

REPORT OF DR. LEE'S PROFESSOR OF CHEMISTRY FOR THE YEAR ENDED

31st JULY 2001

At year's end, one of the more tangible developments in Chemistry is the rapidly emerging framework of the new Chemical Research Laboratories across the road, for which the ground-breaking took place in September 2000. While the PTCL will only be a minor beneficiary of the new building, nonetheless the prospect of the additional space is most welcome as we enter a new year at record levels of research student numbers and of research funding.

We were delighted to hear of Professor Paul Madden's election to the Royal Society, which brings to five the number of research-active FRS's in the PTCL. Professor Gus Hancock was awarded the prestigious 2000 Italgas Prize for Innovation in Science and Technology, while Dr. Colin Bain was honoured with the Royal Society of Chemistry Corday-Morgan Medal and Prize for the year 2000, joining other previous recipients in the Department of this recognition of outstanding younger chemists. We were proud to hear of Professor Graham Richards' appointment as Commander of the British Empire in the Queen's Birthday Honours. Professor John Simons was selected to give the Royal Society Humphry Davy Lecture 2001, and was also chosen the Burton Memorial Lecturer for 2001 at Kings College London. Among our younger members Angus Gray-Weale was awarded a Junior Research Fellowship at Jesus College, and Nathan Lawrence, who did his Part II and is now working towards a D.Phil. with Professor Richard Compton, was awarded the Royal Society of Chemistry Ronald Belcher Memorial Lectureship, recognising outstanding achievements by graduate students.

On a different note, we were sorry to hear of the death of Mr. Andy Whiting in March 2001. Mr. Whiting joined the Department's Mechanical Workshop in 1944 and retired a full fifty years later, including some twenty years as its Supervisor. As generations go others come, and we were happy to see Mr. Roger Bowler and Mr. Paul Mitchell take up their duties as Supervisors in the Mechanical Workshop and the Lab Services Unit respectively.

The Department has also seen several prestigious appointments. Professor Peter Atkins was appointed Chairman of the new IUPAC Committee for Chemical Education, which has worldwide responsibilities for coordinating and developing chemical education and the public appreciation of chemistry.

Professor Keith McLauchlan was named Eminent Scientist at the Institute of Chemical and Physical Research in Tokyo where he lectured on several occasions over the year. Several PTCL colleagues have left us for positions elsewhere. Dr. James Davis was appointed to a lectureship in electrochemistry and analytical chemistry at the University of Surrey, Dr. E.G. Robertson returned to Australia, having been awarded an Australian Research Council Fellowship as well as a Logan Fellowship at Monash University, Dr. Sarah Wilsey, a Glasstone Research Fellow, was appointed to a lectureship at Kings College London, and Dr. Mark Wilson, a Royal Society University Research Fellow, was appointed to a lectureship at University College London. Dr. Stephen Ashworth, a former D.Phil. student with Professor John Brown, was appointed to a lectureship at the University of East Anglia.

During the year we have been fortunate in hosting several distinguished lecturers. Professor Dennis Evans of the Australian National University, Canberra kicked off with the Boys-Rahman Lecture of the Royal Society of Chemistry, while Dr. Bill Price of the Royal Institute of Technology in Stockholm delivered the Rennie Lecture of the Royal Australian Chemical Institute. We were very happy to host Professor Peter Toennies of the Max Planck Institute for Fluid Dynamics, in the Hilary Term, as our Hinshelwood Lecturer

for the year 2001. His six lectures on *Novel Spectroscopies using Helium Atoms, Clusters, and Droplets* were delivered with humour and perception and drew large crowds right to the very end. A Half-Day Symposium of the Faraday Division of the Royal Society of Chemistry, entitled *Spectroscopy in Action: Molecular Dynamics and Structure*, held in our lecture theatre before a packed audience, was opened by this year's Faraday Lecturer, Professor Dick Zare (Stanford University), a former Hinshelwood Lecturer who has been a long-standing friend of the Department; he was followed by the Tilden Lecturer, Professor Klaus Müller-Dethlefs (University of York), with supporting lectures by Dr. Helen Fielding (Kings College London) and Dr. Martin Cockett (University of York). In April the new Dr. Lee's Professor delivered his Inaugural Lecture, *Soft Matter: from Hieroglyphics to Biolubrication*, indicating some of the new directions he intends to pursue.

Research activity has continued unabated. In these days of belt-tightening it is particularly pleasing to note that grants awarded during the year totalled , 3.2M, a clear high for the Department; this included grants of , 0.45M to Professor Graham Richards, , 0.4M to Dr. Colin Bain to set up the new departmental surface characterisation facility (now partly running and being looked after by Dr. Rob Jacobs); and , 0.83M to Professor Jacob Klein. At the same time, at , 2.3M our research grant income over the year is a full 25% larger than even the previous year's record levels. In particular, at the year's end, we looked forward with keen anticipation to welcoming 29 starting graduate students, a new and promising high for the Department.

Once again we have had a distinguished crop of visitors. In addition to our regulars, Professor Ian Beattie (University of Southampton) and Professor Itamar Burak (Tel Aviv University), we were happy to host Professor Zehra Akdeniz (Istanbul) and Professor Paul Brint (University College Cork). From even further afield, we were happy to welcome Professor Walter Balfour (University of Victoria, B.C.), Professor David Chandler from the University of California at Berkeley, and Professor John Lekner from Victoria University, New Zealand, who interacted with many of us during his year here. Other welcome visitors included Professor Tom Dyke (University of Oregon), Professor Peter Harrowell (University of Sydney), Professor Mineo Hiramatsu (Meijo University), Professor S.K. Lai (National University of Taiwan) and Professor Greg Voth (University of Utah), as well as a brief visit by Professor Jacob Israelachvili from the University of California at Santa Barbara.

My first year in the PTCL was marked by a warm welcome and cooperation from all members of the Department, for which I am immensely grateful. I would like to thank in particular Professor Gus Hancock who was Head of Department in the interim period between the two Dr. Lee's Professors, and who >delivered= the PTCL in such very good shape.

