, M.A. **The dynamics of the H+D<sub>2</sub>O→OD+HD reaction at 2.5 eV: experiment and theory.** *J. Chem. Phys.* (2003), 118(3), 1162–1174.

Castillo, J.F.<sup>‡</sup>, Collins, M.A., Aoiz, F.J.\* , Bañares, L.\* **Quasiclassical trajectory study of the dynamics of the H+N<sub>2</sub>O reaction on a new potential energy surface.** *J. Chem. Phys.* (2003), 118(16), 7303–7312.

## Publications

Collins, M.A., Radom, L. **Proton-transport catalysis, proton abstraction, and proton exchange in  $\text{HF}+\text{HOC}^+$  and  $\text{H}_2\text{O}+\text{HOC}^+$  and analogous deuterated reactions.** *J. Chem. Phys.* (2003), 118(14), 6222–6229.

Coote, M.L., Collins, M.A., Radom, L. **Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax.** *Mol. Phys.* (2003), 101(9), 1329–1338.

Crespos, C.<sup>‡</sup>, Collins, M.A., Pijper, E.<sup>\*</sup>, Kroes, G.J.<sup>\*</sup> **Multi-dimensional potential energy surface determination by modified Shepard interpolation for a molecule-surface reaction:  $\text{H}_2 + \text{Pt}(111)$ .** *Chem. Phys. Lett.* (2003), 376, 566–575.

Moyano, G.E., Collins, M.A. **Interpolated potential energy surface and classical dynamics for  $\text{H}_3^+ + \text{HD}$  and  $\text{H}_3^+ + \text{D}_2$ .** *J. Chem. Phys.* (2003), 119(11), 5510–5517.

### Computational Quantum Chemistry, Polymer Chemistry

Barner-Kowollik, C.<sup>\*</sup>, Coote, M.L., Davis, T.P.<sup>\*</sup>, Radom, L., Vana, P.<sup>\*</sup> **The reversible addition-fragmentation chain transfer process and the strength and limitations of modeling: comment on the “Magnitude of the fragmentation rate coefficient”.** *J. Polym. Sci., Part A: Polym. Chem.* (2003), 41, 2828–2832.

Coote, M.L., Collins, M.A., Radom, L. **Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax.** *Mol. Phys.* (2003), 101(9), 1329–1338.

Coote, M.L., Davis, T.P.<sup>\*</sup> **Effect of the copolymer composition on the  $K$  and  $\alpha$  constants of the Mark–Houwink equation: comments on a recent paper by Songkhla and Wootthikanokkhan.** *J. Polym. Sci., Part B: Polym. Phys.* (2003), 41, 655–659.

Coote, M.L., Gordon, D.H.<sup>\*</sup>, Hutchings, L.R.<sup>\*</sup>, Richards, R.W.<sup>\*</sup>, Dalgleish, R.C.<sup>\*</sup> **Neutron reflectometry investigation of polymer–polymer reactions at the interface between immiscible polymers.** *Polymer* (2003), 44, 7689–7700.

Coote, M.L., Pross, A.<sup>\*</sup>, Radom, L. **Variable trends in R–X bond dissociation energies (R = Me, Et, i-Pr, t-Bu).** *Org. Lett.* (2003), 5, 4689–4692.

Coote, M.L., Radom, L. **Ab initio evidence for slow fragmentation in RAFT polymerisation.** *J. Am. Chem. Soc.* (2003), 125, 1490–1491.

Gómez-Balderas, R., Coote, M.L., Henry, D.J., Fischer, H.<sup>\*</sup>, Radom, L. **What is the origin of the contrathermodynamic behavior in methyl radical addition to alkynes versus alkenes.** *J. Phys. Chem. A* (2003), 107, 6082–6090.

### Liquid State Chemical Physics

Delhommelle, J.<sup>\*</sup>, Petravac, J. **Shear viscosity of molten sodium chloride.** *J. Chem. Phys.* (2003), 118(6), 2783–2791.

Delhommelle, J.<sup>\*</sup>, Petravac, J., Evans, D.J. **On the effects of assuming flow profiles in nonequilibrium simulations.** *J. Chem. Phys.* (2003), 119(21), 11005–11010.

