

Amyand David Buckingham 1930–2021*

Sir David C. Clary^A and Brian J. Orr^{B,C}

^ADepartment of Physical and Theoretical Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QZ, UK.

^BEmeritus Professor (Molecular and Optical Physics), Faculty of Science and Engineering, Macquarie University, Sydney, NSW 2109, Australia.

^CCorresponding author. Email: brian.orr@mq.edu.au

Professor A. David Buckingham CBE FRS FAA made fundamental theoretical and experimental 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 took his PhD at the University of Cambridge, UK. He moved to Oxford in 1955 and then in 1965 became Professor of Theoretical Chemistry at the University of Bristol. Finally, he moved back to Cambridge in 1969 for twenty-eight years as Professor of Chemistry and head of a distinguished Department of Theoretical Chemistry. A man of broad interests and achievements, he played first class cricket in the 1950s.

Published online 18 January 2022

Early life and education (1930–53)

David Buckingham (Fig. 1) was born in Sydney on 28 January 1930. He grew up on Sydney's North Shore 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), as shown in Fig. 2. His parents were born in England, emigrating separately to Australia before World War 1 and marrying in 1923. For over forty years, Reginald worked for Dalgety and Co. Limited, serving the rural sector. Grace trained as a nurse in wartime London and came back to Australia in 1920, and was involved in helping to develop the nation's early baby-health clinics; she returned to England eleven years after Reginald's death in 1956. David's first name, Amyand (the 'A' in the 'ADB' acronym used by his colleagues), had Huguenot origins on Grace's side of the family. Among these ancestors was Claudius Amyand, who was elected Fellow of the Royal Society (FRS) in 1716 and was 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 treasured his Australian origins throughout his life.¹

David attended Barker College, where, in 1947, he was both head prefect and dux. He and his brother Michael (who had also been Barker's dux two years earlier) both studied in the Faculty of Science at the University of Sydney. They would each win a University Medal (Michael's in physics and David's in chemistry) before going to England to study for their respective doctorates. Only Michael would return permanently to Australia, as a prominent physicist at the Universities of Sydney and of Western Australia, where he was Professor of Theoretical Physics (1964–92). David has written that he learned from Michael 'the importance of mathematics and fundamentals'—as was amply demonstrated throughout David's career in molecular science.² His talented cohort of first-year undergraduates in 1948 included four future



ADBuckingham

Fig. 1. Professor A. David Buckingham, together with his characteristic signature.

Fellows of the Royal Society (Owen M. Phillips, Alan M. Sargeson, J. Stewart Turner, and him) and others who would become Fellows of the Australian Academy of Science (AAS), including Neville H. Fletcher. The group of science students with whom he took his MSc in 1953 are shown in Fig. 3. During his six years in the Sydney academic community, David overlapped with many students and staff members who were (already or later) pivotal figures in Australian science.

* This article is adapted from a memoir that was commissioned by the Royal Society and will appear in Volume 72 (2022) of *Biographical Memoirs of Fellows of the Royal Society*. It is published here with minor amendments to the original memoir.

¹ Clary and Orr (1997a); Buckingham (1998).

² Buckingham (1998).



Fig. 2. Young David Buckingham (right) aged 9, with sister Joslin and brother Michael.



Fig. 3. Graduating Science students at Sydney University in 1953. David Buckingham is fourth from the right. Second from the right is inorganic chemist Alan Sargeson, another member of the 1948 cohort who was later elected FRS and FAA.

During 1951–3, David's BSc Honours and MSc research projects were supervised by Professor of Chemistry, R. J. W. Le Fèvre, an internationally renowned physical-organic chemist who was a founding member of the AAS in 1954, and was elected FRS in 1959.³ In the Le Fèvre tradition of interpreting electric dipole 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'.⁴ He published as many as eight papers during his two and a half years as a research student at Sydney University.

David excelled at cricket, captaining Barker College's First XI in 1946 and 1947 and gaining a cricket blue at Sydney University.

Early in 1952, after David had graduated with a University Medal in chemistry and the Masson Memorial Scholarship of the Royal Australian Chemical Institute (RACI), a Sydney newspaper published a short item headlined 'Cricketer gets degree'.⁵

PhD at Cambridge (1953–5)

In 1953, David gained a Shell Postgraduate Scholarship at Cambridge in the Department of Theoretical Chemistry headed by Sir John Lennard-Jones—a prominent name in the field of intermolecular forces where David himself would later gain comparable fame. However, because Lennard-Jones was about to leave Cambridge, David became the first PhD student of John Pople, who was

³ Aroney and Buckingham (1988).

