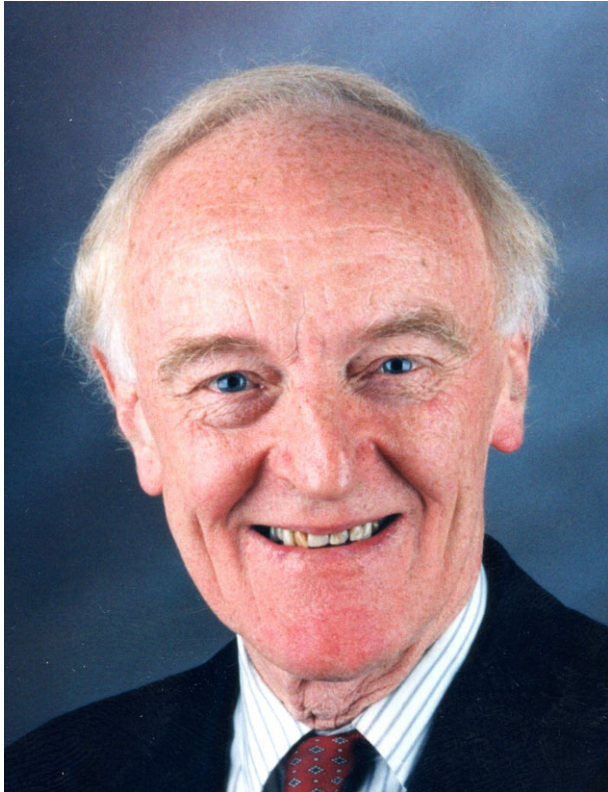


AMYAND DAVID BUCKINGHAM

28 January 1930 — 4 February 2021



A.D. Buckingham



AMYAND DAVID BUCKINGHAM

28 January 1930 — 4 February 2021

Elected FRS 1975

BY SIR DAVID C. CLARY FRS^{1,*} AND BRIAN J. ORR²

¹*Department of Physical and Theoretical Chemistry, University of Oxford,
South Parks Road, Oxford OX1 3QZ, UK*

²*Faculty of Science and Engineering, Macquarie University, Sydney 2109, Australia*

David Buckingham was a chemical physicist and theoretical chemist who made fundamental contributions to the understanding of optical, electric and magnetic properties of molecules. Born in Australia, he was an undergraduate at the University of Sydney and the first PhD research student of John Pople (FRS 1961) at Cambridge, and there he made significant advances in the theory of intermolecular forces and nonlinear optics. He then moved to Oxford, where he and his group performed the first direct measurement of a molecular electric quadrupole moment. He was elected to the first chair of theoretical chemistry at the University of Bristol, where he wrote a particularly influential article on molecular moments, higher-order polarizabilities and intermolecular forces. His next appointment was at the University of Cambridge as the first holder of the 1968 Chair of Chemistry, and he was head of a distinguished department of theoretical chemistry for 28 years. With colleagues he pioneered experiment and theory on vibrational optical activity and developed a powerful model to predict the structures of weakly-bound molecules. A man of broad interests and achievements, he played first class cricket in the 1950s.

EARLY LIFE AND EDUCATION (1930–1953)

Born in Sydney, Australia, David Buckingham grew up there with his parents Reginald and Grace (née Elliot) and his elder sister Joslin and her twin brother Michael (who also became a distinguished physical scientist) (figure 1). His parents were born in England, emigrated separately to Australia before World War I and married in 1923. For over 40 years, Reginald

* david.clary@chem.ox.ac.uk

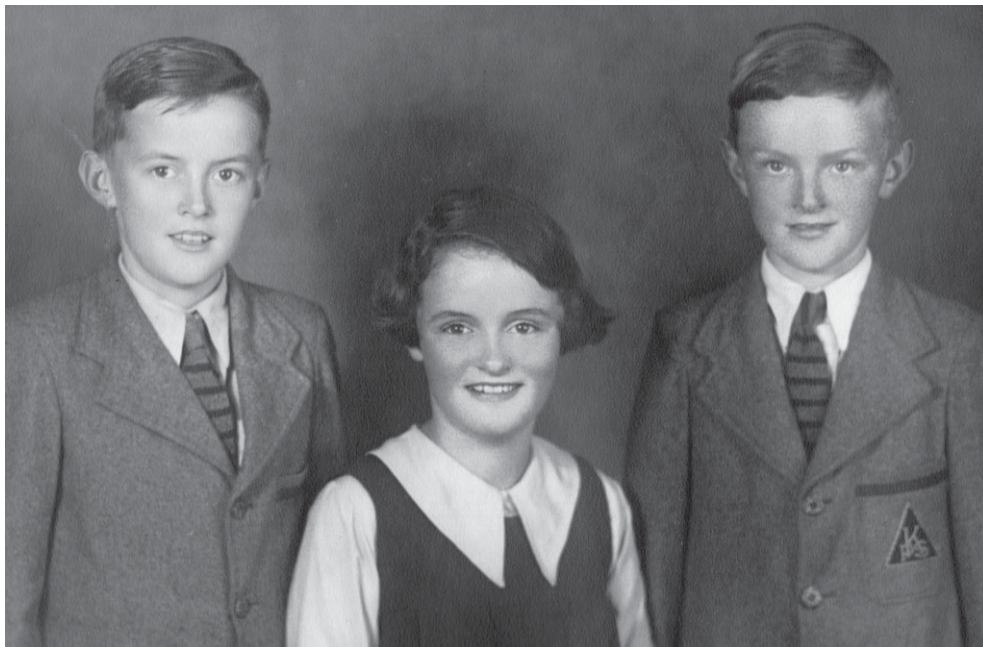


Figure 1. The young David Buckingham (right), aged nine, with sister Joslin and her twin brother Michael.

worked for Dalgety and Company Limited, serving the rural sector. Grace trained as a nurse at King's College Hospital in London and went back to Australia in 1920 to help develop its early baby health clinics; she returned to England 11 years after Reginald's death in 1956. David treasured his Australian origins throughout his life (CO97*) (47)†. His first name, Amyand (the A in the ADB acronym used by his colleagues), had Huguenot origins on Grace's side of the family; among them was Claudius Amyand FRS, surgeon to George I and George II—in 1735, he performed the first recorded successful appendicectomy. Grace's brother, John Amyand Elliot, died in action at Gallipoli in 1915.

David attended Barker College, where, in 1947, he was both head prefect and dux (the top academic achiever). Both he and his brother Michael (who had also been Barker's dux two years earlier) studied at Sydney University's Faculty of Science; they would each win a University Medal (Michael's in physics and David's in chemistry) before going to England to study for doctorates. Only Michael would return permanently to Australia. David wrote (47) that he learned from Michael 'the importance of mathematics and fundamentals'—as was amply demonstrated throughout his career in molecular science.

He was a member of a talented cohort of first-year undergraduates in 1948, which included four future Fellows of the Royal Society. During 1951–1953, David's BSc honours and MSc research projects were supervised by the professor of chemistry, R. J. W. Le Fèvre (FRS 1959), a prominent physical-organic chemist. In the Le Fèvre tradition of interpreting electric dipole

* The abbreviation CO97 designates the much-cited reference [Clary & Orr 1997](#).

† Numbers in this form refer to the bibliography at the end of the text.

moments in terms of molecular structure, David adapted dielectric theories ‘to allow for the influence of molecular shape on the static dielectric constant of a liquid’ (1). He published as many as eight papers during his two and a half years as a research student at Sydney University.

