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David Parker Craig 1919–2015*

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David Craig was an outstanding Australian theoretical chemist whose academic life oscillated between Australia (University of Sydney and Australian National University (ANU)) and the UK (University College London). The Craig Building of the Research School of Chemistry of the ANU was named in his honour in 1995. He was President of the Australian Academy of Science from 1990 to 1994, and the Academy's David Craig Medal, which recognizes outstanding contributions to chemistry research, was inaugurated in his honour. His best-known research is in the fields of quantum theory and spectroscopy of aromatic molecules, molecular crystals, quantum electrodynamics and chirality.

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Family Background

David Parker Craig was born in Sydney, Australia, on 23 December 1919. His father, Andrew Hunter Craig, was born in Nottingham in England in 1886, and emigrated to Australia in 1911 seeking a warmer climate. He was a successful chartered accountant. David's mother, Mary Jane Craig (née Parker), was born in Carlisle, England, in 1887, and emigrated to Australia in 1915. Andrew and Mary married in New Norfolk, Tasmania, in 1915. David was their only son.

David Craig married Veronica (Ronia) Bryden-Brown on 25 August 1948, in Caversham, England. Ronia was the daughter of Cyril Bryden-Brown, who had emigrated from Market Harborough, England, after World War 1 and Kathleen Bryden-Brown

(née Parkinson), who was born in Cooma, New South Wales (Australia). David and Ronia had four children, Andrew (born 1949), Hugh (born 1952), Mary Louise (born 1955) and Douglas (born 1961) (see Fig. 1).

Early Education

David was a pupil at the Knox Grammar School on the North Shore of Sydney (1927–31), and went on to the Sydney Church of England Grammar School in North Sydney (1931–6). He had good memories of the teaching there—the headmaster, a stern ex-World War 1 brigade-major, was also a very good mathematics teacher, and his chemistry and physics masters were also outstanding. The latter, surprisingly, had some knowledge of Linus Pauling's 'resonance' theory of chemical bonding, which was very new at the time. It was a fortunate start to a life in science. David enrolled at the University of Sydney in 1937 with a university exhibition, which paid the tuition fees, studying mathematics, physics and chemistry, and graduating with a BSc with first class honours in 1940. His chemistry honours research project, which was supervised by D. P. Mellor (who had recently returned from an inspiring year with Linus Pauling at CalTech), concerned the magnetochemistry of transition



metal complexes, and this resulted in several publications. During this period, David also had close contact with another chemistry lecturer, Allan Maccoll, which began a life-long personal and scientific association.

World War 2

Having completed his honours degree in 1940, and worked on an MSc into early 1941, David sought to join the part of the Services where his scientific training might be of value, specifically the submarine detection service. However, he failed the colour blindness test and joined the Australian Imperial Force (AIF) instead.

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Figure 1. Craig family portrait (2011). From left to right: Douglas, Veronica (Ronia), Mary Louise Chalmers, David, Andrew and Hugh.



Figure 2. Taken at Ivanhoe Grammar School in Victoria (1942), showing (left to right) Lt-Gen. Iven Mackay, Lt (later Capt.) D. P. Craig and Sgt Eric Codling.

He served as aide-de-camp (ADC) to Lieutenant-General Sir Iven Mackay, which took him to Darwin (immediately after the first Japanese bombing raid) and then to New Guinea, where he saw active service (see Fig. 2). Mackay was a citizen soldier, who in civilian life was a physicist. He gave David his copy of a celebrated biography of James Clerk Maxwell, who had produced a unified theory of electromagnetism.¹ He later introduced him to JA Stratton, who was on a scientific mission, and whose 1941 book on Maxwell's theory,² was a welcome model of clarity on a subject that was to greatly concern David in his future spectroscopic work.