⁴ Buckingham (1953).

⁵ A copy of a press clipping, probably from the *Sydney Morning Herald* in March 1952, has been provided by the Buckingham family.

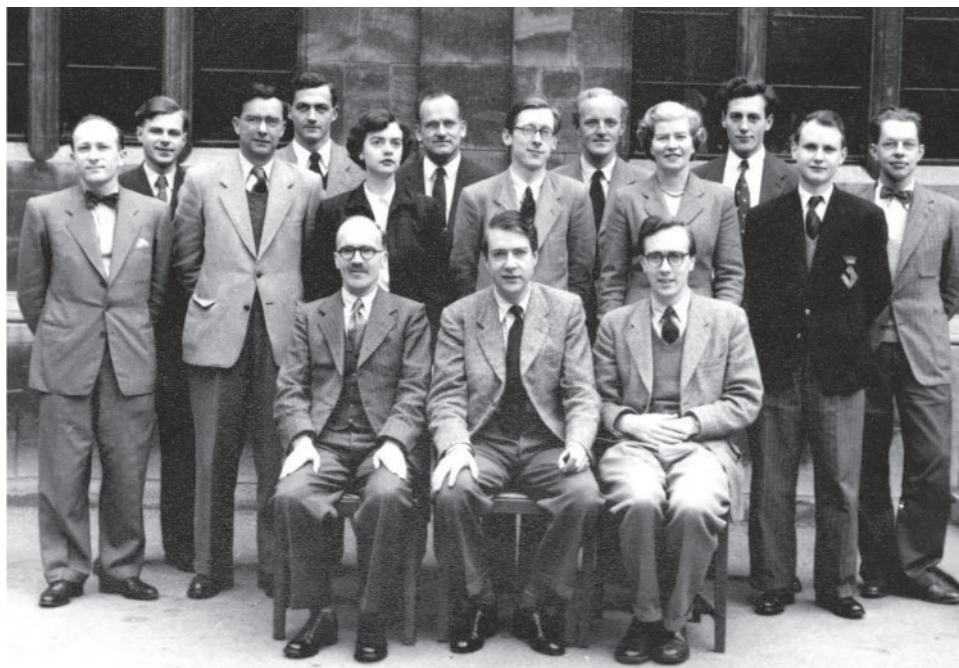


Fig. 4. The theoretical chemists at Cambridge University in 1955. David Buckingham is third from the right in the back row looking over the shoulder of John Pople. In the front row are Frank Boys, Christopher Longuet-Higgins and George Hall.

only four years older than he. Pople, who would win a Nobel Prize in 1998 for computational methods in quantum chemistry, was elected FRS in 1961 and knighted (KBE) in 2003.⁶ The Cambridge theoretical chemistry group of that era is depicted in Fig. 4.

Buckingham and Pople generated many influential publications on dielectric properties of imperfect gases and hyperpolarization of molecules. David has 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’.⁷ Likewise, Pople has extolled David’s leading role in generating their prolific research output and declared: ‘In retrospect, it is hard to imagine a more fortunate start than acquiring someone like David Buckingham as a first student!’⁸

Oxford (1955–65)

After completing his PhD in two years, David moved in 1955 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 expected to be a ‘useful probe of anisotropic intermolecular potentials’.⁹ 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 (who was elected FRS in 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 NMR spectra.

At Oxford, David 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’—an allusion to the so-called Home Counties surrounding Greater London.

From 1959 onwards, David’s experimental work was able to take advantage of superior facilities and technical support at Teddington in the National Physical Laboratory (NPL) where Pople had become superintendent of the Basic Physics Division. There, David¹⁰ and postdoctoral fellow Ray Disch (from Harvard)¹¹

⁶ Buckingham (2006).

⁷ Clary and Orr (1997b), p. 5.

⁸ Pople (1997), p. xiii.

⁹ Buckingham (1998), p. xvii.

¹⁰ Buckingham (1959a); Buckingham (1959b).

¹¹ Buckingham and Disch (1963).