David also excelled at cricket, captaining Barker College’s First XI and gaining a cricket blue at Sydney University. Early in 1952, when he graduated as Australia’s most outstanding chemistry student of that year, a Sydney newspaper published a short item headed ‘Cricketer gets degree’.

PHD AT CAMBRIDGE 1953–1955

In 1953, David gained a Shell postgraduate scholarship at Cambridge in the Department of Theoretical Chemistry headed by Sir John Lennard-Jones FRS—a prominent name in the field of intermolecular forces, where David himself would later gain comparable fame. However, because Lennard-Jones was moving away from Cambridge, David became the first PhD student of John Pople (FRS 1961; KBE 2003), only four years older than he. Pople would later win the 1998 Nobel Prize for chemistry (for computational methods in quantum chemistry). Together they generated many influential publications on dielectric properties of imperfect gases and hyperpolarization of molecules.

David stated that he ‘benefited greatly from the mathematical rigor and elegance’ that Pople ‘brought to bear on some of the problems that [they] worked on’ (47). Likewise, Pople has written: ‘In retrospect, it is hard to imagine a more fortunate start than acquiring someone like David Buckingham as a first student!’ (CO97) (figure 2).

OXFORD 1955–1965

After completing his PhD in two years, in 1955 David moved to Oxford as a senior student of the Royal Commission for the Exhibition of 1851 and as a lecturer of Christ Church Oxford. Initially, he joined the Physical Chemistry Laboratory and set out to complement his theoretical research with experiments on second dielectric virial coefficients of gases, which he and Pople had predicted as a ‘useful probe of anisotropic intermolecular potentials’ (47). In 1958, David became a university lecturer in inorganic chemistry while remaining at Christ Church. Among his DPhil students at Oxford were Roger Raab, Philip Stephens (FRS 2008), James Bridge and David Dunmur. During this period, David published many insightful theoretical papers covering dielectric constants of dense fluids, solvent and pressure effects in infrared spectroscopy, depolarized light scattering from dense fluids, electro-, magneto- and nonlinear-optical effects, and mechanisms of nuclear magnetic resonance (NMR) spectra.

In Oxford, he was an inspiring tutor to undergraduates. Jonathan Connor, who became professor of theoretical chemistry at the University of Manchester, recalls: ‘At Christ Church, he seemed to be an order of magnitude more dynamic than everybody else. He thought quickly, spoke quickly and even walked quickly. You had to almost run to keep up with him.’ He formed a formidable teaching partnership with the organic chemist Paul Kent, and Buckingham and Kent were known as ‘the County Pair’ at Christ Church (figure 3).

From 1959 onwards, David’s experimental research was able to take advantage of superior facilities and technical support at Teddington in the National Physical Laboratory (NPL),

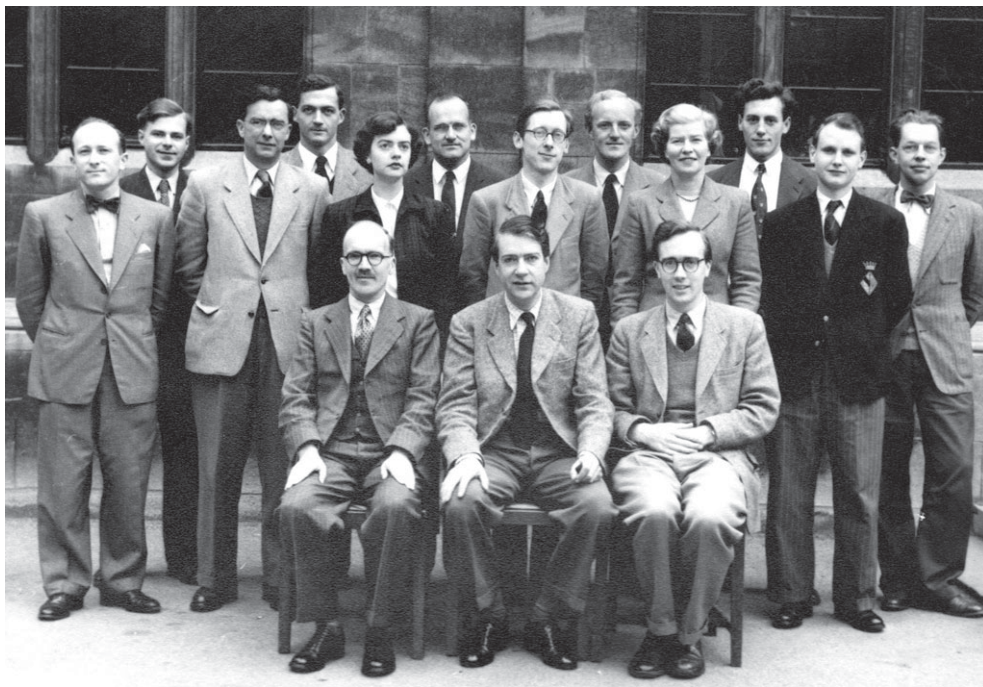


Figure 2. The theoretical chemists at the University of Cambridge in 1955. David Buckingham is third from the right in the back row looking over the shoulder of John Pople. In the front row are Frank Boys, Christopher Longuet-Higgins and George Hall.

where John Pople had become superintendent of the new Basic Physics Division and Gordon Sutherland FRS (Kt 1960) was director. There, David and postdoctoral fellow Ray Disch (from Harvard) realized a novel birefringence experiment (7, 8, 10) to measure directly the electric quadrupole moment of gas-phase carbon dioxide molecules; this led to the cgs unit for electric quadrupole moments being known as ‘the Buckingham’.

David revelled in the colourful company of characters in the senior common room at Christ Church at that time; these included Robert Blake, Hugh Trevor-Roper, Roy Harrod, Lord Cherwell (FRS 1920), Sir George White Pickering (FRS 1960) and the poet W. H. Auden. Auden was interested in science, and one evening borrowed a book that David was reading called *Mr Tompkins in Wonderland* by George Gamow. Nine months later, rather than returning the book, Auden put a poem in David’s college pigeon hole; it was entitled ‘After Reading a Child’s Guide to Modern Physics’, immortalizing in poetry the Buckingham enthusiasm for science. This 10-year immersion in college life, particularly as junior censor (responsible for discipline), and having a set of rooms beautifully furnished and decorated with a painting by Van Dyck, was most influential in heightening David’s appreciation of history, architecture, silver, furniture and fine wine.

In July 1964, David sailed from Southampton to Montréal, bound for research in Ottawa. On this voyage he met Jillian Bowles, a physiotherapist who was heading to a post in British Columbia. They were engaged in January 1965 and married at Christ Church Cathedral six

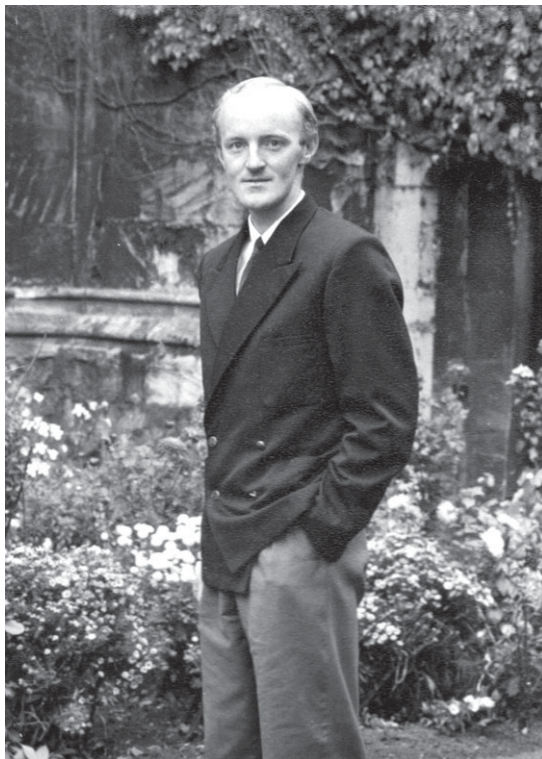


Figure 3. David Buckingham in the gardens of Christ Church, Oxford, in 1955.

months later. Jill was David's discerning and highly supportive partner during more than 55 years of marriage.