As part of his war service, David was later redeployed to the University of Sydney, working with Adrien Albert, the pioneer



Figure 3. David (on the left) at the University of Sydney with Allan Maccoll, Charles Fawcett, Tom Iredale and David Mellor (ca 1944) (from A. Maccoll, 'Australian Chemists at University College London 1899–1988', *Ambix*, 26 (1989), 82–90.

of chemotherapy, who was successfully designing bacteriostatic agents, particularly aminoacridines, which were desperately needed in the Pacific war zone.³ Owing to the large number of ex-soldiers who had elected to go to university, help was needed with the large classes that ensued (to maintain order as well as to instruct), and David was appointed as a lecturer in Chemistry at the University of Sydney in 1944 (see Fig. 3).

University College London, 1946-52

The long-established tradition of Australian graduates going to England for postgraduate work was not resumed until late 1945. At the end of World War 2, David took this path. He was offered fellowships at both Liverpool University and University College London (UCL). He was more attracted by the London offer, where Professor (later Sir) Christopher Ingold had established a very highly regarded department specializing in physical chemistry and chemical physics. He accepted the UCL fellowship in the middle of 1946, arriving in London in October that year. London itself was in a sorry state after the wartime bombing, and UCL had suffered because of its proximity to the King's Cross railway hub. The chemistry laboratories were relatively undamaged but were out of date and short of equipment. However, the standard and quality of work in them was very high and there was intense activity in research. The Department of Chemistry took in 40 undergraduate students each year and, over time, grew to have a standing population of research students of 400. Its reputation at the time was high, and almost every scientific visitor to the UK from Europe or from the USA would call in to give a seminar or to have discussions. It was a period of extraordinary stimulation. After support for two years by the Fellowship (which paid quite well for the time, at £600 per annum), David was appointed to the teaching staff as a lecturer. He was obviously regarded as showing great promise.

On starting at UCL, David registered for a PhD, listing Ingold as his supervisor. In practice, Ingold allowed David to formulate his own research plans. Before leaving Sydney, David had begun theoretical work on the quantum mechanical calculation of the electronic structures and spectra of small aromatic molecules, with the aim of achieving this without making empirical assumptions. This, in fact,



Figure 4. Aromatic hydrocarbons, which figured prominently in David's research, are planar molecules consisting of fused sixmembered rings of carbon atoms, each with an attached hydrogen. In the sequence benzene (B), naphthalene (N) and anthracene (A), the rings are arranged in a linear fashion. The carbon atoms have four valence electrons, three of which are employed to form bonds to the adjacent atoms at each vertex. The fourth electron, called a π -electron, is not bound to a particular nucleus but is delocalized over the whole framework. This confers unusual stability and also gives rise to many excited electronic states. As a result, these hydrocarbons have a rich electronic spectroscopy, which theoreticians have striven from early days to understand.

was to be the unifying theme of his life's work. After beginning with the molecule anthracene, which he soon realized was too large to be tackled without much better computational facilities, he continued with the study of the benzene molecule, the simplest and most symmetric aromatic species.

David's work with aromatic hydrocarbon molecules, such as those in Figure 4, remained a continuing interest. He was intrigued by the question of what the defining property of 'aromatic' structures was. The German chemist Ernst Hückel had advanced 'Hückel's Rules', the simplest of which stated that only molecules with $4n \downarrow \pi$ -electrons (the 'magic numbers') were aromatic. It is easily verified that molecules such as those in Figure 4 satisfy this criterion. David proposed modified rules, which were briefly known as 'Craig's Rules',⁴ but exceptions were soon found. Some of the work was carried out jointly with Allan Maccoll, his colleague from earlier days in Sydney, also later at UCL.⁵ They enjoyed a fruitful collaboration over several years until Maccoll's interests diverged into gas-phase kinetics and mass spectrometry, while David's interests remained in the theory of molecular structure and, increasingly, in experimental spectroscopy (see Fig. 5).⁶



Figure 5. David with colleagues (ca 1950). From left to right: David, Allan Maccoll, Angelo Mangini (Bologna) and Christopher Ingold.

David continued to work within the molecular orbital approach, improving the quality of calculations of individual energy levels. He came to realize, however, that there was a serious shortcoming in the molecular calculations to date. This was associated with the fact that when there were configurational energy levels of the same symmetry and of comparable energy, there would be a coupling between them, which, although well known in atomic calculations, was not being taken into account in the molecular calculations. Indeed, the interconfigurational coupling energy frequently greatly exceeded the difference in energy between the two configurations. In 1950, David published a seminal paper 'Configuration interaction in molecular orbital theory'.⁷ The inclusion of configuration interaction (CI) marked an important milestone in ongoing work on molecular orbital calculations.