- Delhommelle, J.<sup>\*</sup>, Petravac, J., Evans, D.J. **Reexamination of string phase and shear thickening in simple fluids.** *Phys. Rev. E* (2003), 68, 031201/1–6.
- Evans, D.J. **A non-equilibrium free energy theorem for deterministic systems.** *Mol. Phys.* (2003), 101(10), 1551–1554.
- Evans, D.J., Mittag, E.<sup>†</sup> **Time-dependent fluctuation theorem.** *Phys. Rev. E* (2003), 67, 026113/1–5.
- Hess, S.<sup>\*</sup>, Kroger, M.<sup>\*</sup>, Evans, D.J. **Crossover between short- and long-time behaviour of stress fluctuations and viscoelasticity of liquids.** *Phys. Rev. E* (2003), 67, 042201/1–4.
- Petravac, J. **Properties of isolated systems in external fields.** *Phys. Rev. E* (2003), 68, 011104/1–9.
- Petravac, J., Delhommelle, J.<sup>\*</sup> **Conductivity of molten sodium chloride and its supercritical vapor in strong dc electric fields.** *J. Chem. Phys.* (2003), 118(16), 7477–7485.
- Petravac, J., Delhommelle, J.<sup>\*</sup> **Conductivity of molten sodium chloride in an alternating electric field.** *J. Chem. Phys.* (2003), 119(16), 8511–8518.
- Petravac, J., Delhommelle, J.<sup>\*</sup> **Influence of temperature, pressure and internal degrees of freedom on hydrogen bonding and diffusion in liquid ethanol.** *Chem. Phys.* (2003), 286, 303–314.
- Petravac, J., Jepps, O.G.<sup>\*</sup> **Homogeneous shear flow of a hard sphere fluid: analytic solutions.** *Phys. Rev. E* (2003), 67, 021105/1–11.
- Laser and Optical Spectroscopy**
- Åhrling, K.A.<sup>#4</sup>, Peterson, S.<sup>‡</sup> **Light-adaptation of Photosystem II is mediated by the plastoquinone pool.** *Biochemistry* (2003), 42, 7655–7662.
- Krausz, E. **Biophysics and biochemistry of Photosystem II.** *The Physicist* (2003), 40(1), 173–177.
- Lilley, R.McC.<sup>\*</sup>, Wang, X.-Q., Krausz, E., Andrews, T.J.<sup>#4</sup> **Complete spectra of the far-red chemiluminescence of the oxygenase reaction of Mn<sup>2+</sup>-activated ribulose-bisphosphate carboxylase/oxygenase establish Mn<sup>2+</sup> as the source.** *J. Biol. Chem.* (2003), 278(19), 16488–16493.
- Peterson, S.<sup>‡</sup>, Åhrling, K.A.<sup>#4</sup>, Höglblom, J.E.P.<sup>\*</sup>, Styring, S.<sup>\*</sup> **Flash-induced relaxation changes of the EPR signals from the manganese cluster and Y<sub>D</sub> reveal a light-adaptation process of Photosystem II.** *Biochemistry* (2003), 42, 2748–2758.
- Peterson Årsköld, S.<sup>‡</sup>, Masters, V.M., Prince, B., Smith, P.J.<sup>+1</sup>, Pace, R.J.<sup>+1</sup>, Krausz, E. **Optical spectra of synechocystis and spinach Photosystem II preparations at 1.7 K: identification of the D1-pheophytin energies and Stark shifts.** *J. Am. Chem. Soc.* (2003), 125, 13063–13074.
- Riley, M.J.<sup>\*</sup>, Krausz, E.R., Stanco, A.<sup>\*</sup> **New generation MCD spectrometers.** *J. Inorg. Biochem.* (2003), 96, 217.

## Publications

### Computational Quantum Chemistry

Barner-Kowollik, C.<sup>\*</sup>, Coote, M.L., Davis, T.P.<sup>\*</sup>, Radom, L., Vana, P.<sup>\*</sup> **The reversible addition-fragmentation chain transfer process and the strength and limitations of modeling: comment on the “Magnitude of the fragmentation rate coefficient”**. *J. Polym. Sci., Part A: Polym. Chem.* (2003), 41, 2828–2832.

Collins, M.A., Radom, L. **Proton-transport catalysis, proton abstraction and proton exchange in HF + HOC<sup>+</sup> and H<sub>2</sub>O + HOC<sup>+</sup> and analogous deuterated reactions**. *J. Chem. Phys.* (2003), 118, 6222–6229.