BRISTOL 1965–1969

In September 1965, David took up the inaugural chair of theoretical chemistry at the University of Bristol. In his first week he presented the opening paper in a Faraday Discussion on the theory of long-range intermolecular forces (15). This also coincided with the arrival of one of us (BJO) as David's first research student from his native Australia; 12 years apart, our respective first research projects had both been supervised by Le Fèvre. Under the direction of David Dunmur (who had recently completed his DPhil at Oxford), the instruments were moved from NPL to Bristol. The research group in Bristol comprised a lively international brigade, drawn from Argentina, Australia, Canada, Nigeria, The Netherlands and the USA (as well as Scotland and Wales), far outnumbering English locals.

Research carried out in David's department in Bristol had widespread scientific impact. His theoretical insight (20) into higher-order molecular polarizabilities was complemented by refined birefringence measurements of molecular hyperpolarizabilities (relevant to the emerging area of nonlinear optics), prolific NMR studies of molecules oriented in

liquid-crystal media, and mechanisms of atomic and molecular properties and spectra in gases and condensed phases.

David's lectures in Bristol were often attended by other academic staff keen to learn what they could from their new professor. One day, he paused to ask the audience: 'Is that clear?' The response from a senior colleague was: 'No, it is not!' Using his best cricketing skills, David played a straight bat and explained, patiently and respectfully, the point that had escaped his colleague. PhD students who were present regarded this incident with amusement and awe.

By this time, David's research was getting noticed by the top chemistry departments around the world. He had formal offers of tempting positions from several leading universities, including MIT, Toronto, Manchester and Cambridge. The opportunity to return to Cambridge in 1969, where he had completed his PhD 14 years before, was particularly appealing.

CAMBRIDGE 1969–2021

David was elected to the 1968 Chair of Chemistry at the University of Cambridge. The two previous theoretical chemistry professors, Sir John Lennard-Jones and Christopher Longuet-Higgins (FRS 1958), both held John Humphrey Plummer professorships, which were not dedicated to particular subjects. After Longuet-Higgins resigned, the university established in 1968 a statutory professorship in theoretical chemistry. This was based in the chemistry department, which also included at that time organic and inorganic chemistry. Rather remarkably, physical chemistry was separate and the unified Department of Chemistry was not formed until 1988. David was also elected a professorial fellow at Pembroke College in 1970.

In 1969 the other academic staff in his department were Frank Boys (FRS 1972) and Anthony Stone. Boys was a pioneer in developing quantum chemistry methods, but was only a university lecturer. Promotions were then rare in Cambridge and David's first priority was to secure a readership for Boys. Sadly, Boys died just afterwards in the same year that he was elected FRS.

Boys was followed in quantum chemistry by Nicholas Handy (FRS 1990), who became a close colleague of David. Other university appointments that David made included Paul Madden (FRS 2001), David Clary (FRS 1997) and David Wales (FRS 2016). In addition, others who worked in his department and who were elected to the Royal Society include Ruth Lynden-Bell (FRS 2006), Laurence Barron (FRS 2005), Patrick Fowler (FRS 2012), Jeremy Hutson (FRS 2010) and Tim Softley (FRS 2018). With colleagues such as Barron and Softley, David continued with experimental work 'to keep the theoreticians honest', as he often would say.

David considered the weekly seminars in theoretical chemistry to be the heart of his department. He sat in the front row and invariably asked the first question. In addition, he always gave the first seminar at the start of every academic year. His own research lectures were a model of style and clarity. He often quoted the principle that 'people come away from seminars remembering one thing or nothing!' As in Bristol, David gave wise advice and support to the theoretical chemistry students and academics in his department at Cambridge, and followed their careers with interest. He went out of his way to welcome students and postdocs from overseas (figure 4).

In his undergraduate lectures on quantum mechanics, which he presented for over 25 years, he targeted the top students in natural sciences, with the aim of inspiring them to undertake



Figure 4. David Buckingham at work in his office at the University Chemical Laboratory, Lensfield Road, Cambridge. (Online version in colour.)

PhDs in theoretical chemistry. Peter Knowles, who is now professor of theoretical chemistry at Cardiff University says: ‘Most of us found the subject matter of David’s lectures quite impenetrable, but there was an awareness that something special was going on. Each lecture was a polished performance without any notes that started top-left, and finished bottom-right of the blackboard.’ Several undergraduate students who took this course went on to study for their PhDs in his department and were subsequently elected to the Royal Society. These included Sally Price (FRS 2017), David Manolopoulos (FRS 2011) and Ali Alavi (FRS 2015).

At Cambridge, David continued to attract first-rate research students and postdoctoral fellows to his research group. He encouraged his students to develop their own ideas, and allowed some to publish on their own. His collaboration with Laurence Barron on the Raman scattering of circularly polarized light led to the field of vibrational optical activity. With Patrick Fowler he developed a powerful *ab initio* model for predicting the structures of van der Waals molecules.

He was also active on the national academic and scientific scene. He was president of the Faraday Division of the Royal Society of Chemistry from 1987 to 1989. He was appointed to the Advisory Council of the Royal Military College of Science, Shrivenham, for 15 years from 1973, taking the chair for two years during the transition to Cranfield University. From 1975, David was a trustee of the Charles and Julia Henry Fund for 30 years, awarding scholarships to students to study at Harvard and Yale, and was chair for 13 years. At the Royal Society, he was on the Council from 1999 to 2001 and was a member of several committees.



Figure 5. Ahmed Zewail, John Pople, David and Jill Buckingham and Bill Klemperer at the 1997 conference. (Online version in colour.)

David retired in 1997, and a major conference in his honour was held at Pembroke College. A book describing his career, with expert comments on his major papers, was also published (CO97). Figure 5 shows David and Jill Buckingham at the conference with plenary speakers Ahmed Zewail (ForMemRS 2001), John Pople and Bill Klemperer. The conference was timely, as the Nobel Prize for chemistry was awarded to Pople in the next year and to Zewail in the year after that.

David became emeritus professor of chemistry and emeritus fellow of Pembroke in 1997, and was elected honorary fellow of Pembroke in 2005. He continued to publish original papers until shortly before he died. He proposed the detection of chirality by nuclear magnetic resonance (48), and in his last years was involved with colleagues from the Max Planck Society and the Centre National de la Recherche Scientifique in efforts to demonstrate this effect, which he expected would eventually become a valuable tool.