Interestingly, when David presented a seminar on his benzene work at King's College London, the academic home of Charles Coulson, a leading British theoretical chemist at the time, he learned that Coulson and his student Inga Fischer-Hjalmars were using a similar approach for molecular hydrogen. In the event, the two pieces of work were published at about the same time. During the same period, David published a series of important papers demonstrating the relationship of the molecular orbital/CI approach on the one hand and the valence-bond approach on the other, through the inclusion of polar structures.⁸

The molecular orbital calculations for benzene involved evaluation of a very large number of electron-interaction integrals, which was time-consuming and also had to be carefully checked. Robert Parr, a former student of Robert Mulliken, then at the Carnegie Institute of Technology in the USA and working in this field, suggested that David collaborate with him in the computations. David agreed and they did so, together with Ian Ross, David's close friend from Sydney who was now working with him at UCL as a PhD student. In the ensuing paper (famous as 'Craig, Parr and Ross'),⁹ they estimated the values of three- and four-centre integrals and recalculated the energy levels of benzene, achieving improved agreement with experiment. Also in this paper, the term *ab initio* was coined to describe calculations that did not use any experimental information; its use has subsequently become widespread.

These considerations applied to electronic wave functions. However, molecular electronic transitions are accompanied essentially simultaneously by excitation to vibrational energy levels of the excited state. The experimental results of Ingold for the 2600 Å band system of benzene (obtained under very difficult conditions during the war years) showed a dense forest of lines. Vibrational wave functions needed to be introduced in order to interpret the electronic–vibrational (vibronic) spectra.

While weak observed spectral lines had been qualitatively interpreted for 20 years in terms of the Herzberg-Teller principle,¹⁰ and its associated symmetry selection rules, David performed the first quantitative calculations, considering the role of symmetric E_a^+ vibrations in the 2600 Å band system of benzene.¹¹ David realized that these weak transitions embodied a breakdown of the Born-Oppenheimer approximation (underlying the Franck-Condon principle), according to which one can express an electronic-vibrational wave function as a simple product of individual electronic and vibrational functions. In modern language, this results in entanglement of electronic and vibrational wave functions. Entanglement is a profound quantum mechanical property, and David's insight underlies a great deal of modern research in molecular spectroscopy and chemical bonding theory, as well as materials science, for example, solar energy harvesting. This was a topic to which David returned much later, in influential work with G. J. Small.12

As a major research centre in one of the world's main travel hubs, UCL's Department of Chemistry had many visitors. One exceptional visitor was the Hungarian physicist Edward Teller, who, after leaving Europe in the period just before World War 2, had been a visiting



Figure 6. David Craig (front centre) and the other chemistry professors (front row) in the old chemistry building at the University of Sydney in 1955. On David's right is Raymond Le Fèvre; on his left is Arthur Birch.

scientist in the department. He had been offered a place in the laboratories by Ingold and had worked there for a year or two, publishing two highly important papers on the Jahn–Teller effect. David talked to Teller during one of his visits about his paper on the role of perturbing vibrations in benzene spectra,¹³ which was close to Teller's own interests. Teller suggested that David should come and work with him in Chicago, but David remained in London. However, he continued to have extensive discussions with Teller during his visits, and was deeply impressed on every occasion by his extraordinary physical insight and ability to grasp problems quickly. No doubt these talents contributed later to the design of the thermonuclear hydrogen bomb, of which Teller is colloquially known as 'the father'.

David's interaction with Charles Coulson remained close and friendly over many years, until Coulson's untimely death in 1974. His group, then at King's College, and later in Oxford, included many theoreticians who later became well known, such as William Moffitt, Christopher Longuet-Higgins, Roy McWeeny and, occasionally, visiting French workers from the Paris groups of Raymond Daudel and Bernard Pullman. Coulson had a weekly seminar, which David regularly attended, as did Alan Maccoll. The trio published some work conjointly, especially on the theory of small aromatic-type molecules.¹⁴

David's first London period ended in 1952, when he accepted an invitation to return to the University of Sydney as Professor of Physical Chemistry, at the remarkably young age of 31—a welldeserved recognition of his achievements and promise.

