



## PUBLICATIONS

### Key to Symbols Used to Identify Research Workers

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

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

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

### Biological Chemistry

#### *Protein Structure and Function*

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

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

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

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

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

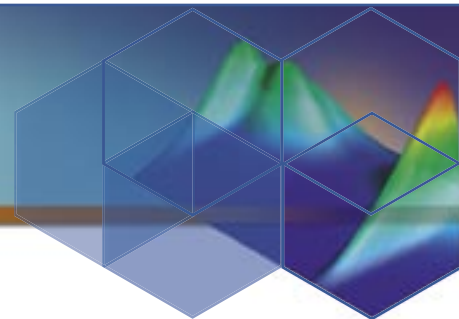
Schaeffer, P., Headlam, M., Dixon, N. Protein-protein interactions in the bacterial replisome. *Aust. Biochemist* (2004) 35(1), 9–12.

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

Wijffels, G.\*, Dalrymple, B.P.\*, Prosselkov, P., Kongsuwan, K.\*, Epa, V.C.\*, Lilley, P.E., Jergic, S., Buchardt, J.\*, Brown, S.E., Alewood, P.F.\*, Jennings, P.A., Dixon, N.E. Inhibition of protein interactions with the  $\beta_2$  sliding clamp of *Escherichia coli* DNA polymerase III by peptides from  $\beta_2$ -binding proteins. *Biochemistry* (2004), 43(19), 5661–5671.

#### *Nuclear Magnetic Resonance*

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



## Structural Biology

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

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

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

<sup>§</sup> Research conducted prior to commencement at RSC

## Protein Crystallography and Engineering

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

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

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

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

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

<sup>#1</sup> IAS (John Curtin School of Medical Research)

## Biomolecular NMR

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

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

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

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

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



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

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

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

<sup>§</sup> Research conducted prior to commencement at RSC

## Inorganic Chemistry

### Coordination Chemistry and Spectro-electro Chemistry

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

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

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

<sup>1</sup> Faculty of Science (Chemistry)

<sup>2</sup> Faculty of Science, (Biochemistry and Molecular Biology)

### Synthetic Organometallic and Coordination Chemistry

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

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

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

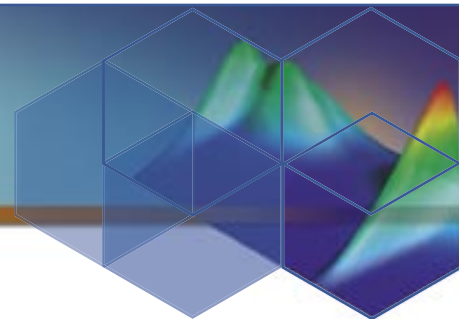
Crossley, I.R., Hill, A.F., Humphrey, E.R., Smith, M.K., Tshabang, N., Willis, A.C. Caveats for poly(methimazolyl)borate chemistry: the novel inorganic heterocycles [H<sub>2</sub>C(mt)<sub>2</sub>BR<sub>2</sub>]Cl (mt = methimazolyl; BR<sub>2</sub> = BH<sub>2</sub>, BH(mt), 9-BBN). *Chem. Commun.* (2004), (16), 1878–1879.

Dewhurst, R.D., Hill, A.F., Smith, M.K. Heterobimetallic C<sub>3</sub> complexes through silylpropargylidyne desilylation. *Angew. Chem.* (2004), 116(4), 482–484; *Angew. Chem., Int. Ed.* (2004), 43(4), 476–478.

Dewhurst, R.D., Hill, A.F., Willis, A.C. A bis(tricarbido) complex of iridium and tungsten: [IrH(C≡CC≡W(CO)<sub>2</sub>{HB(pz)<sub>3</sub>}]<sub>2</sub>(CO)(PPh<sub>3</sub>)<sub>2</sub>]. *Organometallics* (2004), 23(8), 1646–1648.

Dewhurst, R.D., Hill, A.F., Willis, A.C. A mercury bis(tricarbido) complex: [Hg{C≡C–C≡W(CO)<sub>2</sub> Tp}<sub>2</sub>-(dmsO)<sub>4</sub>](dmsO)<sub>2</sub>(Tp = hydrotrispyrazolylborate). *Chem. Commun.* (2004), (24), 2826–2827.

Dewhurst, R.D., Hill, A.F., Willis, A.C. Bi- and tetranuclear tricarbido complexes: μ,σ:σ' and μ,σ:σ':π<sub>1</sub> coordination of bridging C<sub>3</sub> ligands. *Organometallics* (2004), 23(25), 5903–5906.



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

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

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

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

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

### *Inorganic Stereochemistry and Asymmetric Synthesis*

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

Kitto, H.J., Rae, A.D., Willis, A.C., Zank, J., Wild, S.B. Synthesis and structure of the helicate (M)–(–)– $[\text{Pt}_2\{(R,R)\text{-tetraphos}\}_2](\text{CF}_3\text{SO}_3)_4 \cdot 4.5\text{H}_2\text{O}$ . *Z. Naturforsch., B: Chem. Sci.* (2004), 59b(11&12), 1458–1461.

### *Solid State Inorganic Chemistry*

#### 2003:

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

#### 2004:

Bennett, M.A., Bhargava, S.K.\*, Bond, A.M.\*, Edwards, A.J., Guo, S.-X.\*, Privér, S.H.\*, Rae, A.D., Willis, A.C. Synthesis, characterization, and electrochemical relationships of dinuclear complexes of platinum(II) and platinum(III) containing ortho-metallated tertiary arsine ligands. *Inorg. Chem.* (2004), 43(24), 7752–7763.

Brink, F.J., Norén, L.H., Withers, R.L. Electron diffraction evidence for continuously variable, composition-dependent O/F ordering in the  $\text{ReO}_3$  type,  $\text{Nb}^{\text{V}}_{1-x}\text{Nb}^{\text{V}}_x\text{O}_{2-x}\text{F}_{1+x}$ ,  $0 \leq x \leq 0.48$ , solid solution. *J. Solid State Chem.* (2004), 177(6), 2177–2182.

Carter, M.\*, Withers, R.L. An electron and X-ray diffraction study of the compositely modulated barium nickel hollandite  $\text{Ba}_x(\text{Ni}_x\text{Ti}_{8-x})\text{O}_{16}$ ,  $1.16 < x < 1.32$ , solid solution. *Z. Kristallogr.* (2004), 219(11), 763–767.

García-García, F.J.\*, Larsson, A.-K.†, Norén, L., Withers, R.L. The crystal structures of  $\text{Co}_3\text{Se}_4$  and  $\text{Co}_7\text{Se}_8$ . *Solid State Sci.* (2004), 6(7), 725–733.

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

James, M.\*, Cassidy, D.\*, Goossens, D.J., Withers, R.L. The phase diagram and tetragonal superstructures of the rare earth cobaltate phases  $\text{Ln}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$  ( $\text{Ln} = \text{La}^{3+}, \text{Pr}^{3+}, \text{Nd}^{3+}, \text{Sm}^{3+}, \text{Gd}^{3+}, \text{Y}^{3+}, \text{Ho}^{3+}, \text{Dy}^{3+}, \text{Er}^{3+}, \text{Tm}^{3+}$  and  $\text{Yb}^{3+}$ ). *J. Solid State Chem.* (2004), 177(6), 1886–1895.