MAJOR SCIENTIFIC CONTRIBUTIONS

David Buckingham made many significant theoretical and experimental contributions to the understanding of optical, electric and magnetic properties of molecules. Covering a wide topical range, they bear the stamp of his scientific vision and determination to gain insight into problems that he saw as inadequately understood. To meet such challenges, David brought mathematical elegance, critical analysis of potentially overlooked mechanisms and a close synergy between theory and experiment. He tackled difficult problems and was always optimistic that there were new phenomena or techniques awaiting discovery. For instance, Kees de Lange (one of David's PhD students in Bristol) has recently commented on 'David's conviction that detailed studies on small well-characterized molecules could never fail to provide breakthroughs somehow'.

Selected examples of David's major research contributions are summarized below.

Imperfect polar gases

With Pople, David published on the second density virial coefficients of imperfect polar gases (2). Their theory went beyond permanent dipole moments to include dipole-induced dipole interactions and quadrupole forces. Detailed expressions were derived for the second virial coefficients from force fields. Second dielectric virial coefficients were also calculated, showing that dipole interactions increase the total polarization (3). Parameters associated with molecular shape were needed to obtain agreement with experiments for molecules such as CH₃F. Quantities such as virial coefficients can now be calculated with sophisticated force fields determined from accurate *ab initio* computations, but these early papers of Buckingham and Pople demonstrated the rich opportunity for relating intermolecular forces to measurements of molecular properties.

Solvent effects on vibrational spectra

In 1960, David advanced understanding of the infrared and Raman spectra of dense fluids (9). Solvent-solute interactions cause these spectra to differ from those in the gas phase and David realized that the spectra of dense fluids could give new information on intermolecular forces. He developed the theory for spectral shifts, widths and intensities using equilibrium statistical mechanics, and was the first to calculate moments for infrared and Raman spectra. Several new predictions agreed with experimental spectral observations. The relative shift in overtone bands was found to match that in the fundamental and to be independent of isotopic substitution. For polyatomics, he predicted redshifts in stretching vibrations and blueshifts in bending modes.

More recently, computer simulations (accounting for all degrees of freedom, including quantum effects, and incorporating increasingly more accurate potential energy surfaces) have enabled detailed prediction of solvent effects (Gray *et al.* 1997). However, David's analytical predictions frequently offer more direct insight than extensive computations on the importance of underlying intermolecular forces.

Experiments with oriented molecules

In 1964, David delivered his Tilden Lecture to the Chemical Society in London (13). Although most of David's publications were specialized, pitched to the scientific cognoscenti, this article was aimed at readers in other areas of chemistry. It is effectively a digest of research progress made in Oxford and a prospectus for future work in Bristol. Classical and quantum orientation mechanisms in external fields, such as birefringence experiments including the electro-optic Kerr effect and measurement of quadrupole moments, are discussed. The final portion of the article (13) is a substantial forward-looking section describing NMR measurements (11) in which the absolute sign of spin-spin coupling is determined by orienting molecules in an electric field.

David also mentions (13) the new observation (Saupe & Englert 1963) that a magnetic field could substantially orient molecules in a liquid-crystal solvent. In Bristol, this became a highly productive research area for PhD students Elliott Burnell and Kees de Lange (18, 35), as reviewed by Burnell (CO97). It is notable that H₂ molecules are partially aligned in a nematic solvent (25), later leading to new research on subtle quantum-rotor effects in liquid-crystal NMR studies of all the H, D and T isotopic variants of hydrogen (Burnell *et al.* 1982, 1997).

Measurement of electric multipole moments

Throughout his career, David studied physical processes influenced by molecular multipole moments (32). His earliest research at Sydney University concerned extraction of ‘true’ electric dipole moments (symbolized by a vector $\boldsymbol{\mu}^{(0)}$) (1), equivalent to those measured in the gas phase, from experiments on small molecules in dilute solution or in dense fluids.

A pioneering contribution comprised experimental evaluation of molecular electric quadrupole moments (symbolized by a second-rank tensor $\boldsymbol{\Theta}^{(0)}$), which indicate the distribution of electric charge in a molecule. The 1936 Nobel Laureate Peter Debye ForMemRS, after whom the pre-SI unit for electric dipole moments is named, proposed in 1963 that Buckingham (B) cgs units (1×10^{-26} e.s.u.) should be used for $\boldsymbol{\Theta}^{(0)}$. Debye was prompted by the ingenious optical measurement of $\boldsymbol{\Theta}^{(0)}$ for carbon dioxide (10). A tiny spatial refractive-index difference was probed over a 1.25 m path in a gas by linearly polarized light passing through a strong electric field gradient in which the uniform electric field strength was zero. This ‘quadrupolar birefringence’ arose primarily by orientation of the anisotropically polarizable molecules. David and his co-workers later published quadrupolar birefringence studies of a variety of atoms and molecules (23), as reviewed by Geoffrey Ritchie (CO97). Remarkably, the current best experimental value of the quadrupole moment of CO₂ is virtually identical to that originally reported by Buckingham & Disch (CO97). David Dunmur, who for his DPhil added a HeNe laser and refined electronics to the NPL apparatus, notes that their paper (23) has even been cited as far afield as mineralogical models of nitrogen adsorption in extraction of Australian shale gas (Ekundayo *et al.* 2021).

Theory of molecular moments and intermolecular forces

In 1966, David ruptured an Achilles tendon when playing squash in Bristol. This put him in plaster for many weeks and gave him time to derive a rigorous semi-classical formalism for electromagnetic scattering from molecules that went beyond the dipole approximation (20). Applications of the theory include those to Raman optical activity, circular dichroism of oriented molecules and the linear effect of an electrostatic field on the scattering of light by gases. Expressions were also derived for long-range intermolecular forces that are nowadays used routinely in simulations of complex systems, including fluids, materials and biomolecules.

This paper chose several common examples, including a point charge interacting with linear and tetrahedral molecules as well as interactions between spherical and tetrahedral molecules and between two linear molecules. The main theory was derived in a Cartesian representation but, for these special cases, the long-range terms in the potential were also expressed usefully in angles of molecular orientation. Advances in *ab initio* quantum chemistry, including work done by David’s colleagues Nicholas Handy and Roger Amos, have allowed accurate computation of the various higher-order moments and polarizabilities that David derived (Amos *et al.* 1988).

First- and higher-order polarizabilities

Associated with permanent electric multipole moments ($\boldsymbol{\mu}^{(0)}$, $\boldsymbol{\Theta}^{(0)}$, ...) are induced moments arising from the interaction of electric, magnetic and radiation fields with molecular

polarizabilities. Power-series expansions of the molecular dipole and quadrupole moments induced by a static electric field vector \mathbf{F} contain the conventional electric dipole polarizability tensor α and hyperpolarizabilities β , γ , ... together with additional quadrupolar tensors \mathbf{A} , \mathbf{B} and \mathbf{C} arising from an electric field gradient \mathbf{F}' (20). Expansions were made of field-dependent electric moment vectors $\boldsymbol{\mu}$ and $\boldsymbol{\Theta}$, as well as the magnetic moment vector \mathbf{m}' (with field-induced terms added to the permanent paramagnetic moment $\mathbf{m}^{(0)}$) in the presence of a semi-classical periodic electromagnetic field; this introduces additional tensors, including diamagnetic susceptibilities. The ‘quadrupole moment paradox’, in which $\boldsymbol{\Theta}^{(0)}$ for a dipolar molecule is found to be origin-dependent, was eventually resolved (21) by identifying an effective quadrupole centre about which the first moment of the polarizability anisotropy is zero; this is defined by tensors \mathbf{A} and \mathbf{G}' , which are cross-term polarizabilities of $\boldsymbol{\mu}$ with $\boldsymbol{\Theta}$ and \mathbf{m} , respectively (20).