University of Sydney, 1952-6

On returning to Sydney in 1952, David joined Professor A. J. Birch, an Australian organic chemist, who had been appointed at about the same time from Oxford. They began a partnership that lasted throughout the whole of their working lives, first in Sydney, then with a short break when Birch went to Manchester and David to London, and finally resuming in 1967, when they together established the Research School of Chemistry of the Australian National University. In Sydney, chemistry was in the process of being reorganized into three departments, headed by Raymond Le Fèvre (who had already arrived), Arthur Birch and David, as Heads of Inorganic, Organic and Physical Chemistry, respectively (see Figs. 6 and 7).

Equipment was in short supply in Sydney, but David started some experimental spectroscopy with a large quartz Hilger spectrograph, and he also continued theoretical work. On the spectroscopic side, he began with the molecule naphthalene in the gas phase, together with M. F. Redies, an MSc student. This laid the foundation for work that later resumed in London on a much more powerful spectrograph, which resulted in the first analysis of the weak naphthalene system at 320 nm,¹⁵ and was also the precursor of studies on the crystal spectrum of this molecule.¹⁶ On the theoretical side, particularly with J. R. Walsh and E. A. Magnusson, David turned to the calculation of the spectra of molecular crystals,¹⁷ and to some ideas on valence theory, focusing on the new concept of 'orbital contraction'.¹⁸ Both efforts led to significant theoretical developments in the hands of many people, particularly in the theory of



Figure 7. Board of Directors of Sydney University Union 1954-5, including David (centre, front row), with Ian Ross on his left.

excitons on the spectroscopic side,¹⁹ and in the valence theory of elements of the second and later rows of the periodic table.²⁰

University College London, 1956-67

In late 1955, David had an invitation from Christopher Ingold in London to re-join the Department of Chemistry at University College London as the first Professor of Chemistry with special reference to Theoretical Chemistry-a signal honour. He accepted, and set out for England in 1956 with his family, by cargo boat with its tiny complement of passengers. They travelled around the north of Australia towards the Suez Canal but, on receiving word that war had broken out in precisely that area, made a U-turn towards the Cape of Good Hope. After an eight-week journey, David was back in London, in time to start work at the beginning of the university session in October. The laboratories were in much better shape than they had been ten years earlier, but they were still somewhat oldfashioned and spread out. A good deal of refurbishing had been done, particularly of the undergraduate laboratories, and the department was now very well equipped. Moreover, the quality of entering students was high, and the graduate students, drawn not only from the College but also from other UK institutions and from abroad, were excellent. David had a research group usually numbering about six individuals, including graduate students and postdocs, for the whole of this second period at UCL.

At this point, David's work entered into a quite new direction, which was to dominate his subsequent spectral investigations. In order to determine the polarization directions of transitions involving excited states, it was necessary to work in a crystal rather than a gaseous environment. This required new experimental techniques. Measurements with P.C. Hobbins of the polarized ultraviolet spectrum of anthracene crystal yielded the information that the second major absorption lay in the molecular plane and was directed along the major axis, in agreement with molecular orbital theory.²¹ Measurement at liquid hydrogen temperature showed improved resolution, adding further weight to the transition moment assignments. Apart from a low-resolution Russian study fourteen years earlier, these were the first detailed measurements of aromatic molecular properties in the crystal state.

But a new feature emerged: splitting of absorption lines was observed as a result of interaction between the excited states of adjoining molecules. This was the start of a line of experimental and theoretical research in David's group that continued for many years. The Soviet physicist A. S. Davydov had shown in 1948 that in a crystal there was electrostatic coupling of transition moments so that one had to consider not simply individual molecular states but combinations of them.²² These were excitons (which, in the pure crystal, associate to form waves) and Davydov's work had laid the foundation for analysis of their structures, which resulted from the particular symmetry of the environment and of the quantum mechanism of the particular excited-state coupling. Extension of these ideas became a major focus of the work of David and his group. He later met and exchanged ideas with Davydov, both in Moscow on a visit to the Soviet Union and in London.