Coote, M.L., Collins, M.A., Radom, L. **Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax**. *Mol. Phys.* (2003), 101(9), 1329–1338.

Coote, M.L., Davis, T.P.<sup>\*</sup> **Effect of the copolymer composition on the *K* and  $\alpha$  constants of the Mark–Houwink equation: comments on a recent paper by Songkhla and Woothikanokkhan**. *J. Polym. Sci., Part B: Polym. Phys.* (2003), 41, 655–659.

Coote, M.L., Gordon, D.H.<sup>\*</sup>, Hutchings, L.R.<sup>\*</sup>, Richards, R.W.<sup>\*</sup>, Dalgleish, R.C.<sup>\*</sup> **Neutron reflectometry investigation of polymer–polymer reactions at the interface between immiscible polymers**. *Polymer* (2003), 44, 7689–7700.

Coote, M.L., Pross, A.<sup>\*</sup>, Radom, L. **Variable trends in R–X bond dissociation energies (R = Me, Et, i-Pr, t-Bu)**. *Org. Lett.* (2003), 5, 4689–4692.

Coote, M.L., Radom, L. **Ab initio evidence for slow fragmentation in RAFT polymerisation**. *J. Am. Chem. Soc.* (2003), 125, 1490–1491.

Corral, I.<sup>##</sup>, Mó, O.<sup>\*</sup>, Yáñez, M.<sup>\*</sup>, Scott, A.P., Radom, L. **Interactions between neutral molecules and Ca<sup>2+</sup>: an assessment of theoretical procedures**. *J. Phys. Chem. A* (2003), 107, 10456–10461.

Croft, A.K.<sup>†</sup>, Easton, C.J., Kociuba, K.<sup>†</sup>, Radom, L. **Strategic use of amino acid *N*-substituents to limit  $\alpha$ -carbon-centered radical formation and consequent loss of stereochemical integrity**. *Tetrahedron: Asymm.* (2003), 14(19), 2919–2926.

Croft, A.K.<sup>†</sup>, Easton, C.J., Radom, L. **Design of radical-resistant amino acid residues: a combined theoretical and experimental investigation**. *J. Am. Chem. Soc.* (2003), 125(14), 4119–4124.

Gómez-Balderas, R., Coote, M.L., Henry, D.J., Fischer, H.<sup>\*</sup>, Radom, L. **What is the origin of the contrathermodynamic behavior in methyl radical addition to alkynes versus alkenes**. *J. Phys. Chem. A* (2003), 107, 6082–6090.

Henry, D.J., Beckwith, A.L.J.<sup>+1</sup>, Radom, L. **Homo-anomeric effect in the 1,2-dimethoxyethyl radical**. *Aust. J. Chem.* (2003), 56, 429–436.

Henry, D.J., Sullivan, M.B.<sup>†</sup>, Radom, L. **G3-RAD and G3X-RAD: modified Gaussian-3 (G3) and Gaussian-3X (G3X) procedures for radical thermochemistry**. *J. Chem. Phys.* (2003), 118, 4849–4860.

Rauk, A.<sup>##</sup>, Boyd, R.J.<sup>##</sup>, Boyd, S.L.<sup>##</sup>, Henry, D.J., Radom, L. **Alkoxy radicals in the gaseous phase:  $\beta$ -scission reactions and formation by radical addition to carbonyl compounds**. *Can. J. Chem.* (2003), 81, 431–442.

Sullivan, M.B.<sup>†</sup>, Iron, M.A.\* , Redfern, P.C.\* , Martin, J.M.L.\* , Curtiss, L.A.\* , Radom, L. **Heats of formation of alkali metal and alkaline earth metal oxides and hydroxides: surprisingly demanding targets for high-level ab initio procedures.** *J. Phys. Chem. A* (2003), 107, 5617–5630.

Wood, G.P.F., Henry, D.J., Radom, L. **Performance of the RB3-LYP, RMP2 and UCCSD(T) procedures in calculating radical stabilization energies for •NHX radicals.** *J. Phys. Chem. A* (2003), 107, 7985–7990.

### Electrochemistry

Webster, R.D. **In situ electrochemical-ATR-FTIR spectroscopic studies on solution phase 2,4,6-tri-substituted phenoxy radicals.** *Electrochem. Commun.* (2003), 5(1), 6–11.