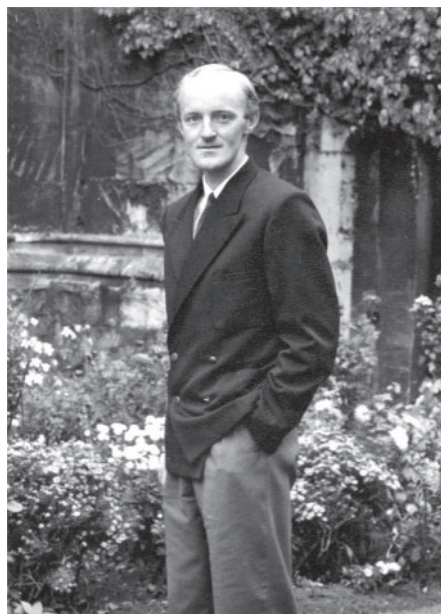


Fig. 5. David Buckingham in the gardens of Christ Church, Oxford in 1955.

realised a novel birefringence experiment to directly measure 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’.

At Oxford (Fig. 5) David revelled in the company of personalities in Christ Church’s Senior Common Room. One of these was the poet W. H. Auden to whom, explaining his scientific interests in 1963, David presented a copy of George Gamow’s book *Mr Tompkins in Wonderland*. DPhil student David Dunmur recalls David’s excitement, nine months later, at receiving from Auden a handwritten poem entitled ‘After Reading a Child’s Guide to Modern Physics’—immortalising in poetry the Buckingham enthusiasm for science. His ten years in college, with beautifully furnished rooms (including a Van Dyck painting), heightened 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 in Oxford at Christ Church Cathedral six months later. Jill was David’s discerning and highly supportive partner during more than fifty-five years of marriage.

Bristol (1965–9)

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 at a Faraday Discussion on the theory of long-range intermolecular forces.¹² This also coincided with the arrival of

one of us (BJO) as David’s first research student from his native Australia; twelve 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 Oxford DPhil research), the instruments were moved from NPL to Bristol. The research group in Bristol comprised a lively international brigade from Argentina, Australia, Canada, Nigeria, the Netherlands, and the USA (as well as Scotland and Wales), with English locals far outnumbered.

Research carried out in David’s department in Bristol had widespread scientific impact. His outstanding theoretical insight 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 mechanistic investigations of atomic and molecular properties and spectra in gases and condensed phases.¹³

David’s lectures in Bristol were often attended by other academic staff who were keen to learn what they could from their new professor. One day, he paused to ask the audience: ‘Is that clear?’. The loud 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 top chemistry departments around the world. He had formal offers of tempting positions from several leading universities such as MIT, Toronto, Manchester, and Cambridge. The opportunity to return to Cambridge in 1969, where he had completed his PhD fourteen 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) had 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; a unified department of chemistry was not formed until 1988. David was elected a Professorial Fellow at Pembroke College in 1970.

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

Boys was followed in quantum chemistry by Nicholas Handy, who became a close colleague of David. Other university appointments that David made included Paul Madden, David Clary, and David Wales. These four were later elected FRS, as were others in David’s department, including Laurence Barron, Ruth Lynden-Bell,

¹² Buckingham (1965b).

¹³ Buckingham (1967); Klemperer (1997).

Patrick Fowler, Jeremy Hutson, and Tim Softley. With colleagues such as Barron and Softley, David continued to promote experimental work ‘to keep the theoreticians honest’, as he would often explain.

David considered the weekly seminars in theoretical chemistry to be the heart of his department. He would sit in the front row and invariably ask the first question. Also, he always gave the first seminar at the beginning of each 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 he had done in Bristol, David gave wise advice and support to the theoretical chemistry students and academics in his department and followed their careers with interest. He went out of his way to welcome students and postdoctoral researchers from overseas (Fig. 6).



Fig. 6. David Buckingham in his office at the University Chemical Laboratory, Lensfield Road, Cambridge.

For over twenty-five years, David presented undergraduate lectures on quantum mechanics, targeting the top students in Natural Sciences to inspire them to undertake PhDs in his department. Peter Knowles, Professor of Theoretical Chemistry at Cardiff University, said: ‘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.’

David continued to attract first-rate PhD students and postdoctoral researchers to his group. He encouraged students to develop their own ideas and sometimes 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 useful *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 (1987–9). He was on the Council of the Royal Society (1999–2001) and served on several of its committees.