James, M.\*, Cassidy, D.\*, Wilson, K.F.\*, Horvat, J.\*, Withers, R.L. Oxygen vacancy ordering and magnetism in the rare earth stabilised perovskite form of "SrCoO<sub>3-δ</sub>". *Solid State Sci.* (2004), 6(7), 655–662.

Kitto, H.J., Rae, A.D., Willis, A.C., Zank, J., Wild, S.B. Synthesis and structure of the helicate (M)–(–)–[Pt<sub>2</sub>{(R,R)-tetraphos}<sub>2</sub>](CF<sub>3</sub>SO<sub>3</sub>)<sub>4</sub>•4.5H<sub>2</sub>O. *Z. Naturforsch., B: Chem. Sci.* (2004), 59b(11&12), 1458–1461.

Liu, Y., Withers, R.L., Brink, F.J., Norén, L.H. Cubic perovskite-related phases in the ternary SrO–CuO–Nb<sub>2</sub>O<sub>5</sub> system. *J. Solid State Chem.* (2004), 177(9), 3140–3148.

Liu, Y., Withers, R.L., Norén, L. The pyrochlore to 'defect fluorite' transition in the Y<sub>2</sub>(Zr<sub>γ</sub>Ti<sub>1-γ</sub>)<sub>2</sub>O<sub>7</sub> system and its underlying crystal chemistry. *J. Solid State Chem.* (2004), 177(12), 4404–4412.

Rae, A.D., Linden, A.\*, Majchrzak, A.\*, Mloston, G.\*, Heimgartner, H.\* Bis(1-chloro-2,2,4,4-tetramethyl-3-oxocyclobutan-1-yl)pentasulfane: an occupancy modulated structure. *Acta Crystallogr., B* (2004), 60(4), 416–423.

Ting, V., Liu, Y., Norén, L., Withers, R.L., Goossens, D.J., James, M.\*, Ferraris, C.\* A structure, conductivity and dielectric properties investigation of A<sub>3</sub>CoNb<sub>2</sub>O<sub>9</sub> (A = Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>) triple perovskites. *J. Solid State Chem.* (2004), 177(12), 4428–4442.

Ting, V., Liu, Y., Withers, R.L., Krausz, E. An electron diffraction and bond valence sum study of the space group symmetries and structures of the photocatalytic 1:1 ordered A<sub>2</sub>InNbO<sub>6</sub> double perovskites (A = Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>). *J. Solid State Chem.* (2004), 177(3), 979–986.

Ting, V., Liu, Y., Withers, R.L., Norén, L. An electron diffraction and bond valence sum study of the space group symmetries and structures of the photocatalytic 1:2 B site ordered A<sub>3</sub>CoNb<sub>2</sub>O<sub>9</sub> perovskites (A = Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>). *J. Solid State Chem.* (2004), 177(7), 2295–2304.

Withers, R.L. Constraints, 'order' and new types of modulated phases. *Ferroelectrics* (2004), 305, 69–74.

Withers, R.L., Brink, F.J., Norén, L.H., Welberry, R.T., Liu, Y. Local strain, structured diffuse scattering and oxygen/fluorine ordering in transition metal oxyfluorides. *Ferroelectrics* (2004), 305, 123–126.

Withers, R.L., Höche, T.\*, Liu, Y., Esmaeilzadeh, S.\*, Keding, R.\*, Sales, B.\* A combined temperature-dependent electron and single-crystal X-ray diffraction study of the fresnoite compound Rb<sub>2</sub>V<sup>4+</sup>V<sup>5+</sup>O<sub>6</sub>. *J. Solid State Chem.* (2004), 177(10), 3316–3323.

Withers, R.L., Liu, Y., Norén, L., Fitz Gerald, J.D.<sup>#2</sup> A TEM study of Ni ordering in the Ni<sub>6</sub>Se<sub>5-x</sub>Te<sub>x</sub>, 0 < x < ~1.7, system. *J. Solid State Chem.* (2004), 177(3), 972–978.

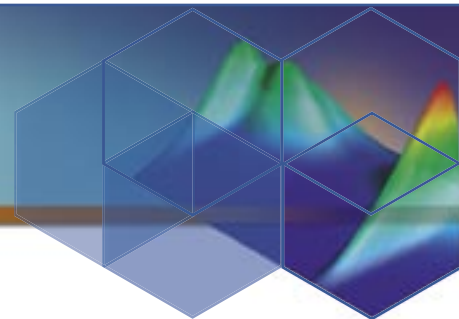
Withers, R.L., Norén, L., Liu, Y. Flexible phases, modulated structures and the transmission electron microscope. *Z. Kristallogr.* (2004), 219(11), 701–710.

Withers, R.L., Vincent, R.\*, Schoenes, J.\* A low-temperature electron diffraction study of structural disorder and its relationship to the Kondo effect in ThAsSe. *J. Solid State Chem.* (2004), 177(3), 701–708.

Withers, R.L., Welberry, T.R., Larsson, A.-K.<sup>#1</sup>, Liu, Y., Norén, L., Rundlöf, H.\*, Brink, F.J. Local crystal chemistry, induced strain and short range order in the cubic pyrochlore (Bi<sub>1.5-α</sub>Zn<sub>0.5-β</sub>)(Zn<sub>0.5-γ</sub>Nb<sub>1.5-δ</sub>)O<sub>(7-1.5α-β-γ-2.5δ)</sub> (BZN). *J. Solid State Chem.* (2004), 177(1), 231–244.

<sup>#1</sup> IAS (Research School of Physical Sciences & Engineering)

<sup>#2</sup> IAS (Research School of Earth Sciences)