PUBLICATIONS

P.W. Atkins

Atkins, P.W. *Elements of Physical Chemistry*, Oxford University Press and W.H. Freeman & Co., 2000.

C.D. Bain

Bain, C.D., Manning-Benson, S. and Darton, R.C. Rates of mass transfer and adsorption of hexadecyltrimethylammonium bromide at an expanding air-water interface. *J. Colloid Interface Sci.* **229**, 247-256, 2000.

Beattie, D.A., Haydock, S. and Bain, C.D. A comparative study of confined organic monolayers by Raman scattering and sum-frequency spectroscopy. *Vibrational Spectroscopy* **24**, 109-123, 2000.

Eastoe, J., Rankin, A, Wat, R. and Bain, C.D. Surfactant adsorption dynamics. *Int. Rev. Phys. Chem.* **20**, 357-386, 2001.

M. Brouard

Aoiz, F.J., Bañares, L., Brouard, M., Castillo, J.F. and Herrero, V.J. The dynamics of the $O(^1D) + HD$ reaction: A quasiclassical trajectory multisurface study. *J. Chem. Phys.* **113**, 5339-5353, 2000.

Aoiz, F.J., Bañares, L., Castillo, J.F., Brouard, M., Denzer, W., Vallance, C., Honvault, P., Launay, J.-M., Dobbyn, A.J. and Knowles, P.J. Insertion and abstraction pathways in the reaction $O(^1D_2) + H_2 \div OH + H$. *Phys. Rev. Lett.* **86**, 1729-1732, 2001.

Brouard, M., Burak, I., Joseph, D.M., Markillie, G.A.J., Minayev, D., O'Keeffe, P. and Vallance, C. The dynamics of the reactions $H + H_2O \div OH + H_2$ and $H + D_2O \div OD + HD$ at 1.4 eV. *J. Chem. Phys.* **114**, 6690-6701, 2001.

Brouard, M., Gatenby, S., Joseph, D.M. and Vallance, C. The $H + H_2O \div OH(^2\Pi_{\Omega}, v\mathbb{N}, M\mathbb{N}) + N_2$ reaction: OH rotational angular momentum polarization. *J. Chem. Phys.* **113**, 3162-3172, 2000.

Brouard, M., O'Keeffe, P., Joseph, D.M. and Minayev, D. NO rotational orientation following 308 nm photodissociation of NO_2 . *Phys. Rev. Lett.* **86**, 2249-2252, 2001.

Brouard, M. and Vallance, C. The dynamics of the light atom transfer reaction $O(^3P_J) + HBr \div OH(v\mathbb{N}, j\mathbb{N}) + Br(^2P_{3/2})$. *Phys. Chem. Chem. Phys.* **3**, 3602-3609, 2001.

M. Brouard and J.P. Simons

Brouard, M., Burak, I., Hughes, D.W., Kalogerakis, K.S., Simons, J.P. and Stavros, V. Product state resolved stereodynamics: Rotational polarization of $OH(^2\Pi; v\mathbb{N}, M\mathbb{N}, \Omega, f)$ scattered from the reaction, $H + CO_2 \div OH + CO$. *J. Chem. Phys.* **113**, 3173-3180, 2000.

J.M. Brown

- Bosch, E., Crozet, P., Ross, A.J. and Brown, J.M. Fourier transform spectra of the $E^2\Pi_u$ - $BX^2\Pi_{g(3/2)}$ system of CuCl_2 . 2. Rovibronic levels of the ground state up to 4000 cm^{-1} . *J. Molec. Spectrosc.* **202**, 253B261, 2000.
- Brown, J.M. The Renner-Teller effect: The effective Hamiltonian approach, in *Computational Molecular Spectroscopy*, eds. P.R. Bunker and P.Jensen. J. Wiley & Sons Ltd., Chichester, 2000, chap.16, pp.517B537.
- Brown, J.M., Buenker, R.J., Carrington, A., Di Lauro, C., Dixon, R.N., Field, R.W., Hougen, J.T., Hüttner, W., Kuchitsu, K., Mehring, M., Merer, A.J., Miller, T.A., Quack, M., Ramsay, D.A., Veseth, L. and Zare, R.N. Remarks on the signs of g factors in atomic and molecular Zeeman spectroscopy. *Molec. Phys.* **98**, 1597B1601, 2000.
- Davidson, S.A., Evenson, K.M. and Brown, J.M. A measurement of the rotational spectrum of the CH radical in the far-infrared. *Astrophys. J.* **546**, 330B337, 2001.
- Kermode, S.M. and Brown, J.M. The ultraviolet spectrum of the FeF radical: A study of the ${}^6\Pi_{BX}^6 \Delta$ and ${}^6\Phi_{BX}^6 \Delta$ band systems at 330 and 323 nm respectively. *J. Molec. Spectrosc.* **207**, 161B171, 2001.
- Tamassia, F., Brown, J.M. and Saito, S. The detection of the free radical FO ($X^2\Pi_{3/2}$) by submillimeter-wave spectroscopy. *J. Chem. Phys.* **112**, 5523B5526, 2000.
- Tamassia, F., Kermode, S.M. and Brown, J.M. A study of the (2B0) overtone bands of the FO, BrO, and IO free radicals by laser magnetic resonance. *J. Molec. Spectrosc.* **205**, 92B101, 2001.

H.M. Cartwright

- Cartwright, H.M. Why should on-line experiments form part of University science courses? CAL-laborate, October 2000, pp.6B9. On-line at <http://science.uniserve.edu.au/pubs/callab/>.
- Cartwright, H.M. Undergraduate projects in the application of Artificial Intelligence to chemistry. II. Self-organizing maps. *Chem. Educator* **5**, 196B204, 2000.
- Cartwright, H.M. Nationalizing Science. Adolph Wurtz and the Battle for French Chemistry: A review. *Chem. Educator* **6**, 139B140, 2001.
- Cartwright, H.M. Physical Chemistry: A review. *Chem. Educator* **6**, 262B263, 2001.
- Cartwright, H.M. Instruments and Experimentation in the History of Chemistry: A review. *Chem. Educator* **6**, 263B264, 2001.
- Cartwright, H.M. and Yiasoumis, L.T. Undergraduate projects in the application of Artificial Intelligence to Chemistry. III. Cellular automata. *Chem. Educator* **6**, 247B254, 2001.
- Cartwright, H.M. and Yiasoumis, L. Chemical and biological remediation: cellular automata studies of bacteria under stress. Proceedings of the 5th World Multiconference on, *Systemics, Cybernetics and Informatics (SCI 2001)*, and 7th International Conference on, *Information Systems, Analysis and Synthesis (ISAS 2001)*, Orlands, Florida, 2001.