By a very fortunate coincidence, one of David's colleagues, E. A. Power (later head of the Department of Mathematics), was at the time working on the theory of propagation of excitation within crystals. His primary interest had been in the spectroscopic properties of molecular crystals and in the origin of the splitting of levels that is produced when free 'guest' molecules are embedded in the pure 'host' crystal. He came to the conclusion that it was necessary to replace the semi-classical method, in which electrons are treated quantum mechanically but radiation is treated classically, with a more general theory for molecular systems. This was molecular quantum electrodynamics (QED).²³

The central theme of QED is that there is a closed system of particles and fields that act on one another, the particles associated with the radiation field being photons. The states of the entire system can be dealt with in a rigorous quantum mechanical way, and its properties, including rates of transition in which the number of particles changes, can be handled as accurately as is desired. David formed a close working relationship with Power, which later included his former student T. Thirunamachandran ('Thiru'), applying QED theory to a range of chemical phenomena. This generalized and massively extended the scope of his previous work.²⁴

Throughout the second period at UCL, David and his research group, many of whom later proceeded to distinguished academic careers, continued to explore the nature of excited molecular states by single- and mixed-crystal low-temperature spectroscopy, with increasingly sophisticated theory and occasional fruitful forays into the inorganic structural area. During the period 1952-67, there was concurrent activity in the experimental chemistry and photochemistry of the organic solid state to go along with the theoretical developments. Topochemistry was accepted as the method for the photochemical formation of dimers in a molecular crystal in which the dimer was generally preformed by arrangement of monomers in the perfect lattice.²⁵ In addition, it was known that photodimerization of anthracene began at surface dislocations. There was a need for study of the connections between disordered lattice packing and the course of photochemical change, including migration to traps in the energy surface due to photon absorption.

A new feature of scientific life, which had been lacking during David's earlier time in London, was the ability to travel relatively easily overseas, with the support not only of home institutions, such as UCL, but also of US agencies, such as the Office of Naval Research, the Office of Army Research and the US Air Force, to all of whom at various times David was contracted for specific research tasks. These offices provided funds that were mainly, though not exclusively, for travel to the USA, though visits to Europe were also supported. During the same period, David was invited by the British Council to undertake four-week lecture tours in the USSR (1958) (see Fig. 8) and in Czechoslovakia (1964). Scientific trips to the Iron Curtain countries were not a novelty at that time, although they were fraught with bureaucratic overregulation. University College London took a relaxed view of absences, accepting the idea that visits abroad for the purpose of speaking about research in the College were a necessary part of the duties of a professor. The provost of the College, Sir Ifor Evans, told David on one occasion that, while the College had no formal arrangements for study leave, he expected his professors to be in the College two terms out of three! David recalled that lecture loads were light, with thirty a year on average.



Figure 8. David (ca 1958) preparing for his forthcoming trip to the USSR.

There was a vigorous research programme in Inorganic Chemistry at UCL during the times that David was there (the dominant figure being another Australian Sir Ronald Nyholm), and he interacted with several of the researchers, as well as with some colleagues outside UCL, on theoretical aspects of bonding in inorganic molecules and complexes.²⁶ In particular, two 1954 papers with A. Maccoll, R. S. Nyholm, L. E. Orgel and L. E. Sutton,²⁷ which discussed chemical bonds involving d-orbitals, showing how they overlap with π -orbitals, attracted considerable attention.²⁸

Australian National University, 1967-85

David Craig's final academic move was in response to an ambitious initiative of the Australian National University (ANU). Founded in 1946 to provide an Australian centre of research excellence, the ANU was rapidly becoming recognized internationally as such. The Government and the ANU now wanted to create a school for research in chemistry, which would also be of a sufficiently high standard that it could attract back some of the cohort of promising scientists who had left Australia to work in the USA or in Britain.

