

# **REPORT OF THE HEAD OF THE PHYSICAL AND THEORETICAL CHEMISTRY LABORATORY FOR THE YEAR ENDED 31<sup>ST</sup> JULY 2006**

As is thankfully (and deservedly) the norm for the PTCL, we have many honours and distinctions to note for the past year. First amongst these comes the election of John Eland as a Fellow of the Royal Society, distinguished for his “seminal conceptual, instrumental and methodological contributions to the study of molecular ionization by photon and electron impact.” A splendid dinner in Corpus was attended by academic and support staff to celebrate John’s achievements and to honour the contribution made to them by the technical expertise which has for long been a feature of the Department. The PTCL continues to feature well in the current lists of Oxford Chemistry academic and emeritus staff with FRSSs. We congratulate Mark Brouard on his promotion from Reader to Professor in the Recognition of Distinction exercise here in Oxford, and, further from home, Honorary Professorships were conferred upon Dr Bob Thomas by the China Petroleum University and Professor Peter Atkins by Mendeleev University, Moscow. Professor Atkins was also elected as Foreign Member of the Accademia delle Scienze dell’Istituto di Bologna. Professor David Clary was elected President of the Faraday Division of the Royal Society of Chemistry, and has started his Presidency by arranging a star studded meeting of RSC prize winners to be held in the PTCL in early January 2007. Professor David Logan was elected as the Tilden Lecturer of the RSC, and will follow in the footsteps of Professor Richard Compton who delivered the 2005/6 Tilden series. Professor Compton was also awarded the Breyer Medal of the Royal Australian Chemical Institute. Professor Mark Child was appointed to the Boys Rahman lectureship of the RSC, and Professor John Brown was awarded the Sir David Bates prize of the Institute of Physics.

This has been a year of considerable change in the PTCL. Two of our distinguished and long serving colleagues, Professors John Eland and Richard Wayne, both retired at the end of the 2006 academic year, having spent the vast majority of their academic careers in the PTCL. Both are internationally recognised figures in gas phase photochemistry, kinetics and dynamics. Both have given unhesitatingly of their time and abilities to help to make this Department flourish, and to continue to be the success that has marked it out for many years, and both will both be hard acts to follow. We wish them both happiness in their official “retirements”, and know that they will always be welcome back in the Department. Another change is that Professor Jacob Klein came to the end of his five year appointment as Head of Department, and I take this opportunity of thanking him for the positive things that he has done for us over the past years.

The year has been an exciting one for new appointments. As reported last year, Professor David Logan was elected as the Coulson Professor of Theoretical Chemistry, and took up his post in October 2005. Two newly elected Lecturers, Drs Claire Vallance and Mark Wallace have joined the PTCL, and four new appointments were announced during the year. In the theoretical group, Drs William Barford and Jonathan Doye, from Sheffield and Cambridge respectively, will become tutors at Balliol and Queen's. Dr Grant Ritchie, a Royal Society University Research Fellow in the PTCL, becomes Lecturer and Tutor at Worcester, and Dr Dirk Aarts, presently a Marie Curie Fellow at l'Ecole Normale Supérieure in Paris, but formerly from Utrecht University, will become Lecturer and Student of Christ Church in early 2007. Longevity of service is something that is a feature of the PTCL. Richard Wayne retired after 41 years, Roger Bowler and Charlie Jones from the Mechanical Workshop are still going extremely strongly, and have reached 45 and 40 years respectively, and in a slightly different vein we celebrated John Rowlinson's 80<sup>th</sup> birthday with a dinner in Trinity, where we were joined by several retirees from the Rowlinson age, all in very good form. We note also the importance of "value added" indicators by the PTCL for our young members of the Department. Dr Chris Skylaris was appointed to a lectureship in Southampton, Dr Dmitri Shalashilin to a lectureship in Leeds and Dr Craig Banks to a lectureship in Nottingham Trent University. Further afield, Dr Rebecca Jockusch was appointed to an Assistant Professorship in the University of Toronto, and Dr Pierre Çarçabal to a CNRS Researcher position at the Université Paris-sud. Two of our members were elected to Junior Research Fellowships, Gregory Wildgoose at St John's and Martin Galpin at Worcester. Magnetic resonance featured in two young scientists' awards: Janet Banham, working with Chris Timmel, received the JEOL prize of the Royal Society of Chemistry ESR group, and Lars Kuhn, from Peter Hore's group, was awarded the Magnetic Resonance in Chemistry Award for Young Scientists, donated by John Wiley and Sons. We congratulate them all.