### Disordered Materials

Bonin, M.\* , Welberry, T.R., Hostettler, M.\* , Gardon, M.\* , Birkedal, H.\* , Chapuis, G.\* , Möckli, P.\* , Ogle, C.A.\* , Schenk, K.J.\* **Urotropin azelate: a rather unwilling co-crystal.** *Acta Crystallogr., Sect. B* (2003), 59, 72–86.

Kreisel, J.\* , Bouvier, P.\* , Dkhil, B.\* , Thomas, P.A.\* , Glazer, A.M.\* , Welberry, T.R., Chaabane, B.\* , Mezouar, M.\* **High-pressure X-ray scattering of oxides with a nano-scaled local structure: application to Na<sub>1/2</sub>Bi<sub>1/2</sub>TiO<sub>3</sub>.** *Phys. Rev. B* (2003), 68, 014113/1–7.

Welberry, T.R., Goossens, D.J., David, W.I.F.\* , Gutmann, M.J.\* , Bull, M.J.\* , Heerdegen, A.P. **Diffuse neutron scattering from in benzil, C<sub>16</sub>D<sub>10</sub>O<sub>2</sub>, using the time-of-flight Laue technique.** *J. Appl. Crystallogr.* (2003), 36, 1440–1447.

Welberry, T.R., Goossens, D.J., Haeffner, D.R.\* , Lee, P.L.\* , Almer, J.\* **High-energy diffuse scattering on the 1-ID beamline at the Advanced Photon Source.** *J. Synchrotron Rad.* (2003), 10, 284–286.

Welberry, T.R., Heerdegen, A.P. **Diffuse X-ray scattering from 4,4'-dimethoxybenzil, C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>: analysis via automatic refinement of a Monte Carlo model.** *Acta Crystallogr., Sect. B* (2003), 59, 760–769.

Withers, R.L., Welberry, T.R., Brink, F.J., Norén, L. **Oxygen/fluorine ordering, structured diffuse scattering and the local crystal chemistry of K<sub>3</sub>MoO<sub>3</sub>F<sub>3</sub>.** *J. Solid State Chem.* (2003), 170(2), 211–220.

### Solid State Molecular Science

De Bruyn, H.\* , Gilbert, R.G.<sup>†</sup>, White, J.W., Schulz, J.C.\* **Characterization of electrosterically stabilized polystyrene latex; implications for radical entry kinetics.** *Polymer* (2003), 44, 4411–4420.

Devonshire, A.L.\* , Heidari, R., Bell, K.L.\* , Campbell, P.M.\* , Campbell, B.E.\* , Odgers, W.A.\* , Oakeshott, J.G.\* , Russell, R.J.\* **Kinetic efficiency of mutant carboxylesterases implicated in organophosphate insecticide resistance.** *Pestic. Biochem. Physiol.* (2003), 76, 1–13.

Henderson, M.J., King, D., White, J.W. **The growth of self-assembled titania-based films at the air-water interface.** *Aust. J. Chem.* (2003), 56, 933–939.

## Publications

Holt, S.A.<sup>†</sup>, Ruggles, J.L.<sup>†</sup>, Reynolds, P.A., White, J.W. **Structural development of silicated films self-assembled at the air-water interface.** *Physica B* (2003), 336, 193–203.

Reynolds, P.A., McGillivray, D.<sup>†</sup>, Gilbert, E.P.<sup>†</sup>, Holt, S.A.<sup>†</sup>, Henderson, M.J., White, J.W. **Neutron and X-ray reflectivity from polyisobutylene-based amphiphiles at the air-water interface.** *Langmuir* (2003), 19, 752–761.

Ruggles, J.L.<sup>†</sup>, Gilbert, E.P.<sup>†</sup>, Holt, S.A.<sup>†</sup>, Reynolds, P.A., White, J.W. **Expanded mesoporous silicate films grown at the air-water interface by addition of hydrocarbons.** *Langmuir* (2003), 19, 793–800.

## Technical Services

Wheate, N.J.\* , Evison, B.J.\* , Herlt, A.J., Phillips, D.R.\* , Collins, J.G.\* **DNA binding of the anti-cancer platinum complex *trans*-[Pt(NH<sub>3</sub>)<sub>2</sub>Cl]<sub>2</sub>m-dpzm]<sup>2+</sup>.** *Dalton Trans.* (2003), (18), 3486–3492.