The anisotropy $\Delta\alpha$ of the molecular optical polarizability is needed to interpret birefringence experiments, such as the above electric quadrupole moment measurements (10, 23). For his DPhil, James Bridge refined techniques to measure depolarization ratios of Rayleigh light scattering to yield various $\Delta\alpha$ values (12, 17, 41), as reviewed by Martin Bogaard (CO97). A review of electric dipole polarizabilities and hyperpolarizabilities in a volume edited by David (Bogaard & Orr 1975) covered interests of his Oxford and Bristol research groups. Polarizability-anisotropy derivatives with respect to internuclear distance were also evaluated (43), as reviewed by Bogaard (CO97), by measuring intensity ratios for depolarized and polarized Raman scattering from diatomic molecules on specific rotational lines. Later work on vibrational contributions to hyperpolarizabilities such as β and γ (Bishop 1994; Shelton & Rice 1994) is also relevant.

Differential light scattering and optical activity

David’s fascination with chiral effects (in both molecules and light) led to a collaboration in Cambridge with postdoctoral fellow Laurence Barron. Together, they developed semi-classical theories of Rayleigh and Raman scattering from optically active molecules (30) and magnetic optical activity in light scattering from achiral molecules (31). These, as well as vibrational optical activity, are highly relevant to studies of biomolecules and have been the subject of several reviews (37, 46, 51), including some by Barron alone (Barron 2015; CO97). The first successful Raman circular intensity differential experiments were performed in Cambridge by Barron, Bogaard and Buckingham (33, 34).

Nonlinear optics

For his PhD, David predicted observables of gas-phase electric birefringence (electro-optic Kerr effect) experiments (4, 5). Added to conventional contributions from molecular components of $\boldsymbol{\mu}$ and α were extra terms involving hyperpolarizabilities β and γ . The advent of lasers in 1960 gave rise to the new field of nonlinear optics (Franken & Ward 1963)—a feature of modern technology. The above static-field forms of β and γ are closely related to the susceptibilities intrinsic to nonlinear-optical processes (13) (Bogaard & Orr 1975). Moreover, David was the first to propose an all-optical variant of the Kerr effect (6), in which an intense light beam causes birefringence via components of α and γ ; this was a precursor for various four-wave mixing processes in nonlinear optics and optical telecommunications, as reviewed by J. F. Ward (CO97).

Motivated by David's Kerr effect theory (4, 5), fixed-temperature gas-phase measurements of atoms and quasi-spherical molecules yielded γ values (24), while T -dependence studies of non-spherical molecules (22, 26) enabled terms involving μ , α , β and γ to be separated. As in the case of quadrupolar birefringence (14), quantum-statistical corrections needed to be made to the classically predicted T -dependence of the Kerr effect; these were verified experimentally (22). Nonlinear-optical diagrammatic perturbation theory led to divergent formulae for γ when zero static-field frequencies replaced optical frequencies, although realistic results could be derived by double perturbation theory (19). A collaboration, largely by correspondence, that spanned five cities, four countries and five years eventually resulted in a much-cited formulation to resolve that theoretical anomaly (Orr & Ward 1971).

A decade later, David and his PhD student David Shelton devised a novel nonlinear-optical technique to measure hyperpolarizabilities β and γ for static-electric-field-induced second-harmonic generation (ESHG) in fluids (44), as reviewed by Ward (CO97). This yielded more reliable ESHG estimates of β and γ for comparison with computed values, as well as dispersion studies to evaluate vibrational contributions to hyperpolarizability (Shelton & Rice 1994).

Novel spectroscopic techniques

David's insight into the Stark effect (32) and magnetic optical activity (16) promoted collaborations with the group of Donald Ramsay (FRS 1978) at the National Research Council of Canada on high-resolution Stark or Kerr effect spectroscopy (27, 29) and magnetic-rotation spectra (38).

Theoretical work in the emerging area of photoelectron spectroscopy (PES) also resulted in a rotationally resolved formulation of PES for diatomic molecules, exploring whether the angular distribution of photoelectrons might indicate the molecular orbital from which they had been ejected (28). As reviewed by de Lange (CO97), this was later widely cited as 'BOS theory' once high-resolution methods (e.g. zero kinetic energy) had enhanced rotational-state-resolved PES experiments.

Effects of collisions on molecular properties

A seminar by George Tabisz, on sabbatical at Cambridge from Manitoba, led to a major collaborative project on how molecular properties are influenced by collisions (39, 40). Tabisz presented some unexplained features in the Rayleigh scattering of molecules such as CH₄ and CF₄. In the ensuing discussion, David suggested that electric field gradients in the molecular interactions could be responsible. With Tabisz, he then developed this idea into a concept termed collision-induced rotational Raman scattering (39); higher-order molecular properties were determined from observed scattering data. The theory also proposed selection rules for rotational transitions in molecular collisions. Other groups have advanced this research (Bancewicz *et al.* 2004). David often emphasized that his best ideas came from lectures or papers with unexplained observed phenomena that could be understood from underlying intermolecular forces.

Structures of van der Waals molecules

At a Faraday Discussion at Oxford, Bill Klemperer commented on the structure of a weakly-bound complex formed between formaldehyde and hydrogen fluoride (Klemperer 1982). He claimed that electrostatic interactions were not responsible as the dipole-dipole interaction

was almost zero for the observed orientation of the molecules in the dimer. David at once proposed that higher moments such as the quadrupole moment could be important. Klemperer responded by adapting a Samuel Johnson quote ‘the quadrupole moment is the last refuge of a scoundrel!’

This good-humoured interaction inspired a new project for David and Patrick Fowler on an ab initio model to predict the structure of van der Waals molecules (45). They exploited Stone’s distributed multipole analysis to describe the electric charge distribution around each monomer molecule. Short-range repulsive interactions were represented by atom multipoles embedded in hard spheres of appropriate van der Waals radii centred on the nuclei. Their model predicted angular geometries of numerous molecular complexes in good agreement with experiment. Some deviations have been observed for systems with strong repulsive anisotropies, as was shown, somewhat triumphantly, by Klemperer for complexes such as HF–CIF (Baiocchi *et al.* 1983). Nevertheless, subsequent refinements of the model have continued to demonstrate its usefulness and it has even been extended to the structures of biological molecules (Ren *et al.* 2012).

Isotope effects and hydrogen bonding

David extended his deep understanding of intermolecular forces to the important problem of hydrogen bonding (36). With Werner Urland, he suggested that a hydrogen bond is generally weaker than a deuterium bond as the amplitudes of X–H...Y bending vibrations are greater than those for X–D...Y and the linear configuration is optimum for hydrogen bonding. With PhD student George Hentschel, David examined the importance of this effect on the partial miscibility of protonated and deuterated polymers (42). They concluded that, while isotope segregation is unlikely for small hydrocarbons, it becomes more important for larger polymer systems. This prediction has been confirmed in several subsequent experiments (White *et al.* 2010).

A highly cited article with Janet Del Bene and Sean McDowell discussed some other exceptions in hydrogen bonding, including proton-shared and ion-pair bonds (49). By considering harmonic and anharmonic vibrations of X–H in a variety of complexes, it was shown that there is no fundamental difference between blue-shifting and red-shifting bonds. These findings have implications for understanding the structures and properties of water clusters and hydrogen-bonded liquids.