M.S. Child

- Child, M.S., Dong, S.-H. and Wang, X.-G. Quantum states of a sextic potential: hidden symmetry and quantum monodromy. *J. Phys. A: Math. Gen.* **33**, 5653B5661, 2000.
- Jacobson, M.P. and Child, M.S. Spectroscopic signatures of bond-breaking internal rotation. I. Saddle point induced polyad breakdown. *J. Chem. Phys.* **114**, 250B261, 2001.
- Jacobson, M.P. and Child, M.S. Spectroscopic signatures of bond-breaking internal rotation. II. Rotation-vibration level structure and quantum monodromy in HCP. *J. Chem. Phys.* **114**, 262B275, 2001.
- Jacobson, M.P. and Child, M.S. Scaling rules for resonance dynamics near a saddle point: the pendulum as a zero-order model. *J. Phys. Chem. A* **105**, 2834B2841, 2001.
- Shalashilin, D.V. and Child, M.S. Time dependent quantum propagation in phase space. *J. Chem. Phys.* **113**, 10028, 2000.
- Shalashilin, D.V. and Child, M.S. Description of tunneling with the help of coupled frozen Gaussians. *J. Chem. Phys.* **114**, 9296B9304, 2001.

B.A. Coles and R.G. Compton

- Marken, F., Tsai, Y.-C., Coles, B.A., Matthews, S.L. and Compton, R.G. Microwave activation of electrochemical processes: convection, thermal gradients and hot spot formation at the electrode/solution interface. *New J. Chem.* **24**, 653B658, 2000.
- Moorcroft, M.J., Lawrence, N.S., Coles, B.A., Compton, R.G. and Trevani, L.N. High temperature electrochemical studies using a channel flow cell heated by radio frequency radiation. *J. Electroanal. Chem.* **506**, 28B33, 2001.
- Qiu, F., Compton, R.G., Coles, B.A. and Marken, F. Thermal activation of electrochemical processes in a Rf-heated channel flow cell: experiment and finite element simulation. *J. Electroanal. Chem.* **492**, 150B155, 2000.
- Tsai, Y.-C., Coles, B.A., Compton, R.G. and Marken, F. Microwave activation of electrochemical processes: square-wave voltammetric stripping detection of cadmium in the presence of the surfactant Triton X. *Electroanalysis* **13**, 639B645, 2001.

B.A. Coles, R.G. Compton and J.S. Foord

- Marken, F., Tsai, Y.-C., Saterlay, A.J., Coles, B.A., Tibbetts, D., Holt, K., Goeting, C.H., Foord, J.S. and Compton, R.G. Microwave activation of electrochemical processes: enhanced PbO₂ electrodeposition, stripping and electrocatalysis. *J. Solid State Electrochem.* **5**, 313B318, 2001.
- Tsai, Y.-C., Coles, B.A., Holt, K., Foord, J.S., Marken, F. and Compton, R.G. Microwave-enhanced anodic stripping detection of lead in a river sediment sample. A mercury-free procedure employing a boron-doped diamond electrode. *Electroanalysis* **13**, 831B835, 2001.

R.G. Compton

- Ball, J.C., Marken, F., Qui, F., Wadhawan, J.D., Blythe, A.N., Schröder, U., Compton, R.G., Bull, S.D. and Davies, S.G. Voltammetry of electroactive oil droplets. Part II: Comparison of experimental and simulation data for coupled ion and electron insertion processes and evidence for microscale convection. *Electroanalysis* **12**, 1017B1025, 2000.
- Beckett, E.L., Lawrence, N.S., Evans, R.G., Davis, J. and Compton, R.G. Sonoelectrochemically enhanced determination of 5-aminosalicylic acid. *Talanta* **54**, 871B877, 2001.
- Brookes, B.A., Lawrence, N.S. and Compton, R.G. Microdisk electrode voltammetry: theoretical characterization and experimental verification of a novel electrocatalytic mechanism. *J. Phys. Chem. B* **104**, 11258B11267, 2000.
- Davis, J., Del Campo, F.J., Marken, F., Compton, R.G. and Cordemans, E. Stability of mercury film electrodes under the influence of high frequency (500 kHz) ultrasound. *J. Appl. Electrochem.* **31**, 475B480, 2001.
- Davis, J., Moorcroft, M.J., Wilkins, S.J., Compton, R.G. and Cardosi, M.F. Electrochemical detection of nitrate at a copper modified electrode under the influence of ultrasound. *Electroanalysis* **12**, 1363B1367, 2000.
- Del Campo, F.J., Maisonhaute, E, Compton, R.G., Marken, F. and Aldaz, A. Low-temperature sonoelectrochemical processes. Part 3. Electrodimerisation of 2-nitrobenzylchloride in liquid ammonia. *J. Electroanal. Chem.* **506**, 170B177, 2001.
- Del Campo, F.J., Melville, J., Hardcastle, J.L. and Compton, R.G. Differential pulse and chronoamperometric studies of insonated systems: acoustic streaming and cavitation effects. *J. Phys. Chem. A* **105**, 666B674, 2001.
- Hardcastle, J.L. and Compton, R.G. Sonoelectroanalytical determination of heavy metals in fish gill mucus. *Electroanalysis* **13**, 89B93, 2001.
- Hignett, G., Threlfell, S., Wain, A.J., Lawrence, N.S., Wilkins, S.J., Davis, J., Compton, R.G. and Cardosi, M.F. Electroanalytical exploitation of quinoneBthiol interactions: application to the selective determination of cysteine. *Analyst* **126**, 353B357, 2001.
- Ito, S., Watanabe, H., Uno, H., Murashima, T., Ono, N., Tsai, Y.-C. and Compton, R.G. Synthesis and properties of polypyrrole annelated with bicyclo[2.2.2]octene units. *Tetrahedron Letts.* **42**, 707B710, 2001.
- Lawrence, N.S., Davis, J. and Compton, R.G. Analytical strategies for the detection of sulfide: a review. *Talanta* **52**, 771B784, 2000.
- Lawrence, N.S., Davis, J. and Compton, R.G. Electrochemical detection of thiols in biological media. *Talanta* **53**, 1089B1094, 2001.
- Lawrence, N.S., Davis, J., Jiang, L., Jones, T.G.J., Davies, S.N. and Compton, R.G. The electrochemical analog of the methylene blue reaction: a novel amperometric approach to the detection of hydrogen sulfide. *Electroanalysis* **12**, 1453B1460, 2000.
- Lawrence, N.S., Davis, J., Jiang, L., Jones, T.G.J., Davies, S.N. and Compton, R.G. Electrochemically initiated reactions of diphenylamines with sulfide: application to the voltammetric detection of hydrogen sulfide. *Electroanalysis* **13**, 143B148, 2001.
- Lawrence, N.S., Davis, J., Jiang, L., Jones, T.G.J., Davies, S.N. and Compton, R.G. Electrochemically