When David retired in 1997 a major conference in his honour was held at Pembroke College. A book describing his career with expert comments on some of his major papers was published.¹⁴ Fig. 7 shows David and Jill Buckingham with plenary speakers Ahmed Zewail, John Pople and Bill Klemperer. This gathering 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. He was elected Honorary Fellow of Pembroke in 2005. He continued to publish original papers until shortly before he died, addressing frontiers such as: nonlinear-optical effects in small chiral molecules; NMR-modulated neutron scattering; time-reversal and molecular properties; discrimination of molecular chirality by NMR.¹⁵



Fig. 7. Ahmed Zewail, John Pople, David Buckingham, Jill Buckingham and Bill Klemperer at the 1997 conference.

¹⁴ Clary and Orr (1997a).

¹⁵ Buckingham (2004).

Major scientific contributions

David Buckingham made many significant theoretical and experimental contributions to the understanding of optical, electric and magnetic properties of molecules. Over 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. 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 about finding new phenomena, insights or techniques. 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 summarised below, as further detailed in the book that celebrates his career,¹⁶ and in an autobiographical review.¹⁷

Imperfect polar gases

With John Pople, David published statistical-mechanical theories of imperfect polar gases, extending beyond permanent electric dipole moments to include dipole-(induced dipole) interactions and quadrupole forces.¹⁸ Detailed expressions were derived for the second density virial coefficients from force fields. Calculations of second dielectric virial coefficients also showed that dipole interactions increase the total polarization and that molecular-shape effects are significant. 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 insight into infrared and Raman spectra of dense fluids.¹⁹ Solvent-solute interactions cause such spectra to differ from those in the gas phase and he realised that spectra of dense fluids could give new information on intermolecular forces. David used equilibrium statistical mechanics to develop a theory for spectral shifts, widths and intensities.²⁰ He was the first to calculate moments for infrared and Raman spectra, yielding new predictions

that agree with experiment. 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 (including all degrees of freedom, quantum effects, and increasingly more accurate potential energy surfaces) have enabled detailed prediction of solvent effects.²¹ However, compared to extensive computations, David's analytical predictions frequently offer more direct insight into underlying intermolecular forces.

Experiments with oriented molecules

In 1964, David delivered his prestigious Tilden Lecture to the Chemical Society in London.²² Although most of his publications were specialised and pitched to the scientific cognoscenti, this article addressed 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. Orientation mechanisms in external fields, such as birefringence experiments including the electro-optic Kerr effect and measurement of quadrupole moments, are discussed. The final part of the paper gives a forward-looking description of NMR measurements in which the absolute sign of spin-spin coupling is determined by orienting molecules in an electric field.²³

David's Tilden Lecture article also mentions what was then the latest observation that a magnetic field could substantially orient molecules in a liquid-crystal solvent.²⁴ In Bristol, this became a highly productive research area for him and his PhD students Elliott Burnell and Kees de Lange.²⁵ It is notable that even H₂ molecules are partially aligned in a nematic solvent,²⁶ leading to new research on subtle quantum-rotor effects in subsequent liquid-crystal NMR studies of all the H, D and T isotopic variants of molecular hydrogen.²⁷

Measurement of electric multipole moments

Throughout his career, David studied physical processes influenced by molecular multipole moments.²⁸ His earliest research at Sydney University concerned extraction of 'true' electric dipole moments (symbolised by a vector $\mu^{(0)}$),²⁹ equivalent to those measured in the gas phase, from experiments on small molecules in dilute solution or in dense fluids.

A major contribution comprised experimental evaluation of molecular electric quadrupole moments (symbolised by a second-

¹⁶ Clary and Orr (1997a). This celebratory book contains expert review chapters by D. A. Dunmur, G. L. D. Ritchie (with R. L. Disch), M. P. Bogaard, A. J. Stone, W. Klemperer, A. C. Legon, C. G. Gray and C. G. Joslin, C. A. de Lange, J. F. Ward, L. D. Barron, C. J. Jameson, and E. E. Burnell, with forewords by J. A. Pople, D. R. Herschbach, J. M. Thomas, and A. H. Zewail. This book was published by Elsevier in recognition of A. D. Buckingham's service as a scientific editor over many years.

¹⁷ Buckingham (1998).

¹⁸ Buckingham and Pople (1955a); Buckingham and Pople (1955b).