## Organic Chemistry

### Synthesis and Mechanism

- Banwell, M.G., Beck, D.A.S., Smith, J.A. The influence of chiral auxiliaries and catalysts on the selectivity of intramolecular conjugate additions of pyrrole to *N*-tethered Michael acceptors. *Org. Biomol. Chem.* (2004), 2(2), 157–159.
- Banwell, M.G., Darnos, P., Hockless, D.C.R. Taxane diterpene synthesis studies. Part 1: chemoenzymatic and enantiodivergent routes to AB-ring substructures of taxoids and *ent*-taxoids. *Aust. J. Chem.* (2004), 57(1), 41–52.
- Banwell, M.G., Edwards, A.J., Harfoot, G.J., Jolliffe, K.A. A chemoenzymatic synthesis of the linear triquinane (–)-hirsutene and identification of possible precursors to the naturally occurring (+)-enantiomer. *Tetrahedron* (2004), 60(3), 535–547.
- Banwell, M.G., Edwards, A.J., Loong, D.T.J. The conversion of certain microbially-derived *cis*- and *trans*-1,2-dihydrocatechols into various tetrahydro- and related-derivatives. *ARKIVOC* (2004), (x), 53–67.
- Banwell, M.G., Edwards, A.J., McLeod, M.D., Stewart, S.G. A chemoenzymatic synthesis of the *cis*-decalin core associated with the novel anti-mitotic agent phomopsidin: some observations concerning a high-pressure-promoted Diels–Alder cycloaddition reaction of (1*S*,2*R*)-3-methyl-*cis*-1,2-dihydrocatechol and the anionic oxy-Cope rearrangement of compounds derived from the adduct. *Aust. J. Chem.* (2004), 57(7), 641–644.
- Banwell, M.G., Harfoot, G.J. A chemoenzymatic and enantioselective route to the tricyclic frameworks associated with the protoilludane and marasmane classes of sesquiterpene. *Aust. J. Chem.* (2004), 57(9), 895–897.
- Banwell, M.G., Hungerford, N.L., Jolliffe, K.A. Synthesis of the sialic acid (–)-KDN and certain epimers from (–)-3-dehydroshikimic acid or (–)-quinic acid. *Org. Lett.* (2004), 6(16), 2737–2740.
- Banwell, M.G., Jury, J.C. Stereoselective syntheses of the methyl esters of (*E*)- and (*Z*)-2-methyl-6-oxohept-2-enoic acid. *Org. Prep. Proced. Int.* (2004), 36(1), 87–91.
- Banwell, M.G., Kelly, B.D. Trimethyl{2-[(tributylstannyl)methyl]-2-propenyl}silane. In *Encyclopedia of Reagents for Organic Synthesis [Online (eEROS)]*. Paquette, L.A., Crich, D., Fuchs, P.L., Wipf, P. Eds. John Wiley & Sons Ltd., (2004), <http://www.mrw.interscience.wiley.com/eros/>.
- Banwell, M.G., Kelly, B.D. 3-[(Trimethylsilyl) methyl]-3-butenic acid methyl ester. In *Encyclopedia of Reagents for Organic Synthesis [Online (eEROS)]*. Paquette, L.A., Crich, D., Fuchs, P.L., Wipf, P. Eds. John Wiley & Sons Ltd., (2004), <http://www.mrw.interscience.wiley.com/eros/>.
- Banwell, M.G., Loong, D.T.J. A chemoenzymatic total synthesis of the phytotoxic undecenolide (–)-cladospolide A. *Org. Biomol. Chem.* (2004), 2(14), 2050–2060.
- Banwell, M.G., Loong, D.T.J. Stereoselective total synthesis of the nonenolide (+)-microcarpalide. *Heterocycles* (2004), 62, 713–734.
- Banwell, M.G., Lupton, D.W., Ma, X., Renner, J., Sydnes, M.O. Synthesis of quinolines, 2-quinolones, phenanthridines, and 6(5*H*)-phenanthridinones via palladium[0]-mediated Ullmann cross-coupling of 1-bromo-2-nitroarenes with  $\beta$ -halo-enals, -enones, or -esters. *Org. Lett.* (2004), 6(16), 2741–2744.



Banwell, M.G., McLeod, M.D., Riches, A.G. Taxane diterpene synthesis studies. Part 2: towards taxinine – enantiospecific construction of an AB-ring substructure incorporating both quaternary carbon centers and attempts to annulate the C-ring. *Aust. J. Chem.* (2004), 57(1), 53–66.

Banwell, M.G., Renner, J. Bis[(trimethylsilyl)methyl]zinc. In *Encyclopedia of Reagents for Organic Synthesis [Online (eEROS)]*. Paquette, L.A., Crich, D., Fuchs, P.L., Wipf, P. Eds. John Wiley & Sons Ltd., (2004), <http://www.mrw.interscience.wiley.com/eros/>.

Banwell, M.G., Renner, J. 2-(Trimethylsilyl)ethanesulfonamide. In *Encyclopedia of Reagents for Organic Synthesis [Online (eEROS)]*. Paquette, L.A., Crich, D., Fuchs, P.L., Wipf, P. Eds. John Wiley & Sons Ltd., (2004), <http://www.mrw.interscience.wiley.com/eros/>.

Banwell, M.G., Sydnese, M.O. Utilization of 1-aryl-2,2-dibromocyclopropanes in synthetic approaches to phenanthroquinolizidine and phenanthroindolizidine alkaloids. *Aust. J. Chem.* (2004), 57(6), 537–548.

### Patents:

#### 2003:

Armitt, D.J., Banwell, M.G. Process for synthesising C-glycosides. International Patent Number WO 03/102007 A1, (2003), 27 pp.

#### 2004:

Banwell, M.G., Lupton, D.W. A method of indole synthesis. International Patent Number WO 2004/096766 A1, (2004), 34 pp.

### Biochemical Reactions and Molecular Recognition

Barr, L., Dumanski, P.G., Easton, C.J., Harper, J.B., Lee, K., Lincoln, S.F.<sup>‡</sup>, Meyer, A.G., Simpson, J.S. Cyclodextrin molecular reactors. *J. Inclusion Phenom. Macrocyclic Chem.* (2004), 50(1–2), 19–24.

Barratt, B.J.W., Easton, C.J., Henry, D.J., Li, I.H.W., Radom, L., Simpson, J.S. Inhibition of peptidylglycine  $\alpha$ -amidating monooxygenase by exploitation of factors affecting the stability and ease of formation of glyceryl radicals. *J. Am. Chem. Soc.* (2004), 126(41), 13306–13311.

Cieslinski, M.M. Cyclodextrins and stilbenes as components of supramolecular structures. *Aust. J. Chem.* (2004), 57(8), 815.

Coghlan, P.A., Easton, C.J.  $\beta$ -Nitro- $\alpha$ -amino acids as latent  $\alpha,\beta$ -dehydro- $\alpha$ -amino acid residues in solid-phase peptide synthesis. *ARKIVOC* (2004), (x), 101–108.

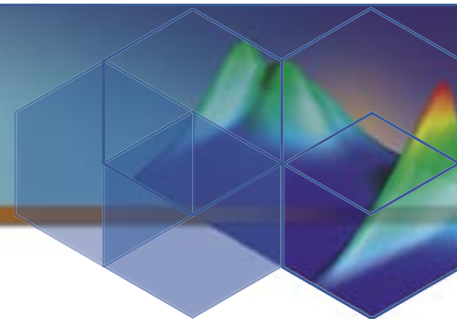
Croft, A.K., Easton, C.J. Anchimeric assistance in hydrogen-atom transfer to bromine. *Aust. J. Chem.* (2004), 57(7), 651–654.

Easton, C.J., Lincoln, S.F.<sup>‡</sup>, Barr, L., Onagi, H. Molecular reactors and machines: applications, potential, and limitations. *Chem. Eur. J.* (2004), 10(13), 3120–3128.

Garson, M.J.\*., Simpson, J.S. Marine isocyanides and related natural products – structure, biosynthesis and ecology. *Nat. Prod. Rep.* (2004), 21(1), 164–179.

Lock, J.S.\*., May, B.L.\*., Clements, P.\*., Lincoln, S.F.<sup>‡</sup>, Easton, C.J. Cyclodextrin complexation of a stilbene and the self-assembly of a simple molecular device. *Org. Biomol. Chem.* (2004), 2(3), 337–344.