## Single Crystal X-ray Diffraction Unit (External Collaborations)

### 2002

Hartnell, R.D.\* , Edwards, A.J., Arnold, D.P.<sup>‡</sup> **Peripherally-metallated porphyrins: *meso*-η<sup>1</sup>-porphyrinylplatinum(II) complexes of 5,15-diaryl- and 5,10,15-triarylporphyrins.** *J. Porphyrins and Phthalocyanines* (2002), 6(11 & 12), 695–707.

### 2003

Bhargava, S.K.\* , Mohr, F.\* , Willis, A.C. **Expect the unexpected. Isolation and characterisation of some unusual organometallic gold(I) complexes.** *Inorg. Chim. Acta* (2003), 352, 19–23.

Chai, C.L.L.<sup>†,+1</sup>, Edwards, A.J., Wilkes, B.A.<sup>+1</sup>, Woodgate, R.C.J.<sup>+1</sup> **Directed 1,3-dipolar cycloadditions of ylidene piperazine-2,5-diones.** *Tetrahedron* (2003), 59(44), 8731–8739.

Chaplin, J.H.<sup>+1</sup>, Edwards, A.J., Flynn, B.L.<sup>†,+1</sup> **An enantioselective double Diels–Alder approach to the tetracyclic framework of colombiasin A.** *Org. Biomol. Chem.* (2003), 1(11), 1842–1844.

Dickie, A.J.\* , Hockless, D.C.R.<sup>†</sup>, Willis, A.C., McKeon, J.A.\* , Jackson, W.G.<sup>‡</sup> **A unique mechanism for base catalyzed hydrolysis of pentaaminocobalt(III) complexes containing picolyl residues.** *Inorg. Chem.* (2003), 42(12), 3822–3834.

Kelly, A.E.\* , Macgregor, S.A.<sup>†</sup>, Willis, A.C., Nelson<sup>‡</sup>, J.H., Wenger, E.<sup>‡</sup>, **Insertion reactions of unsymmetrical ester-activated alkynes with *o*-benzylamine palladacycles: a regioselectivity study.** *Inorg. Chim. Acta* (2003), 352, 79–97.

Matthews, C.J.\* , Broughton, V.\* , Bernardinelli, G.\* , Melich, X.\* , Brand, G.\* , Willis, A.C., Williams, A.F.<sup>‡</sup> **Molecular bricklaying: the protonated benzimidazole moiety as a synthon for crystal engineering.** *New J. Chem.* (2003), 27(2), 354–358.

Powell, C.E.<sup>+1</sup>, Cifuentes, M.P.<sup>+1</sup>, McDonagh, A.M.<sup>+1</sup>, Hurst, S.K.<sup>+1</sup>, Lucas, N.T.<sup>+1</sup>, Delfs, C.D.<sup>†</sup>, Stranger, R.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Houbrechts, S.\* , Asselberghs, I.\* , Persoons, A.\* , Hockless, D.C.R.<sup>†</sup> **Organometallic complexes for nonlinear optics. Part 27. Syntheses and optical**

**properties of some iron, ruthenium and osmium alkynyl complexes.** *Inorg. Chim. Acta* (2003), 352, 9–18.

Usher, A.J.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Willis, A.C. **Mixed-metal cluster chemistry. 24. Isocyanide derivatives of [MoIr<sub>3</sub>(μ-CO)<sub>3</sub>(CO)<sub>8</sub>(η-C<sub>5</sub>H<sub>5</sub>)] and [Mo<sub>2</sub>Ir<sub>2</sub>(μ-CO)<sub>3</sub>(CO)<sub>7</sub>(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>]; X-ray crystal structures of [MoIr<sub>3</sub>(μ-CO)<sub>3</sub>(CO)<sub>7</sub>(L)(η-C<sub>5</sub>H<sub>5</sub>)] (L = CNBu<sup>t</sup>, CNC<sub>6</sub>H<sub>3</sub>Me<sub>2</sub>-2,6) and [Mo<sub>2</sub>Ir<sub>2</sub>(μ-CO)<sub>2</sub>(CNBu<sup>t</sup>)<sub>2</sub>(CO)<sub>6</sub>(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>]. *J. Organomet. Chem.* (2003), 678(1–2), 72–81.**