The PTCL hosts numerous seminars throughout the term as well as conferences and specialised symposia. Our Hinshelwood lectures this year were given by Professor Rich Saykally from the University of California, Berkeley, on the theme "Water Music – Some New Notes in a Favourite Composition". The lectures ranged from Rich's original interests in spectroscopy as applied to gas phase water clusters, to measurements using both X Rays and non-linear spectroscopies of structures of ions at water interfaces. The lectures were a true tour de force: those who know Rich also appreciated the understated dress style and musical taste which accompanied them. Our Hinshelwood Lecturer for next year will be Professor Michele Parrinello from the ETH in Lugano. We also hosted several meetings over the year. At the 9<sup>th</sup> International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena in September 2005, the final session was a Symposium in honour of Professor Keith McLauchlan, where he was awarded a Fellowship of the International EPR (ESR) Society. In the same month the 5<sup>th</sup> Cavity Ring Down User

Meeting, and a Young Materials Modellers' Forum were held in the PTCL. The Department hosted the Bourke Lecture of the Royal Society of Chemistry, given by Professor Marsha Lester of the University of Pennsylvania. Events aimed at school students took place throughout the year, organized with customary enthusiasm by Hugh Cartwright. These included the Science Open Days (600 attendees over two days), the Science Information Day, the Sutton Trust Summer School, a Salters Company Challenge, and four *Hands on Science* events, which attracted 700 school students. One of the latter programmes was webcast live to schools who could not attend. Members of the Department are often audibly reminded of Hugh's lecture demonstrations, and we owe him a debt of gratitude for continuing to bring Oxford Chemistry to the attention of potential applicants.

Our visitors included Dr Elaine Marzluff (Grinnell College), Prof. Martin Goetz (Halle), Professor Javier Aoiz (Madrid), Prof. Andrew Cooksy (San Diego State), Prof. Minal Sanyal, Prof. Ian Beattie (Southampton), Dr Reider Lund (Forschungszentrum Jülich), Professor Jose Gonzalez (Alicante University), Prof. John Tully (Yale), Prof. David Nesbitt (University of Colorado, Boulder), Professor Nikita N. Lukzen and Dr Konstantin Ivanov (International Tomography Center, Novosibirsk), Prof. P. Majumdar, (Harish-Chandra Research Institute, Allahabad), Prof. A. Raychaudhuri (S N Bose National Center for Basic Science, India), Professor Peter J. Rossky (University of Texas at Austin) and Professor Bastiaan J. Braams (Emory University, Atlanta, Georgia).

In past issues of the Report we have commented on the Journals edited from the Department. Here we mention three special editions, produced in honour of members of the PTCL. An edition of Molecular Physics was published in July 2005 to honour Professor John Simons' contribution to Photochemistry and Reaction Dynamics, in November 2005 the same journal published an issue on Spin Chemistry to honour Professor Keith McLauchlan's contribution to the subject, and the Journal of Photochemistry and Photobiology published a special edition in December 2005 to honour Professor Richard Wayne's contribution to Atmospheric Chemistry. Other members of the Department contributed articles to all these *festschriften*.

The Department's finances continue to be reasonably buoyant in turbulent times for funding; grant income continues to rise, and it looks as if the introduction of Full Economic Costing will have a beneficial effect on the department in the coming years. As always the Departmental Head's job is made easy by dedicated staff and collaborative colleagues, and I am grateful to all those who have made my transition to the HoD office a smooth and straightforward one.

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