SCIENTIFIC EDITING

David was the editor of *Molecular Physics* (1968–1972) and *International Reviews in Physical Chemistry* (1981–1989). However, he is best remembered as editor of *Chemical Physics Letters* (1978–1999) (52). He started as editor before the advent of email and the internet, and corresponded with his perfect handwriting. He received over 1000 papers each year, which he checked and corrected meticulously. As many as 15 authors who published in *Chemical Physics Letters* when David was editor went on to win a Nobel Prize.

Ahmed Zewail from the California Institute of Technology had submitted many of his pioneering papers on femtochemistry to *Chemical Physics Letters*. In 1990, he joined David as an editor and this enabled a close friendship to develop. Zewail was awarded the Nobel Prize for Chemistry in 1999 while he and David were still editors of the journal.



Figure 6. Former England cricket captain Ted Dexter makes a presentation to David Buckingham in 1998. (Online version in colour.)

OTHER INTERESTS

Science took David all over the world. He took great pleasure in his travels and had an encyclopaedic knowledge of the United States. There were frequent visits to Australia, including a four-month family visit in 1979. In later years, Jill and David were able to travel to many fascinating places, ranging from South America and the Falkland Islands to Libya and Lebanon.

Following David's achievements in cricket at school and university in Australia, he was very much involved in this sport in the UK. As a Cambridge graduate student, he played first class cricket with or against some of the greatest English players, including Peter May, Jim Laker, 'Fiery' Fred Trueman, Brian Close, Bill Edrich and Ted Dexter. He was an opening batsman and occasionally an off-break bowler. At Oxford, while a don at Christ Church, he also played first class cricket for the Free Foresters and was treasurer of the Oxford University Cricket Club. When he returned to Cambridge as professor of chemistry, he also became treasurer of the Cambridge University Cricket Club and, for 19 years from 1990, was its elected president (figure 6).

David's early appreciation of silver artefacts (e.g. at Christ Church, Oxford) extended to looking after the fine silver collection at Pembroke College, Cambridge, having it repaired when required and presenting an annual exhibition in the Old Library. He wrote an article for the Silver Society, with Jayne Ringrose, about the Pembroke Foundress's Cup (50).

David greatly valued his family life (figure 7). Jill and David's children, Lucy and Mark, were born in Bristol; Alice completed the family after they moved to Cambridge. They recall David as a playful father when they were young: reading and inventing stories, playing board



Figure 7. Jill and David Buckingham, daughter Lucy and son-in-law James Binney FRS, Jill's sister Susan Enderby and brother-in-law John Enderby FRS. Picture taken at the Royal Society in 2000 on the day of the admission of James Binney. (Online version in colour.)

games. He wanted them to have ball skills and, more importantly, to learn sportsmanship. A car or bicycle ride to school with David was an adventure; he would spot exotic creatures that always just evaded a child's gaze or imagine unlikely details of the lives of people in the street, as well as patiently drilling them on their multiplication tables. Family meals were important to him; he encouraged conversation about current affairs over breakfast. He helped and encouraged his children with their maths schoolwork, he fixed the family bicycles and taught the children to fix their own. He was a faithful supporter at Mark's and Alice's sports matches. Especially after taking on the editorship of *Chemical Physics Letters* in 1978, David worked long hours in his study at home. His children recall him walking past the family television to reach the study, and asking them 'What are you watching? Rubbish?'

During 1981–1993, David and Jill owned a second home in Suffolk, a sixteenth-century farmhouse with 15 acres. David was able to relax there, working physically rather than mentally, including using his carpentry skills. It was a thrill to discover and restore features such as an inglenook fireplace and mullion windows, which had been hidden over the centuries. Teamwork on cutting wood, clearing the pond, and bonfires was a way to connect with his teenagers. The agriculture-industry career of David's son Mark developed from an interest that began there. Other lovely homes followed, large enough



Figure 8. David and Jill Buckingham in 1993. (Online version in colour.)

to accommodate the expanding family of eight grandchildren, and Christmases, birthdays and weddings. Jill and David were tremendous hosts in their homes in Bristol, Cambridge and Newmarket, where they entertained students, colleagues, academic visitors and friends (figure 8).

David Buckingham was an exceptionally talented person who sought excellence in everything he did. His intellectual and athletic agility served him well in science, sport and daily life. His legacy is a formidable body of scientific theory and knowledge, together with the enduring example of his dynamic personality.

MAJOR AWARDS

- 1959 Harrison Memorial Prize of the Chemical Society
- 1964 Tilden Lecturer of the Chemical Society
- 1974 Theoretical Chemistry and Spectroscopy Prize of the Chemical Society
- 1975 Fellow of the Royal Society
- 1978 Fellow of the Optical Society of America
- 1979 Docteur Honoris Causa de l'Université de Nancy I
- 1985 Member of the International Academy of Quantum Molecular Science
- 1986 Fellow of the American Physical Society

- 1992 Foreign Associate of the National Academy of Sciences (USA)
- 1992 Foreign Honorary Member of the American Academy of Arts and Sciences
- 1993 Doctor of Science (Honoris Causa), University of Sydney
- 1994 Doctor of Science (Honoris Causa), University of Antwerp
- 1995 Harrie Massey Medal and Prize of the Institute of Physics
- 1996 Hughes Medal of the Royal Society
- 1996 Foreign Member of the Royal Swedish Academy of Sciences
- 1997 Commander of the Order of the British Empire (CBE)
- 1998 Faraday Lectureship and Prize of the Royal Society of Chemistry
- 2001 C. H. Townes Award of the Optical Society of America
- 2007 Ahmed Zewail Prize in Molecular Sciences
- 2008 Corresponding Member of the Australian Academy of Science

ACKNOWLEDGEMENTS

The authors much appreciate the assistance from Jill Buckingham and the Buckingham family for providing photographs and material used in this memoir. Helpful comments from Laurence Barron, Elliott Burnell, Jonathan Connor, Kees de Lange, David Dunmur, Katharine Hunt, Peter Knowles, David Logan, Sean McDowell, Tim Softley and George Tabisz are also gratefully acknowledged.

All photographs, including the portrait frontispiece, were kindly provided by the Buckingham family (copyright details unknown).

AUTHOR PROFILES

Sir David Clary FRS

David Clary is a professor of chemistry at the University of Oxford working on the quantum theory of chemical reactions. He was a PhD student (1974–1977), lecturer and then reader (1983–1996) in David Buckingham's Department of Theoretical Chemistry at Cambridge. After a professorship at UCL (1996–2002), he was head of the Division of Mathematical and Physical Sciences at the University of Oxford from 2002 to 2005 and then became president of Magdalen College, Oxford, from 2005 to 2020. He was elected FRS in 1997 and was knighted in 2016.



Brian J. Orr



Brian Orr, pictured with David Buckingham in 2016, is emeritus professor in the Macquarie University's Department of Physics and Astronomy in Sydney, Australia. Like David, he grew up in northern Sydney, and studied science at the University of Sydney with early research supervised by Professor R. J. W. Le Fèvre. He then gained a scholarship for research in Bristol (1965–1968), where he was David's first Australian PhD student. After postdoctoral work in Ottawa, he returned to Sydney as an academic at the University

of New South Wales (1969–1988) and then as professor of chemistry at Macquarie University (1989–2002). His 58-year research career has spanned studies of quantum-resolved molecular energetics, high-resolution optical spectroscopy, nonlinear optics and laser-based atmospheric sensing.