Lock, J.S.\*., May, B.L.\*., Clements, P.\*., Lincoln, S.F.<sup>‡</sup>, Easton, C.J. Cyclodextrin complexation of the stilbene 4-(2-(4-tert-butylphenyl)ethen-1-yl)-benzoate and the self-assembly of molecular devices. *J. Inclusion Phenom. Macrocyclic Chem.* (2004), 50(1–2), 13–18.



Lock, J.S.\*, May, B.L.\*, Clements, P.\*, Lincoln, S.F.‡, Easton, C.J. Intra- and intermolecular complexation in C(6) monoazacoronand substituted cyclodextrins. *Org. Biomol. Chem.* (2004), 2(9), 1381–1386.

Simpson, J.S., Brust, A.\*, Garson, M.J.\* Biosynthetic pathways to dichloroimines; precursor incorporation studies on terpene metabolites in the tropical marine sponge *Stylotella aurantium*. *Org. Biomol. Chem.* (2004), 2(6), 949–956.<sup>§</sup>

Simpson, J.S., Garson, M.J.\* Biosynthetic pathways to isocyanides and isothiocyanates; precursor incorporation studies on terpene metabolites in the tropical marine sponges *Amphimedon terpenensis* and *Axinyssa n.sp.* *Org. Biomol. Chem.* (2004), 2(6), 939–948.<sup>§</sup>

Topf, M.‡, Sandala, G.M., Smith, D.M.‡, Schofield, C.J.‡, Easton, C.J., Radom, L. The unusual bifunctional catalysis of epimerization and desaturation by carbapenem synthase. *J. Am. Chem. Soc.* (2004), 126(32), 9932–9933.

Wyness, O.\*, May, B.L.\*, Clements, P.\*, Lincoln, S.F.‡, Easton, C.J. Diazacoronand-linked  $\alpha$ - and  $\beta$ -cyclodextrin dimer complexes of the brilliant yellow tetraanion. *Aust. J. Chem.* (2004), 57(6), 571–576.

### Patent:

#### 2004:

Barratt, B.J.W., Easton, C.J., Simpson, J.S. Enzyme inhibitors. International Patent Number WO 2004/007417 A1, (2004), 47 pp.

<sup>§</sup> Research conducted prior to commencement at RSC

### Organic Synthesis

Beck, E.J., Twitchin, B., Mander, L.N. Radio labelling of the gibberellin plant growth inhibitor 16,17-dihydro-GA<sub>5</sub>. *Can. J. Chem.* (2004), 82(2), 293–300.

Herlt, A., Mander, L., Rombang, W.\*, Rumampuk, R.\*, Soemitro, S.\*, Steglich, W.\*, Tarigan, P.\*, von Nussbaum, F.\* Alkaloids from marine organisms. Part 8: Isolation of bisdemethylaaptamine and bisdemethylaaptamine-9-O-sulfate from an Indonesian *Aaptos* sp. marine sponge. *Tetrahedron* (2004), 60(29), 6101–6104.

Hisamatsu, T.\*, Koshioka, M.\*, Mander, L.N. Regulation of gibberellin biosynthesis and stem elongation by low temperature in *Eustoma grandiflorum*. *J. Hort. Sci. Biotechnol.* (2004), 79(3), 354–359.

King, R.W.\*, Junttila, O.\*, Mander, L.N., Beck, E.J. Gibberellin structure and function: biological activity and competitive inhibition of gibberellin 2- and 3-oxidases. *Physiol. Plant.* (2004), 120(2), 287–297.

Liu, J., Mander, L.N. Koshioka, M.\* Methodology for the synthesis of 11,13-dihydroxy gibberellins. *ARKIVOC* (2004), (x), 68–79.

O'Connor, P.D., Mander, L.N., McLachlan, M.M.W. Synthesis of the himandrine skeleton. *Org. Lett.* (2004), 6(5), 703–706.

Ubukawa, M.\*, Fukuda, N.\*, Oyama-Okubo, N.\*, Koshioka, M.\*, Mander, L.N., Sase, S.\*, Nishimura, S.\* Effect of light source and quality on endogenous gibberellin level and GA<sub>3</sub> response of petunia (*Petunia x hybrida* Vilm.). *J. Jpn. Soc. Hort. Sci.* (2004), 73(5), 441–446.

Williams, C.M.\*, Mander, L.N. Guaiacol transprotection. Replacement of the phenoxy isopropyl protecting function by acetyl. *Tetrahedron Lett.* (2004), 45(4), 667–669.





## Organic Synthesis, Methodology and Host-guest Chemistry

Barrett, E.S., Irwin, J.L.\*, Edwards, A.J., Sherburn, M.S. Superbowl container molecules. *J. Am. Chem. Soc.* (2004), 126(51), 16747–16749.

Fischer, J.\*, Reynolds, A.J.\*, Sharp, L.A., Sherburn, M.S. Radical carboxylation approach to lignans. Total synthesis of (–)-arctigenin, (–)-matairesinol, and related natural products. *Org. Lett.* (2004), 6(9), 1345–1348.

Irwin, J.L.\*, Sinclair, D.J., Edwards, A.J., Sherburn, M.S. Chiral conjoined cavitands. *Aust. J. Chem.* (2004), 57(4), 339–343.

## Physical and Theoretical Chemistry

### Theoretical Chemical Physics

Castillo, J.F.\*, Aoiz, F.J.\*, Bañares, L.\*, Collins, M.A. The  $\text{H} + \text{N}_2\text{O} \rightarrow \text{OH} + \text{N}_2$  reaction dynamics on an interpolated QCISD potential energy surface. A quasiclassical trajectory study. *J. Phys. Chem. A* (2004), 108(32), 6611–6623.

Crespos, C.\*, Collins, M.A., Pijper, E.\*, Kroes, G.J.\* Application of the modified Shepard interpolation method to the determination of the potential energy surface for a molecule–surface reaction:  $\text{H}_2 + \text{Pt}(111)$ . *J. Chem. Phys.* (2004), 120(5), 2392–2404.

Evenhuis, C.R., Collins, M.A. Interpolation of diabatic potential energy surfaces. *J. Chem. Phys.* (2004), 121(6), 2515–2527.

Moyano, G.E., Collins, M.A. Molecular potential energy surfaces by interpolation: Strategies for faster convergence. *J. Chem. Phys.* (2004), 121(20), 9769–9775.

Moyano, G.E., Pearson, D., Collins, M.A. Interpolated potential energy surfaces and dynamics for atom exchange between H and  $\text{H}_3^+$ , and D and  $\text{H}_3^+$ . *J. Chem. Phys.* (2004), 121(24), 12396–12401.

### Computational Quantum Chemistry, Polymer Chemistry

Barner-Kowollik, C.\*, Davis, T.P.\*, Coote, M.L., Matyjaszewski, K.\*, Vana, P.\* Copolymerization. In *Encyclopedia of Polymer Science and Technology*, 3rd Ed., Vol. 9, Mark, H.F., Ed. John Wiley & Sons: New York (2004), pp. 394–445.