- initiated 1,4-nucleophilic substitutions: a general strategy for the analytical detection of hydrogen sulfide. *Electroanalysis* **13**, 432B436, 2001.
- Lawrence, N.S., Davis, J., Marken, F., Jiang, L., Jones, T.G.J., Davies, S.N. and Compton, R.G. Electrochemical detection of sulphide: a novel dual flow cell. *Sensors and Actuators B* **69**, 189B192, 2000.
- Macfie, G. and Compton, R.G. Characterisation of the sonicated ring-pellet reactor and sono-ring-disc electrodes. *J. Electroanal. Chem.* **503**, 125B132, 2001.
- Marken, F., Blythe, A.N., Wadhawan, J.D., Compton, R.G., Bull, S.D., Aplin, R.T. and Davies, S.G. Voltammetry of electroactive liquid redox systems: anion insertion and chemical reactions in microdroplets of *para*-tetrakis(6-methoxyhexyl)phenylenediamine, *para*- and *meta*-tetrahexylphenylenediamine. *J. Solid State Electrochem.* **5**, 17B22, 2001.
- Melville, J.L. and Compton, R.G. The simulation of differential pulse voltammetry. *Electroanalysis* **13**, 123B130, 2001.
- Melville, J.L. and Compton, R.G. Pulse voltammetry at the rotating disc electrode. *J. Electroanal. Chem.* **501**, 114B127, 2001.
- Miles, A.B. and Compton, R.G. The theory of square wave voltammetry at uniformly accessible hydrodynamic electrodes. *J. Electroanal. Chem.* **487**, 75B89, 2000.
- Miles, A.B. and Compton, R.G. Simulation of square-wave voltammetry at a channel electrode: E, EC and ECE processes. *J. Electroanal. Chem.* **499**, 1B16, 2001.
- Moorcroft, M.J., Davis, J. and Compton, R.G. Detection and determination of nitrate and nitrite: a review. *Talanta* **54**, 785B803, 2001.
- Moorcroft, M.J., Nei, L., Davis, J. and Compton, R.G. Enhanced electrochemical detection of nitrite and nitrate at a Cu-30Ni alloy electrode. *Analytical Letts.* **33**, 3127B3137, 2000.
- Powell, M., Ball, J.C., Tsai, Y.-C., Suárez, M.F. and Compton, R.G. Square wave anodic stripping voltammetry at mercury-plated electrodes. Simulation of surface morphology effects on electrochemically reversible, irreversible, and quasi-reversible processes: comparison of thin films and microdroplets. *J. Phys. Chem. B* **104**, 8268B8278, 2000.
- Qiu, F., Ball, J.C., Marken, F., Compton, R.G. and Fisher, A.C. Voltammetry of electroactive oil droplets. Part I: Numerical modelling for three mechanistic models using the dual reciprocity finite element method. *Electroanalysis* **12**, 1012B1016, 2000.
- Qiu, F., Gooch, K.A., Fisher, A.C., Stevens, N.P.C. and Compton, R.G. Computer-aided design and experimental investigation of a hydrodynamic device: the microwire electrode. *Anal. Chem.* **72**, 3480B3485, 2000.
- Saterlay, A.J., Tibbetts, D.F. and Compton, R.G. Comparative study to evaluate the feasibility of *sono*-anodic and *sono*-cathodic stripping voltammetry for the determination of Pb in a Cu-Pb alloy. *Analytical Sciences* **16**, 1055B1060, 2000.
- Schröder, U., Compton, R.G., Marken, F., Bull, S.D., Davies, S.G. and Gilmour, S. Electrochemically driven ion insertion processes across liquid/liquid boundaries: neutral versus ionic redox liquids. *J. Phys. Chem. B* **105**, 1344B1350, 2001.
- Schröder, U., Wadhawan, J.D., Compton, R.G., Marken, F., Suarez, P.A.Z., Consorti, C.S., de Souza, R.F. and Dupont, J. Water-induced accelerated ion diffusion: voltammetric studies in 1-methyl-3-