The essential first step in this endeavour was to persuade three highly eminent expatriates to return to lead such a school. The ANU targeted Arthur Birch from the University of Manchester as the organic chemist, David as the physical chemist and Ronald Nyholm (also from UCL) as the inorganic chemist. For the purpose of designing the new chemistry building, the University sent an architect and an architect's draftsman to London. There were clandestine meetings in Brown's Hotel, Half Moon Street, between the three 'advisers' to the project and the architect and his draftsman, to discuss the details of what was required. After about six weeks, they had achieved agreed working drawings and, following some hold-ups, the project came to fruition. The result was an excellent and impressive building with many innovations, one unusual and valuable one being the absence of internal walls, which facilitated adaptation of space



Figure 9. Arthur Birch, David, and Ray Martin in David's office in the Research School of Chemistry, ANU (ca 1972).

for new purposes. Unfortunately, Nyholm did not take up the Inorganic chair, but David and Arthur Birch were soon in residence. Ray Martin was subsequently appointed as Professor of Inorganic Chemistry in 1970. The new Research School of Chemistry flourished, and became a major focus for Australian chemistry (see Figs. 9 and 10).

David quickly established an energetic research group. He continued to focus on the exploration of the nature of ground and excited states of molecules, usually in the crystal state, both experimentally and theoretically, in collaboration with many co-workers. An authoritative review of exciton theory was provided in his 1968 book with S. H. Walmsley.²⁹ Basic QED theory continued to be explored, including in collaboration with E. A. Power on the Casimir–Polder potential,³⁰ and in studies of the retarded potential with P. D. Dacre and L. A. Dissado.³¹ David also continued his research on aromatic molecules and on so-called pseudo-aromatic molecules.³²

Chirality now became a strong focus of David's interest. This was a major extension of his fundamental QED work. The basic question of the nature of external or internal fields that could induce chiral discrimination, i.e. a difference in the energy of interaction of the *dextro* and *laevo* forms of a chiral molecule when they interact with a second chiral system, had been brought to his attention very early in Sydney by his undergraduate research supervisor, D. P. Mellor, with reference to this phenomenon in transition metal complexes. David asked how a molecule with an achiral group could have its symmetry lowered to that of a chiral group (e.g. D_{2d} to D_2), and realized that this could result from linear coupling to a vibrational mode, i.e. via the Jahn–Teller effect. Predictions of such an effect were made in collaboration with P. J. Stiles and with a group in Bologna.³³ Intramolecular chiral discrimination was studied with L. Radom and P. J. Stiles.³⁴ Circular dichroism and chirality continued to be a focus of interest.³⁵ Thus, the experimental observations of Pasteur, of such immense importance to biology, at last began to yield their secrets.

The Craig Building at ANU was named in David's honour in 1995 (see Fig. 11). His last published scientific paper, in collaboration with T. Thirunamachandran, long after his formal retirement, is entitled 'New approaches to chiral discrimination in coupling between molecules'.³⁶

Comments on Computing

Paul Dirac famously remarked that the invention of quantum mechanics in principle reduced studies such as chemistry to applied physics, although, having made this statement before the advent of computers, he naturally doubted at the time whether it would be feasible in practice. The history of the progress of theoretical chemistry in fact parallels advances in computer technology. David remarked in a 1999 review that he found it intriguing that his career in theoretical chemical physics spanned the entire period of the development of computers up to the supercomputer level.³⁷ In Sydney in 1945, he relied on an extended slide rule in the form of a spiral on a cylinder some two inches in diameter and ten times the normal length, known as the Fuller Calculator. In the early days in London, they had handleturning calculators (Brunswiga), then electric calculating machines, of which examples were the Monroe, and later, as a step forward, the Marchant family of machines. A standard calculation for David was the diagonalization of a matrix of up to six rows and columns. On a Marchant calculator, a 6x6 diagonalization required a full day, possibly more, depending on whether errors had been made on the way through (sometimes revealed through identical calculations being carried out both in London and by collaborators in the USA).



Figure 10. Academic and senior technical staff of the Research School of Chemistry, ANU, including Arthur Birch and David in the front row, as well as members of the review committee for the organic section (John Swan and Ralph Raphael) (1979).