Usher, A.J.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Willis, A.C. **Mixed-metal cluster chemistry. 25. Mixed ligand derivatives of MoIr<sub>3</sub>(μ-CO)<sub>3</sub>(CO)<sub>8</sub>(η-C<sub>5</sub>R<sub>5</sub>) (R = H, Me) and Mo<sub>2</sub>Ir<sub>2</sub>(μ-CO)<sub>3</sub>(CO)<sub>7</sub>(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>; X-ray crystal structures of MoIr<sub>3</sub>(μ-CO)<sub>3</sub>(CO)<sub>6</sub>(PPh<sub>3</sub>)<sub>2</sub>(η-C<sub>5</sub>Me<sub>5</sub>) and Mo<sub>2</sub>Ir<sub>2</sub>(μ<sub>4</sub>-η<sup>2</sup>-PhC<sub>2</sub>Ph)(μ-CO)<sub>4</sub>(CNBu<sup>t</sup>)(CO)<sub>3</sub>(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>.** *J. Organomet. Chem.* (2003), 682(1–2), 41–48.

Zhou, X., Day, A.I.<sup>\*</sup>, Willis, A.C., Jackson, W.G.<sup>‡</sup> **The first structurally characterised perchlorato-cobalt(III) complexes, involving the C-bonded macrobicyclic ligand 1,4,8,11-tetraazabicyclo[9.5.2]octadecane.** *Chem. Commun.* (2003), (18), 2386–2387.

### Adjunct Professor Veronica James

James, V.J. **Changes in the diffraction pattern of hair resulting from mechanical damage can occlude the changes that relate to breast cancer.** *Phys. Med. Biol.* (2003), 48(14), L37–L41.

James, V.J. **Fibre diffraction from a single hair can provide an early non-invasive test for colon cancer.** *Med. Sci. Monitor* (2003), 9(8), MT79–MT84.

James, V.J. **The traps and pitfalls inherent in the correlation of changes in the fiber diffraction pattern of hair with breast cancer.** *Phys. Med. Biol.* (2003), 48(2), L5–L9.

James, V.J. **False-positive results in studies of changes in fiber diffraction of hair from patients with breast cancer may not be false.** *J. Natl. Cancer Inst.* (2003), 95(2), 170–171.

James, V.J. **Response to P. Suortti et al.'s and K. D. Rogers et al.'s Comments on Synchrotron fibre diffraction identifies and locates fetal collagenous breast tissue associated with breast carcinoma by V. J. James (2002).** *J. Synchrotron Rad.* 9, 71–76. *J. Synchrotron Rad.* (2003), 10, 200–201.

### Visiting Fellows (Post-retirement)

Henry, D.J., Beckwith, A.L.J.<sup>‡</sup>, Radom, L. **Homoanomeric effect in the 1,2-dimethoxyethyl radical.** *Aust. J. Chem.* (2003), 56, 429–436.

Bennett, M.A.<sup>‡</sup>, Byrnes, M.J.<sup>†</sup>, Willis, A.C. **(Ethene)bis(acetylacetonato) complexes of divalent and trivalent ruthenium.** *Organometallics* (2003), 22(5), 1018–1028.

Bennett, M.A.<sup>‡</sup>, Kopp, M.R.<sup>##</sup>, Wenger, E.<sup>‡</sup>, Willis, A.C. **Generation of nickel(0)-aryne and nickel(II)-biphenyldiyl complexes via in situ dehydrohalogenation of arenes. Molecular structures of [Ni(2,2'-C<sub>6</sub>H<sub>4</sub>C<sub>6</sub>H<sub>4</sub>)(dcpe)] and C<sub>2</sub>-hexabenzotriphenylene.** *J. Organomet. Chem.* (2003), 667(1–2), 8–15.

Shin, R.Y.C.<sup>\*</sup>, Bennett, M.A.<sup>‡</sup>, Goh, L.Y.<sup>##</sup>, Chen, W.<sup>\*</sup>, Hockless, D.C.R.<sup>†</sup>, Leong, W.K.<sup>\*</sup>, Mashima, K.<sup>##</sup>, Willis, A.C. **Arene–ruthenium complexes of an acyclic thiolate-thioether and tridentate thioether derivatives resulting from ring-closure reactions.** *Inorg. Chem.* (2003), 42(1), 96–106.