- [2,6-(*S*)-dimethylocten-2-yl]imidazolium tetrafluoroborate, 1-butyl-3-methylimidazolium tetrafluoroborate and hexafluorophosphate ionic liquids. *New J. Chem.* **24**, 1009B1015, 2000.
- Thiemann, T., Ohira, D., Arima, K., Sawada, T., Mataka, S., Marken, F., Compton, R.G., Bull, S.D. and Davies, S.G. Photochemical and electrochemical behavior of thiophene-*S*-oxides. *J. Phys. Org. Chem.* **13**, 648B653, 2000.
- Tibbetts, D.F., David, J. and Compton, R.G. Sonoelectroanalytical detection of lead at a bare copper electrode. *Fresenius J. Anal. Chem.* **368**, 412B414, 2000.
- Tsai, Y.-C., Davis, J. and Compton, R.G. Sono-anodic stripping voltammetric determination of cadmium in the presence of surfactant. *Fresenius J. Anal. Chem.* **368**, 415B417, 2000.
- Tsai, Y.-C., Davis, J., Compton, R.G., Ito, S. and Ono, N. Polypyrrole coated mercury film electrodes for sono-ASV analysis of cadmium and lead. *Electroanalysis* **13**, 7B12, 2001.
- Wadhawan, J.D., Compton, R.G., Marken, F., Bull, S.D. and Davies, S.G. Photoelectro-chemically driven processes at the *N,N,N',N'*-tetrahexylphenylenediamine microdroplet/electrode/aqueous electrolyte triple interface. *J. Solid State Electrochem.* **5**, 301B305, 2001.
- Wadhawan, J.D., Marken, F., Compton, R.G., Bull, S.D. and Davies, S.G. Sono-emulsion electrosynthesis: electrode-insensitive Kolbe reactions. *Chem. Commun.* 87B88, 2001.
- Wadhawan, J.D., Schröder, U., Neudeck, A., Wilkins, S.J., Compton, R.G., Marken, F., Consorti, C.S., de Souza, R.F. and Dupont, J. Ionic liquid modified electrodes. Unusual partitioning and diffusion effects of $\text{Fe}(\text{CN})_6^{-/3-}$ in droplet and thin layer deposits of 1-methyl-3-(2,6-(*S*)-dimethylocten-2-yl)-imidazolium tetrafluoroborate. *J. Electroanal. Chem.* **493**, 75B83, 2000.
- Wilkins, S.J., Compton, R.G., Taylor, M.A. and Viles, H.A. Channel flow cell studies of the inhibiting action of gypsum on the dissolution kinetics of calcite: a laboratory approach with implications for field monitoring. *J. Coll. Interface Sci.* **236**, 354B361, 2001.

R.G. Compton and J.S. Foord

- Foord, J.S., Holt, K.B., Compton, R.G., Marken, F. and Kim, D.-H. Mechanistic aspects of the sonoelectrochemical degradation of the reactive dye Procion Blue at boron-doped diamond electrodes. *Diamond Rel. Matt.* **10**, 662B666, 2001.
- Marken, F., Compton, R.G., Goeting, C.H., Foord, J.S., Bull, S.D. and Davies, S.G. Fast electrochemical triple-interface processes at boron-doped diamond electrodes. *J. Solid State Electrochem.* **5**, 88B93, 2001.
- Saterlay, A.J., Marken, F., Foord, J.S. and Compton, R.G. Sonoelectrochemical investigation of silver analysis at a highly boron-doped diamond electrode. *Talanta* **53**, 403B415, 2000.
- Saterlay, A.J., Wilkins, S.J., Goeting, C.H., Foord, J.S., Compton, R.G. and Marken, F. Sonoelectrochemistry at highly boron-doped diamond electrodes: silver oxide deposition and electrocatalysis in the presence of ultrasound. *J. Solid State Electrochem.* **4**, 383B389, 2000.
- Saterlay, A.J., Wilkins, S.J., Holt, K.B., Foord, J.S., Compton, R.G. and Marken, F. Lead dioxide deposition and electrocatalysis at highly boron-doped diamond electrodes in the presence of ultrasound. *J. Electrochem. Soc.* **148**, E66BE72, 2001.

J.H.D. Eland

- Aitchison, D. and Eland, J.H.D. Dissociative ionisation of CS₂ and the formation of S₂⁺. *Chem. Phys.* **263**, 449B457, 2001.
- Eland, J.H.D., Takahashi, M. and Hikosaka, Y. Photoelectron-fragment ion correlations and fixed-molecule photoelectron angular distributions from velocity imaging coincidence experiments. *Faraday Discuss.* **115**, 119B126, 2000.
- Hikosaka, Y. and Eland, J.H.D. Molecular-frame photoelectron angular distributions in inner-valence photoionization of N₂. *J. Phys. B: At. Mol. Opt. Phys.* **33**, 3137B3147, 2000.
- Hikosaka, Y. and Eland, J.H.D. Molecular frame photoelectron angular distributions in inner valence photoionisation of CO. *Phys. Chem. Chem. Phys.* **2**, 4663B4668, 2000.
- Hikosaka, Y. and Eland, J.H.D. New results on photoion pair formation from application of the velocity imaging photoionisation coincidence technique. *Rapid Commun. Mass Spectrom.* **14**, 2305B2311, 2000.

J.S. Foord

- Foord, J.S., Hian, L.C. and Jackman, R.B. An investigation of the surface reactivity of diamond photocathodes with molecular atomic oxygen species. *Diamond Rel. Mat.* **10**, 710B714, 2001.
- Foord, J.S., Wang, J., Lau, C.H., Hiramatsu, M., Vickers, J. and Jackman, R.B. Influence of surface properties on the quantum photoyield of diamond photocathodes. *Phys. Stat. Sol. (a)* **186**, 227B233, 2001.
- Gaudin, O., Whitfield, M.D., Foord, J.S. and Jackman, R.B. Deep level transient spectroscopy of CVD diamond: the observation of defect states in hydrogenated films. *Diamond Rel. Mat.* **10**, 610B614, 2001.
- Marken, F., Gerrard, M.L., Mellor, I.M., Mortimer, R.J., Madden, C.E., Fletcher, S., Holt, K., Foord, J.S., Dahm, R.H. and Page, F. Voltammetry at carbon nanofiber electrodes. *Electrochem. Commun.* **3**, 177B180, 2001.
- Riedel, D., Hernandez-Pozos, J.L., Palmer, R.E., Baggott, S., Kolasinski, K.W. and Foord, J.S. Tunable pulsed vacuum ultraviolet light source for surface science and materials spectroscopy based on high order harmonic generation. *Rev. Sci. Instrum.* **72**, 1977B1983, 2001.
- Williams, O.A., Whitfield, M.D., Jackman, R.B., Foord, J.S., Butler, J.E. and Nebel, C.E. Formation of shallow acceptor states in the surface region of thin film diamond. *Appl. Phys. Letts.* **78**, 3460B3462, 2001.
- Williams, O.A., Whitfield, M.D., Jackman, R.B., Foord, J.S., Butler, J.E. and Nebel, C.E. Carrier generation within the surface region of hydrogenated thin film polycrystalline diamond. *Diamond Rel. Mat.* **10**, 423B428, 2001.