Figure 11. David at the opening of the Craig Building in 1995.

Historical Records of Australian Science

By 1952, when David moved back to Sydney, electronic computers began to be available, but he had no access, and again a mammoth task of computation for those days was undertaken by his student J. R. Walsh, who worked out lattice dipole sums for several simple molecular crystals in order to calculate and predict the exciton spectra for comparison with experiments. In the three years of his thesis work, Walsh spent most of his time on the computation of these quantities on an electric calculator. On a modern electronic computer, the entire task, including programming and production of the results, would probably be over in a few days. Moreover, once the program was written, it could be used for further computations taking less than a second in each case.

On returning to London in 1956, David found his situation transformed in that he had access to the Ferranti PEGASUS and then, soon after, to the MERCURY. Tasks that had previously seemed totally out of reach now became straightforward, although the job of programming these early machines was not trivial. At UCL, David became Chairman of the Computer Committee, and was involved in all the College's purchases of computer equipment, and then in the establishment of the University of London computing centre. UCL changed from UK-manufactured machines (after ATLAS) to US machines, the first being an IBM 360.

On joining the ANU in 1967, David became Chairman of the ANU Computer Committee, and had an important role in computer purchases and the establishment of the computer centre. Shortly after retirement, he became Chairman of the Time Allocation Committee of the newly purchased FUJITSU supercomputer, which in 1989 was ANU's most powerful machine. Even more spectacular advances have been made since then, with calculations to 'chemical accuracy' now being routine up to an increasing level of complexity. Had Dirac lived longer, what would his reaction have been to being proved both right and wrong?



Figure 12. David with Thiru (Canberra, ca 1976).

Elder Statesman Post-retirement

David formally retired from his position as Professor of Physical and Theoretical Chemistry in 1984, and became first an ANU University Fellow for a three-year term and then a Visiting Fellow in the Department of Chemistry, also returning on a regular basis to UCL, again as a Visiting Fellow. He continued to work, especially in collaboration with his former UCL colleague T. Thirunamachandran (see Fig. 12), on problems in quantum electrodynamics, with a particular interest in optical activity.

In 1968, David was elected to Fellowship of the Royal Society, and in the following year to Fellowship of the Australian Academy of Science. In 1985 he became Treasurer of the Academy, always a demanding role, but particularly so during David's tenure as a large donation (the Becker Bequest) had been made by a longtime supporter, but its receipt been delayed by legal challenges. These were subsequently resolved. After completing his term as Treasurer, David was elected as President of the Academy, a role he held with distinction from 1990 to 1994. A major achievement during this term was the setting-up of the Australian Foundation for Science, which provided the Academy with a firm base of funds for developing its resources. To honour David's outstanding contributions to chemical research, the Academy inaugurated the David Craig Medal in 2000. David was appointed Chairman of the Prime Minister's Science and Engineering Council, whose meetings were regularly attended by the Prime Minister of the day, Bob Hawke. His expertise was also harnessed by the Government in his appointment to the Executive of the Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia's national research body (1989–95).

David was a very friendly and approachable man. His manner was unfailingly courteous and the phrase 'true gentleman' comes to mind. He was highly respected and warmly liked by all his colleagues and friends. His clarity of thought and expression made him an outstanding lecturer and an ideal person from whom to seek advice. His students and postdocs described him as an outstanding supervisor. They appreciated the freedom that he gave them in their research, while always being there to provide guidance when needed.

Outside science and academia, David enjoyed tennis (which he played into his eighties), reading (including novels in French), cars, dogs, watching movies (especially Westerns) and listening to classical music and opera. He and his family particularly enjoyed their magnificent home, originally built by the ANU for Sir Mark Oliphant (see Fig. 13). David's services to Australian science, drawing on his background of wide experience in Europe and the USA, were of immense value and were highly acclaimed as such by his colleagues.



Figure 13. David with his granddaughter Lizzie in the grounds of his family home (ca 1993).

David passed away in Canberra on 1 July 2015. A symposium in his memory was held at the ANU on 17 June 2016.

Conflicts of interest

The authors declare no conflicts of interest.

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