REFERENCES TO OTHER AUTHORS

- Amos, R.D., Gaw, J. F., Handy, N. C. & Carter, S. 1988 The accurate calculation of molecular properties by *ab initio* methods. *J. Chem. Soc. Faraday Trans. II* **84**, 1247–1261. (doi:10.1039/f29888401247)
- Baiocchi, F. A., Reiher, W. & Klemperer, W. 1983 Do electrostatic interactions predict structures of van der Waals molecules? *J. Chem. Phys.* **79**, 6428–6429. (doi:10.1063/1.445722)
- Bancewicz, T., Nowicka, K., Godet, J. L. & Le Duff, Y. 2004 Multipolar polarizations of methane from isotropic and anisotropic collision-induced light scattering. *Phys. Rev. A* **69**, 062704. (doi:10.1103/PhysRevA.69.062704)
- Barron, L. D. 2015 The development of biomolecular Raman optical activity spectroscopy. *Biomed. Spectr. Imag.* **4**, 223–253. (doi:10.3233/BSI-150113)
- Bishop, D. M. 1994 Aspects of non-linear-optical calculations. In *Advances in quantum chemistry*, vol. 25 (ed. P.-O. Löwdin), pp. 1–45. San Diego, CA: Academic Press.
- Bogaard, M. P. & Orr, B. J. 1975 Electric dipole polarisabilities of atoms and molecules. In *International review of science: physical chemistry*, Ser. II, vol. 2 (ed. A. D. Buckingham), pp. 149–194. London, UK: Butterworths.
- Burnell, E. E., de Lange, C. A. & Snijders, J. G. 1982 Nuclear magnetic resonance study of H₂, HD and D₂ in nematic solvents. *Phys. Rev. A* **25**, 2339–2350. (doi:10.1103/PhysRevA.25.2339)
- Burnell, E. E., de Lange, C. A., Segre, A. L., Capitani, D., Angelini, D., Lilla, G. & Barnhoorn, J. B. S. 1997 Tritium nuclear magnetic resonance study of T₂, HT and DT dissolved in nematic solvents. *Phys. Rev. E* **55**, 496–503. (doi:10.1103/PhysRevE.55.496)
- Clary, D. C. & Orr, B. J. (eds). 1997 *Optical, electric and magnetic properties of molecules: a review of the work of A. D. Buckingham*. Amsterdam, The Netherlands: Elsevier.
- Ekundayo, J. M., Rezaee, R. & Fan, C. 2021 Experimental investigation and mathematical modelling of shale gas adsorption and desorption hysteresis. *J. Nat. Gas Sci. Engng.* **88**, 103761. (doi:10.1016/j.jngse.2020.103761)
- Franken, P. A. & Ward, J. F. 1963 Optical harmonics and nonlinear phenomena. *Rev. Mod. Phys.* **35**, 23–39. (doi:10.1103/RevModPhys.35.23)
- Gray, C. G., Gubbins, K. E. & Joslin, C. G. 1997 *Theory of molecular fluids*, vol. 2. Oxford, UK: Clarendon Press.
- Klemperer, W. 1982 Conference discussion. *Faraday Discuss. Chem. Soc.* **73**, 126.
- Orr, B. J. & Ward, J. F. 1971 Perturbation theory of the non-linear optical polarization of an isolated system. *Mol. Phys.* **20**, 513–526. (doi:10.1080/00268977100100481)

- Ren P., Chun, J., Thomas, D. G., Schnieders, M. J., Marucho, M., Zhang, J. & Baker, N. A. 2012 Bio-molecular electrostatics and solvation: a computational perspective. *Q. Rev. Biophys.* **45**, 427–491. (doi:10.1017/S003358351200011X)
- Saupe, A. & Englert, G. 1963 High-resolution nuclear magnetic resonance spectra of orientated molecules. *Phys. Rev. Lett.* **11**, 462–464. (doi:10.1103/PhysRevLett.11.462)
- Shelton, D. P. & Rice, J. E. 1994 Measurements and calculations of the hyperpolarizabilities of atoms and small molecules in the gas phase. *Chem. Rev.* **94**, 3–29. (doi:10.1021/cr00025a001)
- White, R. P., Lipson, J. E. G. & Higgins, J. S. 2010 Effect of deuterium substitution on the physical properties of polymer melts and blends. *Macromolecules* **43**, 4287–4293. (doi:10.1021/ma902707u)

BIBLIOGRAPHY

The following publications are those referred to directly in the text. A full bibliography is available as electronic supplementary material at <https://doi.org/10.1098/rsbm.2021.0026>.

- (1) 1953 The dielectric constant of a liquid. *Aust. J. Chem.* **6**, 93–103. (doi:10.1071/CH9530093)
- (2) 1955 (With J. A. Pople) The statistical mechanics of imperfect polar gases. I: Second virial coefficients. *Trans. Faraday Soc.* **51**, 1173–1179. (doi:10.1039/TF9555101173)
- (3) (With J. A. Pople) The statistical mechanics of imperfect polar gases. II: Dielectric polarization. *Trans. Faraday Soc.* **51**, 1179–1183. (doi:10.1039/TF9555101179)
- (4) (With J. A. Pople) Theoretical studies of the Kerr effect I: Deviations from a linear polarization law. *Proc. Phys. Soc. A* **68**, 905–909. (doi:10.1088/0370-1298/68/10/307)
- (5) (With J. A. Pople) Theoretical studies of the Kerr effect II: The influence of pressure. *Proc. Phys. Soc. A* **68**, 910–919. (doi:10.1088/0370-1298/68/11/525)
- (6) 1956 Birefringence resulting from the application of an intense beam of light to an isotropic medium. *Proc. Phys. Soc. B* **69**, 344–349. (doi:10.1088/0370-1301/69/3/309)
- (7) 1959 Direct method of measuring molecular quadrupole moments. *J. Chem. Phys.* **30**, 1580–1585. (doi:10.1063/1.1730242)
- (8) Molecular quadrupole moments. *Q. Rev. Chem. Soc. Lond.* **13**, 183–214. (doi:10.1039/qr9591300183)
- (9) 1960 Solvent effects in vibrational spectroscopy. *Trans. Faraday Soc.* **56**, 733–760. (doi:10.1039/TF9605600753)
- (10) 1963 (With R. L. Disch) The quadrupole moment of the carbon dioxide molecule. *Proc. R. Soc. Lond. A* **273**, 275–289. (doi:10.1098/rspa.1963.0088)
- (11) (With K. A. McLauchlan) The absolute sign of the spin-spin coupling constant. *Proc. Chem. Soc.* **1963**, 144. (doi:10.1039/PS9630000125)
- (12) 1964 (With N. J. Bridge) Polarization of laser light scattered by gases. *J. Chem. Phys.* **40**, 2733–2734. (doi:10.1063/1.1725590)
- (13) 1965 Experiments with oriented molecules (Chemical Society Tilden Lecture). *Chem. Brit.* **1**, 54–59.
- (14) 1966 (With M. Pariseau) Molecular quadrupole moments: quantum corrections to the classical formula. *Trans. Faraday Soc.* **62**, 1–6. (doi:10.1039/TF9666200001)
- (15) Theory of long-range dispersion forces. *Discuss. Faraday Soc.* **40**, 232–238. (doi:10.1039/df9654000232)
- (16) (With P. J. Stephens) Magnetic optical activity. *Annu. Rev. Phys. Chem.* **17**, 399–432. (doi:10.1146/annurev.pc.17.100166.002151)
- (17) (With N. J. Bridge) The polarization of laser light scattered by gases. *Proc. R. Soc. Lond. A* **295**, 334–349. (doi:10.1098/rspa.1966.0244)
- (18) 1967 (With K. A. McLauchlan) High resolution nuclear magnetic resonance in partially oriented molecules. *Prog. Nucl. Magn. Reson. Spectrosc.* **2**, 63–109. (doi:10.1016/0079-6565(67)80003-7)
- (19) (With M. P. Bogaard & B. J. Orr) Kerr dispersion of atomic sodium and lithium. *Mol. Phys.* **13**, 533–545. (doi:10.1080/00268976700101461)