¹⁹ Buckingham (1960).

²⁰ Gray and Joslin (1997).

²¹ Gray, Gubbins and Joslin (2011).

²² Buckingham (1965a).

²³ Buckingham and McLauchlan (1963).

²⁴ Saupe and Englert (1963).

²⁵ Buckingham and McLauchlan (1967); Buckingham (1974); Burnell (1997).

²⁶ Buckingham, Burnell and de Lange (1968).

²⁷ Burnell and others (1982); Snijders and others (1983); Burnell and others (1997); Burnell (1997).

²⁸ Buckingham (1970); Buckingham (1972).

²⁹ Buckingham (1953).

rank tensor $\Theta^{(0)}$, which indicate the distribution of electric charge in a molecule. The 1936 Nobel Laureate Peter Debye, 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 $\Theta^{(0)}$. Debye was prompted by the ingenious optical measurement of $\Theta^{(0)}$ for carbon dioxide,³⁰ where 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 anisotropically polarizable molecules. David and his co-workers published later quadrupolar birefringence results.³¹ David Dunmur, who for his DPhil added a HeNe laser and refined electronics to the NPL apparatus, notes that their paper has been cited in mineralogical modelling of nitrogen adsorption in extraction of Australian shale gas.³² Remarkably, the current experimental value of the quadrupole moment of CO₂ is virtually identical to that originally reported.³³

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 semiclassical formalism for electromagnetic scattering from molecules that went beyond the electric-dipole approximation.³⁴ This landmark paper has been reviewed by Bill Klemperer.³⁵

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. Also, David’s expressions for long-range intermolecular forces are nowadays used routinely in simulations of complex systems including fluids, materials and biomolecules. This paper chose several examples: a point charge interacting with linear and tetrahedral molecules; 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 by David’s colleagues Nicholas Handy and Roger Amos,³⁶ later enabled accurate computation of various higher-order moments and polarizabilities that David’s group had previously derived from experimental measurements.

First- and higher-order polarizabilities

Associated with permanent electric multipole moments ($\mu^{(0)}$, $\Theta^{(0)}$, ...) 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 and γ , ... together with additional quadrupolar tensors \mathbf{A} , \mathbf{B} and \mathbf{C} arising from an electric field gradient \mathbf{F}' .³⁷ Expansions were made of field-dependent electric-moment vectors μ and Θ , as well as the magnetic-moment vector \mathbf{m}' (with field-induced terms added to the permanent paramagnetic moment $\mathbf{m}^{(0)}$) in a semiclassical periodic electromagnetic field; this introduces additional tensors, including diamagnetic susceptibilities. The ‘quadrupole moment paradox’, in which $\Theta^{(0)}$ for a dipolar molecule is origin-dependent, was finally resolved³⁸ in terms of an effective quadrupole centre about which the first moment of polarizability anisotropy is zero; this is defined by real tensors \mathbf{A} and \mathbf{G} , which are cross-term polarizabilities of μ with Θ and \mathbf{m} , respectively.

The anisotropy $\Delta\alpha$ of the molecular optical polarizability is needed to interpret birefringence experiments, such as the above-mentioned electric quadrupole-moment measurements.³⁹ For his DPhil, James Bridge refined techniques to measure depolarization ratios of Rayleigh light scattering to yield various $\Delta\alpha$ values,⁴⁰ which were later expanded by Martin Bogaard and others.⁴¹ A review of electric-dipole polarizabilities and hyperpolarizabilities in a volume edited by David covered interests of his Oxford and Bristol research groups.⁴² Polarizability anisotropy derivatives with respect to internuclear distance were also evaluated,⁴³ by measuring intensity ratios for depolarized and polarized Raman scattering from diatomic molecules on specific rotational lines. Later significant research on vibrational contributions to hyperpolarizabilities such as β and γ is also relevant.⁴⁴

Differential light scattering and optical activity

David’s fascination with chiral effects (in both molecules and light) led to a fruitful collaboration in Cambridge with postdoctoral fellow Laurence Barron. Together, they developed semi-classical theories of Rayleigh and Raman scattering from optically active molecules,⁴⁵ and magnetic optical activity in light scattering from achiral molecules.⁴⁶ These, as well as vibrational optical activity, are

³⁰ Buckingham and Disch (1963).

³¹ Buckingham, Disch and Dunmur (1968).