G.H. Grant and W.G. Richards

- Allen, B.C.P., Grant, G.H. and Richards, W.G. Similarity calculations using two-dimensional molecular representations. *J. Chem. Inf. Comput. Sci.* **41**, 330B337, 2001.

G. Hancock

Barry, H.R., Corner, L., Hancock, G., Peverall, R. and Ritchie, G.A.D. Cavity-enhanced absorption spectroscopy of methane at 1.73 μm . *Chem. Phys. Letts.* **333**, 285B289, 2001.

Breheny, C., Hancock, G. and Morrell, C. The rate constant for the recombination reaction between CF_3 and O_2 measured between 2 and 110 Torr. *Zeit. Phys. Chem.* **215**, 305B317, 2001.

Breheny, C., Hancock, G. and Morrell, C. The $\text{CF}_3 + \text{NO}_2$ rate constant measured between 1.5 and 110 Torr and between 251 and 295 K by time resolved infrared emission. *Phys. Chem. Chem. Phys.* **2**, 5105B5112, 2000.

Hancock, G., Johnson, R.D., Pinot de Moira, J.C., Ritchie, G.A.D. and Tyley, P.L. The photodissociation dynamics of tropospheric ozone, in *Atomic and Molecular Beams*, ed. R. Campargue, Springer, 2000, pp.331B342.

Ritchie, G.A.D. and Sivia, D.S. Foundations of Physics for Chemists, No.93 in *Oxford Chemistry Primers*, Oxford University Press, 2000.

P.J. Hore

Fursman, C.E., Bittl, R., Zech, S.G. and Hore, P.J. 95 GHz ESEEM of radical pairs: a source of radical separations and relative orientations. *Chem. Phys. Letts.* **342**, 162B168, 2001.

P.J. Hore and C.R. Timmel

Timmel, C.R., Cintolesi, F., Brocklehurst, B. and Hore, P.J. Model calculations of magnetic field effects on the recombination reactions of radicals with anisotropic hyperfine interactions. *Chem. Phys. Letts.* **334**, 387B395, 2001.

P.J. Hore, K.A. McLauchlan and C.R. Timmel

Eveson, R.W., Timmel, C.R., Brocklehurst, B., Hore, P.J. and McLauchlan, K.A. The effects of weak magnetic fields on radical recombination reactions in micelles. *Int. J. Radiat. Biol.* **76**, 1509B1522, 2000.

Stass, D.V., Woodward, J.R., Timmel, C.R., Hore, P.J. and McLauchlan, K.A. Radiofrequency magnetic field effects on chemical reaction yields. *Chem. Phys. Letts.* **329**, 15B22, 2000.

Timmel, C.R., Woodward, J.R., Hore, P.J., McLauchlan, K.A. and Stass, D.V. A zero-field electron spin resonance spectrometer for the study of transient radical ion pairs. *Meas. Sci. Technol.* **12**, 635B643, 2001.

B.J. Howard

Dennis, C.R., Whitham, C.J. and Howard, B.J. A theory for the magnetic hyperfine interactions in the microwave spectrum of NOBHf. *J. Chem. Phys.* **115**, 1355B1365, 2001.

Dennis, C.R., Whitham, C.J. and Howard, B.J. An analysis of the magnetic hyperfine interactions in the microwave spectrum of NOBHf: Evidence of electron transfer. *J. Chem. Phys.* **115**, 1367B1377, 2001.

King, A.K. and Howard, B.J. A high-resolution microwave study of the conformations of butan-2-ol in a supersonic expansion. *J. Molec. Spectrosc.* **205**, 38B42, 2001.

D.E. Logan

Dickens, N.L. and Logan, D.E. On the scaling spectrum of the Anderson impurity model. *J. Phys.: Condens. Matter* **13**, 4505B4517, 2001.

Logan, D.E. and Dickens, N.L. Magnetic properties of the Anderson model: A local moment approach. *Europhys. Lett.* **54**, 227B233, 2001.

Schäfer, S. and Logan, D.E. Spectral properties of a narrow-band Anderson model. *Phys. Rev. B* **63**, 045122, 1B9, 2001.

K.A. McLauchlan

Davies, M.N., Gilbert, B.C. and McLauchlan, K.A., Senior Reporters. *Electron Paramagnetic Resonance, Volume 17*. RSC Special Periodical Report, 2000.

McLauchlan, K.A. Herbert Marcus Powell. *Biog. Mems. Fell. Roy. Soc. Lond.* **46**, 425B442, 2000.

P.A. Madden

Bernasconi, L. and Madden, P.A. Optimally localized Wannier functions within the Vanderbilt ultrasoft pseudo-potential formalism. *J. Mol. Struct: THEOCHEM* **544**, 49B60, 2001.

Domene, C., Fowler, P.W., Jemmer, P. and Madden, P.A. Dipole-induced-dipole polarizabilities of symmetric clusters. *Molec. Phys.* **98**, 1391B1407, 2000.

Jesson, B.J. and Madden, P.A. *Ab initio* determination of the melting point of aluminium by thermodynamic integration. *J. Chem. Phys.* **113**, 5924B5934, 2000.

Jesson, B.J. and Madden, P.A. Structure and dynamics at the aluminium solid-liquid interface: an *ab initio* simulation. *J. Chem. Phys.* **113**, 5935B5946, 2000.

P.A. Madden and M. Wilson

Castiglione, M.J., Wilson, M., Madden, P.A. and Grey, C.P. Ion mobility in α -PbF₂: a computer simulation study. *J. Phys.: Condens. Matter* **13**, 51B66, 2001.