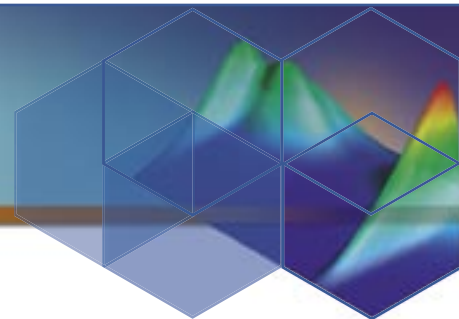
Beare, K.D., Coote, M.L. What influences barrier heights in hydrogen abstraction from thiols by carbon-centered radicals? A curve-crossing study. *J. Phys. Chem. A* (2004), 108(35), 7211–7221.

Coote, M.L. Computational quantum chemistry for free-radical polymerization. In *Encyclopedia of Polymer Science and Technology*, 3rd Ed., Vol. 9, Mark, H.F., Ed. John Wiley & Sons: New York (2004), pp. 319–371.

Coote, M.L. Reliable theoretical procedures for the calculation of electronic-structure information in hydrogen abstraction reactions. *J. Phys. Chem. A* (2004), 108(17), 3865–3872.

Coote, M.L. Ab initio study of the addition-fragmentation equilibrium in RAFT polymerization: When is polymerization retarded? *Macromolecules* (2004), 37(13), 5023–5031.

Coote, M.L. A quantum-chemical approach to understanding reversible addition fragmentation chain-transfer polymerization. *Aust. J. Chem.* (2004), 57(12), 1125–1132.



Coote, M.L., Pross, A.\*, Radom, L. Understanding alkyl substituent effects in R–O bond dissociation reactions in open- and closed-shell systems. In *Fundamental World of Quantum Chemistry: A Tribute to the memory of Per-Olov Löwdin*, Vol. 3, Brändas, E.J., Kryachko, E.S., Eds. Kluwer–Springer: Dordrecht (2004), pp. 563–579.

Coote, M.L., Radom, L. Substituent effects in xanthate-mediated polymerization of vinyl acetate: ab initio evidence for an alternative fragmentation pathway. *Macromolecules* (2004), 37(2), 590–596.

Feldermann, A.\*, Coote, M.L., Stenzel, M.H.\*, Davis, T.P.\*, Barner-Kowollik, C.\* Consistent experimental and theoretical evidence for long-lived intermediate radicals in living free radical polymerization. *J. Am. Chem. Soc.* (2004), 126(48), 15915–15923.

Gómez-Balderas, R., Coote, M.L., Henry, D.J., Radom, L. Reliable theoretical procedures for calculating the rate of methyl radical addition to carbon–carbon double and triple bonds. *J. Phys. Chem. A* (2004), 108(15), 2874–2883.

Henry, D.J., Coote, M.L., Gómez-Balderas, R., Radom, L. Comparison of the kinetics and thermodynamics for methyl radical addition to C=C, C=O and C=S double bonds. *J. Am. Chem. Soc.* (2004), 126(6), 1732–1740.

Sandala, G.M., Smith, D.M.†, Coote, M.L., Radom, L. Suicide inactivation of dioldehydratase by glycolaldehyde and chloroacetaldehyde: an examination of the reaction mechanism. *J. Am. Chem. Soc.* (2004), 126(39), 12206–12207.

### Liquid State Chemical Physics

Bright, J.N., Sansom, M.S.P.\* Kv channel S6 helix as a molecular switch: simulation studies. *IEE Proc.-Nanobiotechnol.* (2004), 151(1), 17–27.

Carberry, D.M., Reid, J.C., Wang, G.M., Sevick, E.M., Searles, D.J.\*, Evans, D.J. Fluctuations and irreversibility: an experimental demonstration of a second-law-like theorem using a colloidal particle held in an optical trap. *Phys. Rev. Lett.* (2004), 92(14), 140601/1–4.

Carberry, D.M., Williams, S.R., Wang, G.M., Sevick, E.M., Evans, D.J. The Kawasaki Identity and the Fluctuation Theorem. *J. Chem. Phys.* (2004), 121(17), 8179–8182.

Delhommelle, J.\*, Petracic, J., Evans, D.J. Non-Newtonian behavior in simple fluids. *J. Chem. Phys.* (2004), 120(13), 6117–6123.

Jepps, O.G.\*, Evans, D.J., Searles, D.J.\* The fluctuation theorem and Lyapunov weights. *Physica D* (2004), 187(1–4), 326–337.

Jepps, O.\*, Petracic, J. Color conductivity of hard spheres. *Mol. Phys.* (2004), 102(5), 513–523.

Petravic, J. Influence of strain on transport in dense Lennard–Jones systems. *J. Chem. Phys.* (2004), 120(15), 7041–7049.

Petravic, J. Shear stress relaxation in liquids. *J. Chem. Phys.* (2004), 120(21), 10188–10193.

Petravic, J., Delhommelle, J.\* Nonequilibrium molecular dynamics simulations of molten sodium chloride. *Int. J. Thermophys.* (2004), 25(5), 1375–1393.

Reid, J.C., Carberry, D.M., Wang, G.M., Sevick, E.M., Evans, D.J., Searles, D.J.\* Reversibility in nonequilibrium trajectories of an optically trapped particle. *Phys. Rev. E* (2004), 70 (1–2), 016111/1–9.

Searles, D.J.\*, Evans, D.J. Fluctuations relations for nonequilibrium systems. *Aust. J. Chem.* (2004), 57(12), 1119–1123.



Williams, S.R., Searles, D.J.\*, Evans, D.J. Independence of the transient fluctuation theorem to thermostating details. *Phys. Rev. E* (2004), 70, 066113/1–6.

### *Theoretical Quantum Chemistry*

Besley, N.A.\*, Gill, P.M.W. Atomic and molecular intracules for excited states. *J. Chem. Phys.* (2004), 120(16), 7290–7297.<sup>§</sup>

Gilbert, A.T.B.\*, Gill, P.M.W., Taylor, S.W.\* Extracting atoms from molecular electron densities via integral equations. *J. Chem. Phys.* (2004), 120(17), 7887–7893.<sup>§</sup>

Gill, P.M.W., Gordon, M.S.\*, Head-Gordon, M.\*, Radom, L. Remembrance: John A. Pople (1925–2004). *J. Chem. Phys.* (2004), 120(20), 9445.<sup>§</sup>

Gill, P.M.W., Besley, N.A.\*, O'Neill, D.P.\* Wigner intracule for the Kellner helium-like ions. *Int. J. Quantum Chem.* (2004), 100(2), 166–171.<sup>§</sup>

Gill, P.M.W. Quadrature schemes for integrals of density functional theory. In *Molecular quantum mechanics: Selected papers of N.C. Handy*, Clary, D.C., Colwell, S.M., Schaefer III, H.F., Eds. Taylor & Francis: London (2004), pp 229–230.<sup>§</sup>

Gribakin, G.F.\*, Gill, P.M.W. The role of vibrational doorway states in positron annihilation with large molecules. *Nucl. Instrum. Methods Phys. Res., Sect. B* (2004), 221, 30–35.<sup>§</sup>

Lin, C.Y.\*, George, M.W.\*, Gill, P.M.W. EDF2: A density functional for predicting vibrational frequencies. *Aust. J. Chem.* (2004), 57(4), 365–370.<sup>§</sup>

<sup>§</sup> Research conducted prior to commencement at RSC

### *Laser and Optical Spectroscopy*

Hughes, J.L., Pace, R.J.<sup>+1</sup>, Krausz, E. The exciton contribution to the Faraday *B* term MCD of molecular dimers. *Chem. Phys. Lett.* (2004), 385(1–2), 116–121.