## Publications

Weberndörfer, B.<sup>\*</sup>, Henig, G.<sup>†</sup>, Hockless, D.C.R.<sup>†</sup>, Bennett, M.A.<sup>‡</sup>, Werner, H.<sup>\*</sup> **Synthesis, molecular structure, and reactivity of neutral and cationic areneosmium(II) complexes with diarylcarbenes as ligands.** *Organometallics* (2003), 22(4), 744–758.

Widegren, J.A.<sup>\*</sup>, Bennett, M.A.<sup>‡</sup>, Finke, R.G.<sup>\*</sup> **Is it homogeneous or heterogeneous catalysis? Identification of bulk ruthenium metal as the true catalyst in benzene hydrogenations starting with the monometallic precursor, Ru(II)(*h*<sup>6</sup>-C<sub>6</sub>Me<sub>6</sub>)(OAc)<sub>2</sub>, plus kinetic characterization of the heterogeneous nucleation, then autocatalytic surface-growth mechanism of metal film formation.** *J. Am. Chem. Soc.* (2003), 125(34), 10301–10310.

Bennett, S.A., Rickards, R.W.<sup>‡</sup> **Factors controlling the biomimetic triple cyclisation of xylulose β-keto-esters to syringolides. Part 1: Synthesis of 4'-deoxysyringolide 2.** *Tetrahedron Lett.* (2003), 44(36), 6927–6930.

Bennett, S.A., Rickards, R.W.<sup>‡</sup> **Erratum to "Factors controlling the biomimetic triple cyclisation of xylulose β-keto-esters to syringolides. Part 1: Synthesis of 4'-deoxysyringolide 2" [*Tetrahedron Lett.* 44 (2003) 6927].** *Tetrahedron Lett.* (2003), 44(41), 7691.

### Patents:

Rickards, R.W.<sup>‡</sup>, Smith, G.D.<sup>+2</sup>, Kirk, K.<sup>+2</sup> **Compounds and therapeutic methods.** US Patent 6,632,822 (2003).

Rickards, R.W.<sup>‡</sup>, Trowell, S.C.<sup>\*</sup>, Zhao, C.<sup>\*</sup> **Antimicrobial compounds.** Australian Provisional Patent Application 900555 (2003).

Brown, K.N.<sup>†</sup>, Geue, R.J.<sup>†</sup>, Hambley, T.W.<sup>\*</sup>, Hockless, D.C.R.<sup>†</sup>, Rae, A.D., Sargeson, A.M.<sup>‡</sup> **Specificity in template syntheses of hexaaza-macrobicyclic cages: [Pt(Me<sub>5</sub>-tricosatrieneN<sub>6</sub>)]<sup>4+</sup> and [Pt(Me<sub>5</sub>-tricosaneN<sub>6</sub>)]<sup>4+</sup>.** *Org. Biomol. Chem.* (2003), 1(9), 1598–1608.

Hegetschweiler, K.<sup>#</sup>, Maas, O.<sup>\*</sup>, Zimmer, A.<sup>\*</sup>, Geue, R.J.<sup>†</sup>, Sargeson, A.M.<sup>‡</sup>, Harmer, J.<sup>\*</sup>, Schweiger, A.<sup>\*</sup>, Buder, I.<sup>\*</sup>, Schwitzgebel, G.<sup>\*</sup>, Reiland, V.<sup>\*</sup>, Frank, W.<sup>\*</sup> **The coordination chemistry of the pentadentate 2,2,6,6-tetrakis(aminomethyl)-4-azaheptane (ditame).** *Eur. J. Inorg. Chem.* (2003), (7), 1340–1354.

Walker, G.W.<sup>†</sup>, Geue, R.J.<sup>†</sup>, Haller, K.J.<sup>‡</sup>, Rae, A.D., Sargeson, A.M.<sup>‡</sup> **New synthetic routes to hexa-aza cages using cobalt(III) tris(1,2-diamine) templates.** *Dalton Trans.* (2003), (3), 279–281.

Walker, G.W.<sup>†</sup>, Geue, R.J.<sup>†</sup>, Sargeson, A.M.<sup>‡</sup>, Behm, C.A.<sup>+2</sup> **Surface-active cobalt cage complexes: synthesis, surface chemistry, biological activity, and redox properties.** *Dalton Trans.* (2003), (15), 2992–3001.