³² Ekundayo, Rezaee and Fan (2021).

³³ Ritchie and Disch (1997).

³⁴ Buckingham (1967).

³⁵ Klemperer (1997).

³⁶ Amos and others (1988).

³⁷ Buckingham (1967).

³⁸ Buckingham and Longuet-Higgins (1968).

³⁹ Buckingham and Disch (1963); Buckingham, Disch and Dunmur (1968); Ritchie and Disch (1997).

⁴⁰ Bridge and Buckingham (1964); Bridge and Buckingham (1966).

⁴¹ Bogaard and others (1978); Bogaard (1997).

⁴² Bogaard and Orr (1975).

⁴³ Buckingham, Hamaguchi and Suzuki (1981); Bogaard (1997).

⁴⁴ Shelton and Rice (1994); Bishop (1994).

⁴⁵ Barron and Buckingham (1971).

⁴⁶ Barron and Buckingham (1972).

addressed in various reviews,⁴⁷ including high relevance to studies of biomolecules. The first successful Raman circular intensity differential experiments were realised in Cambridge by Barron, Bogaard and Buckingham.⁴⁸

Nonlinear optics

For his PhD, David predicted observables of gas-phase electric birefringence (electro-optic Kerr effect) experiments.⁴⁹ Added to conventional contributions from molecular components of μ and α were extra terms involving hyperpolarizabilities β and γ . The advent of lasers in 1960 led to the new field of nonlinear optics on which much of modern telecom now relies.⁵⁰ It was soon recognised that the above static-field forms of β and γ are closely related to the susceptibilities intrinsic to nonlinear-optical processes.⁵¹

Moreover, David was first to propose an all-optical variant of the Kerr effect,⁵² in which intense light induces birefringence via components of α and γ ; this was a precursor for various four-wave mixing processes in nonlinear optics and optical telecommunications.⁵³

Motivated by David's Kerr-effect theory,⁵⁴ fixed-temperature gas-phase measurements of atoms and quasi-spherical molecules yielded γ values,⁵⁵ while T -dependence studies of non-spherical molecules enabled terms involving μ , α , β and γ to be separated.⁵⁶ As in the case of quadrupolar birefringence,⁵⁷ quantum-statistical corrections are needed to the classically predicted T -dependence of the Kerr effect; these were verified experimentally.⁵⁸

Nonlinear-optical diagrammatic perturbation theory was found to yield divergent formulae for γ when zero static-field frequencies replaced optical frequencies, although realistic results could be derived by double perturbation theory.⁵⁹ A collaboration by one of us (BJO) with John Ward (largely by correspondence and spanning five cities, four countries and five years) eventually resulted in a much-cited formulation to resolve that theoretical anomaly.⁶⁰

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.⁶¹ 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.⁶²

Novel spectroscopic techniques

David's insight into the Stark effect⁶³ and magnetic optical activity⁶⁴ promoted fruitful collaborations on high-resolution Stark or Kerr-effect spectroscopy⁶⁵ and magnetic-rotation spectra⁶⁶ with the group of Donald Ramsay at the National Research Council of Canada.

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.⁶⁷ This speculative paper was later widely cited as 'BOS theory' once high-resolution methods such as ZEKE had enabled rotational-state-resolved PES studies.⁶⁸

Effects of collisions on molecular properties

A seminar by George Tabisz, on sabbatical at Cambridge from Manitoba, led to a major collaboration on how molecular properties are influenced by collisions. Tabisz presented some unexplained features in the Rayleigh scattering of molecules such as CH₄ and CF₄. David's suggestion that electric field gradients in the molecular interactions could be responsible led to what is now known as collision-induced rotational Raman scattering,⁶⁹ higher-order molecular properties were determined from observed scattering data as well as selection rules for rotational transitions in molecular collisions. Other groups advanced this research.⁷⁰ Many of David's

⁴⁷ Barron and Buckingham (1975); Buckingham (1994); Barron (1997); Barron and Buckingham (2010); Barron (2015).

⁴⁸ Barron, Bogaard and Buckingham (1973a); Barron, Bogaard and Buckingham (1973b).

⁴⁹ Buckingham and Pople (1955c); Buckingham and Pople (1955d); Dunmur (1997).

⁵⁰ Franken and Ward (1963).

⁵¹ Buckingham (1965a); Bogaard and Orr (1975).