Hughes, J.L., Prince, B.J., Krausz, E., Smith, P.J.<sup>+1</sup>, Pace, R.J.<sup>+1</sup>, Riesen, H.\* Highly efficient spectral hole-burning in oxygen-evolving photosystem II preparations. *J. Phys. Chem. B* (2004), 108(29), 10428–10439.

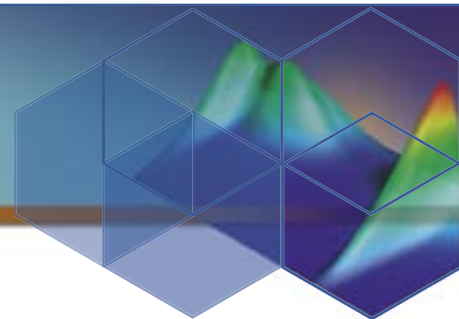
Hughes, J.L., Prince, B.J., Peterson Årsköld, S., Krausz, E., Pace, R.<sup>+1</sup>, Picorel, R.\*, Seibert, M\*. Photo-conversion of chlorophylls in higher-plant CP43 characterized by persistent spectral hole burning at 1.7 K. *J. Lumin.* (2004), 108(1–4), 131–136.

Hughes, J.L., Prince, B.J., Peterson Årsköld, S., Smith, P.J.<sup>+1</sup>, Pace, R.J.<sup>+1</sup>, Riesen, H.\*, Krausz, E. The native reaction centre of photosystem II: a new paradigm for P680. *Aust. J. Chem.* (2004), 57(12), 1179–1183.

Peterson Årsköld, S., Prince, B.J., Krausz, E., Smith, P.J.<sup>+1</sup>, Pace, R.J.<sup>+1</sup>, Picorel, R.\*, Seibert, M\*. Low-temperature spectroscopy of fully active PSII cores. Comparisons with CP43, CP47, D1/D2/cyt  $b_{559}$  fragments. *J. Lumin.* (2004), 108(1–4), 97–100.

Prince, B.J., Krausz, E., Peterson Årsköld, S., Smith, P. J.<sup>+1</sup>, Pace, R.J.<sup>+1</sup> Persistent spectral hole burning in oxygen-evolving photosystem II cores from cyanobacteria and higher plants. *J. Lumin.* (2004), 108(1–4), 101–105.

Samoc, A.<sup>#1</sup>, Samoc, M.<sup>#1</sup>, Luther-Davies, B.<sup>#1</sup>, Kelly, J.F., Krausz, E.R., Willis, A.C. New second-order nonlinear octupolar materials. *Mol. Cryst. Liq. Cryst.* (2004), 415, 179–195.



Ting, V., Liu, Y., Withers, R.L., Krausz, E. An electron diffraction and bond valence sum study of the space group symmetries and structures of the photocatalytic 1:1 ordered  $A_2\text{InNbO}_6$  double perovskites ( $A = \text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ). *J. Solid State Chem.* (2004), 177(3), 979–986.

<sup>†1</sup> Faculty of Science (Chemistry)

<sup>#1</sup> IAS (Research School of Physical Sciences and Engineering)

### Computational Quantum Chemistry

Barratt, B.J.W., Easton, C.J., Henry, D.J., Li, I.H.W., Radom, L., Simpson, J.S. Inhibition of peptidylglycine  $\alpha$ -amidating monooxygenase by exploiting factors affecting the stability and ease of formation of glyceryl radicals. *J. Am. Chem. Soc.* (2004), 126(41), 13306–13311.

Chan, B.\*, Radom, L. Understanding metal-free catalytic hydrogenation: A systematic theoretical study of the hydrogenation of ethene. *Aust. J. Chem.* (2004), 57(7), 659–663.

Coote, M.L., Radom, L. Substituent effects in xanthate-mediated polymerization of vinyl acetate: Ab initio evidence for an alternative fragmentation pathway. *Macromolecules* (2004), 37(2), 590–596.

Coote, M.L., Pross, A.\*, Radom, L. Understanding alkyl substituent effects in R–O bond dissociation reactions in open- and closed-shell systems. In *Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin, Vol. 3*, Brändas, E.J., Kryachko, E.S., Eds. Kluwer-Springer: Dordrecht (2004), pp. 563–579.

Corral, I.\*, Mó, O.\*, Yáñez, M.\*, Salpin, J.-Y.\*, Tortajada, T.\*, Radom, L. Gas-phase reactions between urea and  $\text{Ca}^{2+}$ : the importance of Coulomb explosions. *J. Phys. Chem. A* (2004), 108(46), 10080–10088.

Gill, P.M.W.\*, Gordon, M.S.\*, Head-Gordon, M.\*, Radom, L. Remembrance: John A. Pople (1925–2004). *J. Chem. Phys.* (2004), 120(20), 9445.

Gómez-Balderas, R., Coote, M.L., Henry, D.J., Radom, L. Reliable theoretical procedures for calculating the rate of methyl radical addition to carbon-carbon double and triple bonds. *J. Phys. Chem. A* (2004), 108(15), 2874–2883.

Henry, D.J., Coote, M.L., Gómez-Balderas, R., Radom, L. Comparison of the kinetics and thermodynamics for methyl radical addition to C=C, C=O, and C=S double bonds. *J. Am. Chem. Soc.* (2004), 126(6), 1732–1740.

Sandala, G.M., Smith, D.M.<sup>‡</sup>, Coote, M.L., Radom, L. Suicide inactivation of dioldehydratase by glycolaldehyde and chloroacetaldehyde: an examination of the reaction mechanism. *J. Am. Chem. Soc.* (2004), 126(39), 12206–12207.

Topf, M.<sup>‡</sup>, Sandala, G.M., Smith, D.M.<sup>‡</sup>, Schofield, C.J.<sup>‡</sup>, Easton, C.J., Radom, L. The unusual bifunctional catalysis of epimerization and desaturation by carbapenem synthase. *J. Am. Chem. Soc.* (2004), 126(32), 9932–9933.

### Polymers and Soft Condensed Matter

Carberry, D.M., Reid, J.C., Wang, G.M., Sevick, E.M., Searles, D.J.\*, Evans, D.J. Fluctuations and irreversibility: an experimental demonstration of a second law-like theorem using a colloidal particle held in an optical trap. *Phys. Rev. Lett.* (2004), 92(14), 140601/1–4.

Carberry, D.M., Williams, S.R., Wang, G.M., Sevick, E.M., Evans, D.J. The Kawasaki Identity and the Fluctuation Theorem. *J. Chem. Phys.* (2004), 121(17), 8179–8182.

Reid, J.C., Carberry, D.M., Wang, G.M., Sevick, E.M., Evans, D.J., Searles, D.J.\* Reversibility in nonequilibrium trajectories of an optically trapped particle. *Phys. Rev. E* (2004), 70, 016111/1–9.