- (20) Permanent and induced molecular moments and long-range intermolecular forces. *Adv. Chem. Phys.* **12**, 107–142. (doi:10.1002/9780470143582.ch2)
- (21) 1968 (With H. C. Longuet-Higgins) The quadrupole moments of dipolar molecules. *Mol. Phys.* **14**, 63–72. (doi:10.1080/00268976800100051)
- (22) (With B. J. Orr) Electric birefringence in molecular hydrogen. *Proc. R. Soc. Lond. A* **305**, 259–269. (doi:10.1098/rspa.1968.0117)
- (23) (With R. L. Disch & D. A. Dunmur) The quadrupole moments of some simple molecules. *J. Am. Chem. Soc.* **90**, 3104–3107. (doi:10.1021/ja01014a023)
- (24) (With D. A. Dunmur) Kerr effect in inert gases and sulphur hexafluoride. *Trans. Faraday Soc.* **64**, 1776–1783. (doi:10.1039/TF9686401776)
- (25) (With E. E. Burnell & C. A. de Lange) NMR spectra of hydrogen in a nematic phase. *Chem. Commun.* **1968**, 1408–1409. (doi:10.1039/c1968001408b)
- (26) 1969 (With B. J. Orr) Kerr effect in methane and its four fluorinated derivatives. *Trans. Faraday Soc.* **65**, 673–681. (doi:10.1039/TF9696500673)
- (27) 1970 (With D. A. Ramsay & J. Tyrrell) Electric dipole moment of formaldehyde in the first 3A_2 excited state. *Can. J. Phys.* **48**, 1242–1253. (doi:10.1139/p70-156)
- (28) (With B. J. Orr & J. M. Sichel) Angular distribution and intensity in molecular photoelectron spectroscopy. I: General theory for diatomic molecules. *Phil. Trans. R. Soc. Lond. A* **268**, 147–157. (doi:10.1098/rsta.1970.0068)
- (29) 1971 (With J. M. Brown & D. A. Ramsay) Studies of the Kerr effect in high resolution spectroscopy. *Can. J. Phys.* **49**, 914–931. (doi:10.1139/p71-110)
- (30) (With L. D. Barron) Rayleigh and Raman scattering from optically active molecules. *Mol. Phys.* **20**, 1111–1119. (doi:10.1080/00268977100101091)
- (31) 1972 (With L. D. Barron) Rayleigh and Raman scattering by molecules in magnetic fields. *Mol. Phys.* **23**, 145–150. (doi:10.1080/00268977200100121)
- (32) The Stark effect. In *International review of science: physical chemistry*, ser. I, vol. 3 (ed. D. A. Ramsay), pp. 73–117. London, UK: Butterworths.
- (33) 1973 (With L. D. Barron & M. P. Bogaard) Raman scattering of circularly polarized light by optically active molecules. *J. Am. Chem. Soc.* **95**, 603–605. (doi:10.1021/ja00783a058)
- (34) (With L. D. Barron & M. P. Bogaard) Raman scattering of right and left circularly polarized light by asymmetric molecules. *Nature* **241**, 113–114. (doi:10.1038/241113a0)
- (35) 1974 Molecular structure determination by NMR spectroscopy. *Pure Appl. Chem.* **40**, 1–11. (doi:10.1351/pac197440010001)
- (36) 1975 (With W. Urland) Isotope effects on molecular properties. *Chem. Rev.* **75**, 113–117. (doi:10.1021/cr60293a005)
- (37) (With L. D. Barron) Rayleigh and Raman optical activity. *Annu. Rev. Phys. Chem.* **26**, 381–396. (doi:10.1146/annurev.pc.26.100175.002121)
- (38) 1976 (With J. M. Brown & D. A. Ramsay) High resolution studies of magnetic optical activity in the 3A_2 – 1A_1 system of formaldehyde. *Can. J. Phys.* **54**, 895–906. (doi:10.1139/p76-105)
- (39) 1977 (With G. C. Tabisz) Collision-induced rotational Raman scattering. *Opt. Lett.* **1**, 220–222. (doi:10.1364/OL.1.000220)
- (40) 1978 (With G. C. Tabisz) Collision-induced rotational Raman scattering by tetrahedral and octahedral molecules. *Mol. Phys.* **36**, 583–596. (doi:10.1080/00268977800101771)
- (41) (With M. P. Bogaard, R. K. Pierens & A. H. White) Rayleigh scattering depolarization ratio and molecular polarizability anisotropy for gases. *J. Chem. Soc. Faraday Trans. I* **74**, 3008–3015. (doi:10.1039/f19787403008)
- (42) 1980 (With H. G. E. Hentschel) Partial miscibility of liquid mixtures of protonated and deuterated high polymers. *J. Polymer Sci. B Polymer Phys.* **18**, 853–861. (doi:10.1002/pol.1980.180180416)
- (43) 1981 (With H.-O. Hamaguchi & I. Suzuki) Determination of derivatives of the polarizability anisotropy in diatomic molecules I: theoretical considerations on vibration-rotation Raman intensities. *Mol. Phys.* **43**, 963–973. (doi:10.1080/00268978100101791)
- (44) 1982 (With D. P. Shelton) Optical second-harmonic generation in gases with a low-power laser. *Phys. Rev. A* **26**, 2787–2798. (doi:10.1103/PhysRevA.26.2787)

- (45) 1985 (With P. W. Fowler) A model for the geometries of van der Waals complexes. *Can. J. Chem.* **63**, 2018–2025. (doi:10.1139/v85-334)
- (46) 1994 The theoretical background to vibrational optical activity. *Faraday Discuss.* **99**, 1–12. (doi:10.1039/fd9949900001)
- (47) 1998 Molecules in optical, electric and magnetic fields: a personal perspective. *Annu. Rev. Phys. Chem.* **49**, xiii–xxxv. (doi:10.1146/annurev.physchem.49.1.0)
- (48) 2004 Chirality in NMR spectroscopy. *Chem. Phys. Lett.* **398**, 1–5. (doi:10.1016/j.cplett.2004.08.046)
- (49) 2008 (With J. E. Del Bene & S. A. C. McDowell) The hydrogen bond. *Chem. Phys. Lett.* **463**, 1–10. (doi:10.1016/j.cplett.2008.06.060)
- (50) 2009 (With J. Ringrose) The Foundress's Cup of Pembroke College, Cambridge. *Silver Stud.* **25**, 14–19.
- (51) 2010 (With L. D. Barron) Vibrational optical activity. *Chem. Phys. Lett.* **492**, 199–213. (doi:10.1016/j.cplett.2010.03.090)
- (52) 2017 Fifty years of *Chemical Physics Letters*. *Chem. Phys. Lett.* **684**, 443–445. (doi:10.1016/j.cplett.2017.02.061)