Domene, C., Fowler, P.W., Madden, P.A., Wilson, M. and Wheatley, P. Overlap model and *ab initio* cluster calculations of dipole polarization. *Chem. Phys. Letts.* **333**, 403B412, 2001.

Domene, C., Fowler, P.W., Madden, P.A., Xu, J., Wheatley, R.J. and Wilson, M. Short-range contributions to the polarization of cations. *J. Phys. Chem. A* **105**, 4136B4142, 2001.

- Gray-Weale, A., Madden, P.A. and Wilson, M. Induced-dipole contributions to the conductivity and dielectric response of molten ZnCl_2 . *J. Chem. Phys.* **113**, 6782B6787, 2000.
- Hutchinson, F., Wilson, M. and Madden, P.A. Short- and intermediate-range order in molten metal tribromides: a computer simulation study. *J. Phys.:Condens. Matter* **12**, 10389B10410, 2000.
- Hutchinson, F., Wilson, M. and Madden, P.A. A unified description of MCl_3 systems with a polarizable ion simulation model. *Molec. Phys.* **99**, 811B824, 2001.
- Wilson, M. and Madden, P.A. Growth of ionic crystals in carbon nanotubes. *J. Am. Chem. Soc.* **123**, 2101B2102, 2001.

D.E. Manolopoulos

- Alexander, M.H., Manolopoulos, D.E. and Werner, H.-J. An investigation of the $\text{F} + \text{H}_2$ reaction based on a full *ab initio* description of the open-shell character of the $\text{F}(^2P)$ atom. *J. Chem. Phys.* **113**, 11084B11100.
- Rackham, E.J., Huarte-Larranaga, F., and Manolopoulos, D.E. Coupled-channel statistical theory of the $\text{N}(^2D) + \text{H}_2$ and $\text{O}(^1D) + \text{H}_2$ insertion reactions. *Chem. Phys. Letts.* **343**, 356B364, 2001.
- Skodje, R.T., Skouteris, D., Manolopoulos, D.E., Lee, S.-H., Dong, F, and Liu, K. Resonance-mediated chemical reaction: $\text{F} + \text{HD} \div \text{HF} + \text{D}$. *Phys. Rev. Letts.* **85**, 1206B1209, 2000.
- Skouteris, D., Castillo, J.F. and Manolopoulos, D.E. ABC: a quantum reactive scattering program. *Comput. Phys. Commun.* **133**, 128B135, 2000.

W.G. Richards

- Remko, M., Walsh, O.A. and Richards, W.G. Molecular structure and gas-phase reactivity of clonidine and rilmenidine: Two-layered ONIOM calculations. *Phys. Chem. Chem. Phys.* **3**, 901B907, 2001.
- Remko, M., Walsh, O.A. and Richards, W.G. Theoretical study of molecular structure, tautomerism, and geometrical isomerism of moxonidine: two layered ONIOM calculations. *J. Phys. Chem. A* **105**, 6926B6931, 2001.
- Remko, M., Walsh, O.A. and Richards, W.G. Ab initio and DFT study of molecular structure and tautomerism of 2-amino-2-imidazoline, 2-amino-2-oxazoline and 2-amino-2-thiazoline. *Chem. Phys. Letters* **336**, 156B162, 2001.
- Topf, M., Várnai, P. and Richards, W.G. Quantum mechanical/molecular mechanical study of three stationary points along the deacylation step of the catalytic mechanism of elastase. *Theor. Chem. Acc.* **106**, 146B151, 2001.
- Varnai, P. and Richards, W.G. A density functional study of the interconversion of carbonyls and alcohols in solution: comparison of reaction mechanisms involving NADPH, histidine, and tyrosine. *Int. J. Quantum Chem.* **84**, 276B281, 2001.

J.P. Simons

- Butz, P., Kroemer, R.T., Macleod, N.A., Robertson, E.G. and Simons, J.P. Conformational preferences of neurotransmitters: norephedrine and the adrenaline analogue, 2-methylamino 1-phenyl ethanol. *J. Phys. Chem. A* **105**, 1050B1056, 2001.
- Butz, P., Kroemer, R.T. Macleod, N.A. and Simons, J.P. Conformational preferences of neurotransmitters: ephedrine and its diastereoisomer, pseudo-ephedrine. *J. Phys. Chem. A* **105**, 544B551, 2001.
- Hockridge, M.R., Robertson, E.G., Simons, J.P., Borst, D.R., Korter, T.M. and Pratt, D.W. The $S_1 \rightleftharpoons S_0$ electronic transitions of 4- and 5-phenyl imidazole in the gas phase. *Chem. Phys. Letts.* **334**, 31B38, 2001.
- Mons, M., Dimicoli, I., Tardivel, B., Piuze, F., Robertson, E.G. and Simons, J.P. Energetics of the gas phase hydrates of *trans*-formanilide: a microscopic approach to the hydration sites of the peptide bond. *J. Phys. Chem. A* **105**, 969B973, 2001.
- Robertson, E.G., Hockridge, M.R., Jelfs, P.D. and Simons, J.P. IRBUV ion-dip spectroscopy of *N*-benzylformamide clusters: stepwise hydration of a model peptide. *J. Phys. Chem. A* **104**, 11714B11724, 2000.
- Robertson, E.G., Hockridge, M.R., Jelfs, P.D. and Simons, J.P. IRBUV ion-depletion and fluorescence spectroscopy of 2-phenylacetamide clusters: hydration of a primary amide. *Phys. Chem. Chem. Phys.* **3**, 786B795, 2001.
- Robertson, E.G. and Simons, J.P. Getting into shape: conformational and supramolecular landscapes in small biomolecules and their hydrated clusters. (Invited Article) *Phys. Chem. Chem. Phys.* **3**, 1B18, 2001.
- Robertson, E.G. Snoek, L.C., Simons, J.P. and Mons, M. Structural landscapes in hydrogen-bonded biomolecular clusters: resonant ion-dip spectroscopy. Central Laser Facility, Rutherford Appleton Laboratory Annual Report, 1999/2000, pp.124B128.
- Snoek, L.C., Kroemer, R.T., Hockridge, M.R. and Simons, J.P. Conformational landscapes of aromatic amino acids in the gas phase: Infrared and ultraviolet ion dip spectroscopy of tryptophan. *Phys. Chem. Chem. Phys.* **3**, 1819B1826, 2001.