## Disordered Materials

Campbell, B.J.\*, Welberry, T.R., Broach, R.W.\*, Hong, H.\*, Cheetham, A.K.\* Elucidation of zeolite microstructure by synchrotron X-ray diffuse scattering. *J. Appl. Cryst.* (2004), 37(2), 187–192.

Goossens, D.J., Wilson, K.F.<sup>†1</sup>, James, M.\* Magnetic properties of  $\text{Dy}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$  ( $x = 0.67$  to  $0.95$ ). In *Proceedings of the 28th Annual Condensed Matter and Materials Meeting*, (2004), pp. WP17/1–3, <http://www.aip.org.au/wagga2004/>

Goossens, D.J., Wilson, K.F.\*, James, M.\*, Studer, A.J.\*, Wang, X.L.\* Structural and magnetic properties in  $\text{Y}_{0.33}\text{Sr}_{0.67}\text{CoO}_{2.79}$ . *Phys. Rev. B* (2004), 69(13), 134411/1–6.

Goossens, D.J., Robinson, R.A.\*, Telling, M.T.F.\* The antiferromagnetic structure of  $\text{BaPrO}_3$ . *Physica B* (2004), 352(1–4), 105–110.

Hicks, T.J\*, Goossens, D.J., Harker, S.J.\*, Mulders, A.M.\*, Kennedy, S.J.\* Spin resolved neutron spectroscopy from the heavy Fermion compound  $\text{CeCu}_6$ . *Physica B* (2004), 345, 86–88.<sup>§</sup>

James, M.\*, Cassidy, D.\*, Goossens, D.J., Withers, R.L. The phase diagram and tetragonal superstructures of the rare earth cobaltate phases  $\text{Ln}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$  ( $\text{Ln} = \text{La}^{3+}, \text{Pr}^{3+}, \text{Nd}^{3+}, \text{Sm}^{3+}, \text{Gd}^{3+}, \text{Y}^{3+}, \text{Ho}^{3+}, \text{Dy}^{3+}, \text{Er}^{3+}, \text{Tm}^{3+}$  and  $\text{Yb}^{3+}$ ). *J. Solid State Chem.* (2004), 177(6), 1886–1895.

Kreisel, J.\*, Bouvier, P.\*, Dkhil, B.\*, Chaabane, B.\*, Glazer, A.M.\*, Thomas, P. A.\*, Welberry, T.R. Effect of high pressure on the relaxor ferroelectrics  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$  (NBT) and  $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$  (PMN). *Ferroelectrics* (2004), 302, 293–298.

Ting, V., Liu, Y., Norén, L., Withers, R.L., Goossens, D.J., James, M.\*, Ferraris, C.\* A structure, conductivity and dielectric properties investigation of  $\text{A}_3\text{CoNb}_2\text{O}_9$  ( $\text{A} = \text{Ca}^{2+}, \text{Sr}^{2+}, \text{Ba}^{2+}$ ) triple perovskites. *J. Solid State Chem.* (2004), 177(12), 4428–4442.

Welberry, T.R. Diffuse scattering X-ray scattering and models of disorder. *IUCr Monographs on Crystallography, Vol. 16*, Oxford University Press: Oxford, UK (2004), pp. v–266.

Welberry, T.R. The importance of multisite correlations in disordered structures. *Ferroelectrics* (2004), 305, 117–122.

Welberry, T.R. Disorder and diffuse scattering. In *Encyclopedia of Supramolecular Chemistry, Vol. 1*, Marcel Dekker: New York (2004) pp. 457–466.

Withers, R.L., Welberry, T.R., Larsson, A.-K.<sup>†1</sup>, Liu, Y., Norén, L., Rundlöf, H.\*, Brink, F.J. Local crystal chemistry, induced strain and short range order in the cubic pyrochlore  $(\text{Bi}_{1.5-\alpha}\text{Zn}_{0.5-\beta})(\text{Zn}_{0.5-\gamma}\text{Nb}_{1.5-\delta})\text{O}_{(7-1.5\alpha-\beta-\gamma-2.5\delta)}$  (BZN). *J. Solid State Chem.* (2004), 177(1), 231–244.

Withers, R.L., Brink, F.J., Norén, L., Welberry, T.R., Lui, Y. Local strain, structured diffuse scattering and oxygen/fluorine ordering in transition metal oxyfluorides. *Ferroelectrics* (2004), 305, 123–126.

<sup>†1</sup> IAS (Research School of Physical Sciences and Engineering)

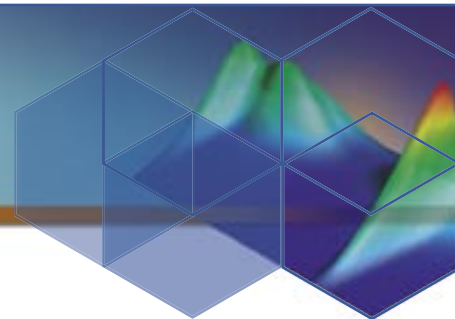
<sup>†1</sup> Faculty of Science (Physics)

<sup>§</sup> Research conducted prior to commencement at RSC

## Solid State Molecular Science

Henderson, M.J., King, D., White, J.W. Time dependent changes in the formation of titania based films at the air–water interface. *Langmuir* (2004), 20(6), 2305–2308.

Reynolds, P.A., Henderson, M.J., White, J.W. A small angle neutron scattering study of the interface between solids and oil–continuous emulsions and oil–based microemulsions. *Colloids Surf., A* (2004), 232(1), 55–65.



## Electrochemistry

Christy, A.G.<sup>+1</sup>, Lowe, A.<sup>+2</sup>, Otieno-Alego, V.<sup>‡</sup>, Stoll, M.<sup>+2</sup>, Webster, R.D. Voltammetric and Raman microspectroscopic studies on artificial copper pits grown in simulated potable water. *J. Appl. Electrochem.* (2004), 34(2), 225–233.

Shin, R.Y.C.\*<sup>‡</sup>, Ng, S.Y.\*<sup>‡</sup>, Tan, G.K.\*<sup>‡</sup>, Koh, L.L.\*<sup>‡</sup>, Khoo, S.B.\*<sup>‡</sup>, Goh, L.Y.\*<sup>‡</sup>, Webster, R.D. Syntheses and X-ray crystal structures of di- and trinuclear trithiolate–thioether bridged complexes of ruthenium. Electrochemistry of mixed-valence triruthenium complexes. *Organometallics* (2004), 23(3), 547–558.

Shin, R.Y.C.\*<sup>‡</sup>, Tan, G.K.\*<sup>‡</sup>, Koh, L.L.\*<sup>‡</sup>, Goh, L.Y.\*<sup>‡</sup>, Webster, R.D.  $[(L_n)Ru\{\eta^3-(tpdt)\}]$  complexes as dithiolate donors to group 10 metal centers: synthetic, single-crystal X-ray diffraction and electrochemical studies  $\{Ln = \eta^6-C_6Me_6$  (HMB) and  $\eta^5-C_5Me_5(Cp^*)$ ;  $tpdt = S(CH_2CH_2S)_2\}$ . *Organometallics* (2004), 23(26), 6108–6115.

Webster, R.D. In situ electrochemical-NMR spectroscopy. Reduction of aromatic halides. *Anal. Chem.* (2004), 76(6), 1603–1610.

Williams, L.L., Webster, R.D. Electrochemically controlled chemically reversible transformation of  $\alpha$ -tocopherol (vitamin E) into its phenoxonium cation. *J. Am. Chem. Soc.* (2004), 126(39), 12441–12450.

<sup>+1</sup> Faculty of Science (Geology)

<sup>+2</sup> Faculty of Science (Engineering)

## Technical Services

Jackson, P. Tandem mass spectrometry study of protonated methanol–water aggregates. *Int. J. Mass Spectrom.* (2004), 232(1), 67–77.

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

Dalton, G.T.<sup>+1</sup>, Willis, A.C., Humphrey, M.G.<sup>+1</sup> Mixed-metal cluster chemistry 27. Coupling of diphenylbuta-1,3-diyne and CO at tungsten–triridium cluster cores. *J. Clust. Sci.* (2004), 15(3), 291–300.

Jackson, W.G.<sup>‡</sup>, Dickie, A.J.\*<sup>‡</sup>, Bhula, R.\*<sup>‡</sup>, McKeon, J.A.\*<sup>‡</sup>, Spiccia, L.\*<sup>‡</sup>, Brudenell, S.J.\*<sup>‡</sup>, Hockless, D.C.R., Willis, A.C. Pyridyl-based pentadentate ligands: base-catalyzed hydrolysis of *asym*-[Co(dmptacn)Cl]<sup>2+</sup>. *Inorg. Chem.* (2004), 43(21), 6549–6556.

Kerr, D.J.<sup>+1</sup>, Willis, A.C., Flynn, B.L.<sup>+1</sup> Multicomponent coupling approach to ( $\pm$ )-frondosin B and a ring-expanded analogue. *Org. Lett.* (2004), 6(4), 457–460.

Rahman, A.F.M.M.\*<sup>‡</sup>, Jackson, W.G.<sup>‡</sup>, Willis, A.C. The first sideways-bonded peroxy complex for a tetraaminecobalt(III) species. *Inorg. Chem.* (2004), 43(24), 7558–7560.

Usher, A.J.<sup>+1</sup>, Dalton, G.T.<sup>+1</sup>, Lucas, N.T.<sup>+1</sup>, Waterman, S.M.<sup>+1</sup>, Petrie, S.<sup>+1</sup>, Stranger, R.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup>, Willis, A.C. Mixed-metal cluster chemistry. 26[1]. Proclivity for "all-terminal" or "plane-of-bridging-carbonyls" ligand disposition in tungsten–triridium clusters. *J. Organomet. Chem.* (2004), 689(1), 50–57.

Willis, A.C., Dalton, G.T.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup> Heptacarbonylbis( $\mu_3$ - $\eta^2$ -diphenylacetylene)( $\eta^5$ -pentamethylcyclopentadienyl)triridiumtungsten. *Acta Crystallogr., Sect. E* (2004), E60(4), m458–m459.

Willis, A.C., Dalton, G.T.<sup>+1</sup>, Morrall, J.P.<sup>+1</sup>, Cifuentes, M.P.<sup>+1</sup>, Humphrey, M.G.<sup>+1</sup> *cis,cis,cis*-Aquaabis[bis(diphenylphosphino)methane- $\kappa^2P,P'$ ]chlororuthenium(II) hexafluorophosphate methanol 1.73-solvate. *Acta Crystallogr., Sect. E* (2004), E60(8), m1122–m1123.

<sup>+1</sup> Faculty of Science (Chemistry)



### Bioinorganic and Medicinal Chemistry

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

Xia, L., Cregan, A.G., Berben, L.A., Brasch, N.E. Studies on the formation of glutathionylcobalamin: Any free intracellular aquacobalamin is likely to be rapidly and irreversibly converted to glutathionylcobalamin. *Inorg. Chem.* (2004), 43(21), 6848–6857.

#### Patent:

Brasch, N.E., Xia, L. Method of synthesis of  $\beta$ -thiolato cobalamin nucleoside compounds. United States patent application 2004/0054128 A1 (2004), 5 pp.

#### Visiting Fellows (Post-retirement)

Adamson, G.A., Beckwith, A.L.J., Chai, C.L.L.<sup>+1</sup> Highly diastereoselective radical reactions of substituted methyl ideneimidazolidinones and related systems. *Aust. J. Chem.* (2004), 57(7), 629–633.

Beckwith, A.L.J., Bowry, V.W., Bowman, W.R.\*, Mann, E.\*, Parr, J.\*, Storey, J.M.D.\* The mechanism of  $\text{Bu}_3\text{SnH}$ -mediated homolytic aromatic substitution. *Angew. Chem.* (2004), 116(1), 97–100; *Angew. Chem., Int. Ed.* (2004), 43(1), 95–98.

Beckwith, A.L.J., Mayadunne, R.T.A. Diastereoselective radical cyclization reactions; the synthesis of *O*-methylcorytenchirine. *ARKIVOC* (2004), (x), 80–93.

<sup>+1</sup> Faculty of Science (Chemistry)

Bennett, M.A., Bhargava, S.K.\*, Bond, A.M.\*, Edwards, A.J., Guo, S.-X.\*, Privér, S.H.\*, Rae, A.D., Willis, A.C. Synthesis, characterization, and electrochemical relationships of dinuclear complexes of platinum(II) and platinum(III) containing ortho-metalated tertiary arsine ligands. *Inorg. Chem.* (2004), 43(24), 7752–7763.

Bennett, M.A., Bhargava, S.K.\*, Hockless, D.C.R., Mohr, F.\*, Watts, K., Welling, L.L., Willis, A.C. Binuclear ten-membered ring cyclometallated complexes of digold(I) and their reactions with iodine and bromine. *Z. Naturforsch., B: Chem. Sci.* (2004), 59b(11&12), 1563–1569.

Bennett, M.A., Byrnes, M.J., Kováčik, I. The fragment bis(acetylacetonato)ruthenium: a meeting-point of coordination and organometallic chemistry. *J. Organomet. Chem.* (2004), 689(24), 4463–4474.

Brown D.J. Quinoxalines: Supplement II. *The Chemistry of Heterocyclic Compounds, Vol. 61*, Taylor, E.C., Wipf, P., and the late Weissberger, A., Eds. John Wiley & Sons: New York (2004), pp. xvi–510.

Williams, J.F. Pentose phosphate pathway, history of. In: *Encyclopedia of Biological Chemistry, Vol. 3*, Lennarz, W.J., Lane, M.D., Eds. Elsevier Science: Oxford, UK. (2004), pp. 216–225.

Zhao, C., Rickards, R.W., Trowell, S.C.\* Antibiotics from Australian terrestrial invertebrates. Part 1: Antibacterial trinervitadienes from the termite *Nasutitermes trididae*. *Tetrahedron* (2004), 60(47), 10753–10759.

#### Patent:

Rickards, R.W., Zhao, C.\*, Trowell, S.C.\* Antimicrobial trinervitane derivatives. PCT International Application no. AU2004/000123, 60 pp.