T.P. Softley

- Dickinson, H., Chelmick, T. and Softley, T.P. $(2 + \infty)$ mass analyzed threshold ionization (MATI) spectroscopy of the CD_3 radical. *Chem. Phys. Letts.* **338**, 37B45, 2001.
- Dickinson, H., Mackenzie, S.R. and Softley, T.P. $(2 + 1)$ Resonance-enhanced multiphoton ionization (REMPI) and $(2 + \infty)$ mass-analyzed threshold ionization (MATI) spectroscopy of H_2O . *Phys. Chem. Chem. Phys.* **2**, 4669B4675, 2000.
- Dickinson, H., Rolland, D. and Softley, T.P. Multichannel quantum defect theory (MQDT) analysis of the $(2 + \infty)$ mass analyzed threshold ionization (MATI) spectroscopy of NH_3 . *J. Phys. Chem. A* **105**, 5590B5600, 2001.
- Monti, O.L.A., Cruse, H.A., Softley, T.P. and Mackenzie, S.R. High resolution photoionisation spectroscopy of vibrationally excited $ArCNO$. *Chem. Phys. Letts.* **333**, 146B152, 2001.
- Procter, S.R., Webb, M.J. and Softley, T.P. The dynamics of high Rydberg states in the presence of time-dependent inhomogeneous fields. *Faraday Discuss.* **115**, 277B294, 2000.

Townsend, D., Goodgame, A.L., Procter, S.R., Mackenzie, S.R. and Softley, T.P. Deflection of krypton Rydberg atoms in the field of an electric dipole. *J. Phys. B: At. Mol. Opt. Phys.* **34**, 439B450, 2001.

R.K. Thomas

- Bai, G.Y., Wang, J.B., Yan, H.K. and Thomas, R.K. Enthalpies of micellization of double chain and gemini cationic surfactants. *J. Coll. Int. Sci.* **240**, 375B377, 2001.
- Bai, G.Y., Wang, J.B., Yan, H.K. and Thomas, R.K. Thermodynamics of molecular self-assembly of cationic gemini and related double chain surfactants in aqueous solution. *J. Phys. Chem. B* **105**, 3105B3108, 2001.
- Bai, G.Y., Yan, H.K. and Thomas, R.K. Microcalorimetric studies on the thermodynamic properties of cationic gemini surfactants. *Langmuir* **17**, 4501B4504, 2001.
- Ederth, T. Computation of Lifshitz-van der Waals forces between alkylthiol monolayers on gold films. *Langmuir* **17**, 3329B3340, 2001.
- Fragneto, G., Su, T.J., Lu, J.R., Thomas, R.K. and Rennie, A.R. Adsorption of proteins from aqueous solutions on hydrophobic surfaces studied by neutron reflection. *Phys. Chem. Chem. Phys.* **2**, 5214B5221, 2000.
- Li, Z.X., Lu, J.R., Thomas, R.K., Weller, A., Penfold, J., Webster, J.R.P., Sivia, D.S. and Rennie, A.R. Conformal roughness in the adsorbed lamellar phase of Aerosol-OT at the air/water and liquid/solid interfaces. *Langmuir* **17**, 5858B5964, 2001.
- Nylander, T., Tiberg, F., Su, T.J., Lu, J.R. and Thomas, R.K. Beta-casein adsorption at the hydrophobized silicon oxide-aqueous solution interface and the effect of added electrolyte. *Biomacromolecules* **2**, 278B287, 2001.
- Penfold, J., Staples, E.J., Tucker, I. and Thomas, R.K. Adsorption of mixed cationic and nonionic surfactants at the hydrophilic silicon surface from aqueous solution: The effect of solution composition and concentration. *Langmuir* **16**, 8879B8883, 2000.

R.P. Wayne

- Andino, J.M., Wallington, T.J., Hurley, M.D. and Wayne, R.P. A classroom demonstration of the formation of aerosols from biogenic hydrocarbons. *J. Chem. Ed.* **77**, 1584B1586, 2000.
- Canosa-Mas, C.E., Dillon, T.J., Sidebottom, H., Thompson, K.C. and Wayne, R.P. A study of the OH-initiated oxidation of chlorinated ethenes in the gas phase. *Phys. Chem. Chem. Phys.* **3**, 542B550, 2001.
- Cotter, E.S.N., Booth, N.J., Canosa-Mas, C.E., Gray, D.J., Shallcross, D.E. and Wayne, R.P. Reactions of Cl atoms with CH₃I, C₂H₅I, 1-C₃H₇I, 2-C₃H₇I and CF₃I: kinetics and atmospheric relevance. *Phys. Chem. Chem. Phys.* **3**, 402B408, 2001.
- Cotter, E.S.N., Booth, N.J., Canosa-Mas, C.E. and Wayne, R.P. Release of iodine in the atmospheric oxidation of alkyl iodides and the fates of iodinated alkoxy radicals. *Atmos. Environ.* **35**, 2169B2178, 2001.
- King, M.D., Canosa-Mas, C.E. and Wayne, R.P. Gas-phase reactions between RO₂ and NO, HO₂ or CH₃O₂: correlations between rate constants and the SOMO energy of the peroxy (RO₂) radical. *Atmos. Environ.* **35**, 2081B2088, 2001.

S.L. Wilsey

Wilsey, S. A computational study of the factors controlling triplet-state reactivity in 1,4-pentadiene. *J. Org. Chem.* **65**, 7878B7888, 2000.

M. Wilson

Walsh, T.R., Wilson, M. and Sutton, A.P. Hydrolysis of the amorphous silica surface. II. Calculation of activation barriers and mechanisms. *J. Chem. Phys.* **113**, 9191B9201, 2000.

Wilson, M. and Walsh, T.R. Hydrolysis of the amorphous silica surface. I. Structure and dynamics of the dry surface. *J. Chem. Phys.* **113**, 9180B9190, 2000.