⁵² Buckingham (1956).

⁵³ Ward (1997).

⁵⁴ Buckingham and Pople (1955c); Buckingham and Pople (1955d); Dunmur (1997).

⁵⁵ Buckingham and Dunmur (1968).

⁵⁶ Buckingham and Orr (1968); Buckingham and Orr (1969).

⁵⁷ Buckingham and Pariseau (1966).

⁵⁸ Buckingham and Orr (1968).

⁵⁹ Buckingham (1962); Bogaard and others (1967).

⁶⁰ Orr and Ward (1971).

⁶¹ Shelton and Buckingham (1982).

⁶² Shelton and Rice (1994).

⁶³ Buckingham (1970); Buckingham (1972).

⁶⁴ Buckingham and Stephens (1966).

⁶⁵ Buckingham and Ramsay (1965); Buckingham, Ramsay and Tyrrell (1970); Brown, Buckingham and Ramsay (1971).

⁶⁶ Brown, Buckingham and Ramsay (1971).

⁶⁷ Buckingham, Orr and Sichel (1970).

⁶⁸ de Lange (1997).

⁶⁹ Buckingham and Tabisz (1977); Buckingham and Tabisz (1978).

⁷⁰ Bancewicz and others (2004).

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 1982 Faraday Discussion in Oxford, Bill Klemperer commented on the structure of a weakly-bound complex formed between formaldehyde and hydrogen fluoride.⁷¹ He discounted electrostatic interactions as the dipole-dipole interaction was almost zero for the observed orientation of molecules in the dimer. David at once proposed that higher moments such as the quadrupole 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.⁷² Stone’s distributed multipole analysis scheme was used 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 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–ClF.⁷³ Nevertheless, subsequent refinements of the model have continued to demonstrate its utility and it has even been extended to the structures of biological molecules.⁷⁴

Isotope effects and hydrogen bonding

David’s understanding of intermolecular forces was applied to the important problem of hydrogen bonding.⁷⁵ He and Werner Urland suggested that hydrogen bonds are generally weaker than deuterium bonds, as bending-vibrational amplitudes for X–H ... Y are greater than for X–D ... Y and the linear configuration is optimum for hydrogen bonding. David and his PhD student George Hentschel examined the importance of this effect on the partial miscibility of protonated and deuterated polymers.⁷⁶ 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.⁷⁷

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.⁷⁸ By considering harmonic and anharmonic vibrations of X–H in various complexes, no fundamental difference was found between blue-shifting and red-shifting bonds. These findings are relevant to structure and properties of water clusters and hydrogen-bonded liquids.

Chirality in NMR spectroscopy

David’s sense of research adventure is well illustrated by his expectation that NMR spectroscopy might be used to discern molecular chirality (that is, to distinguish mirror-image forms of an optically active molecule). The abstract of his first paper on this topic, published in 2004, is reproduced below to demonstrate David’s remarkable ability to deliver an incisive message about a set of complicated physical concepts:

Nuclear magnetic resonance spectra are blind to chirality unless the environment discriminates D and L enantiomers. However, a nuclear magnetic moment in the *x*-direction combined with the strong magnetic field $B_z^{(0)}$ induces, through an odd-parity coupling in a freely tumbling chiral molecule, an electric dipole moment in the *y*-direction. Estimates of the rotating electric polarization at the NMR frequency following a $\pi/2$ pulse indicate that it should be detectable in favourable cases, foreshadowing a new dimension for the NMR spectroscopy of chiral molecules.⁷⁹

In his last years, David was passionate about this quest for an adaptation of NMR that would be ‘of particular interest in the study of molecules of biological importance’. He was involved with colleagues from the Max Planck Society and CNRS in efforts to prove this.

Scientific editing

David was Editor of *Molecular Physics* (1968–72) and *International Reviews in Physical Chemistry* (1981–89). However, he is best remembered as Editor of *Chemical Physics Letters* (1978–99).⁸⁰ He started as editor before the advent of e-mail 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 fifteen authors who published in *Chemical Physics Letters* when David was editor went on to win the Nobel Prize (including his fellow Editor and close friend, Ahmed Zewail).

David Buckingham’s connections with Australia

Throughout his distinguished career, David retained an active interest in Australia’s science (not to mention its cricket and politics!) He was a fellow of the RACI and had won its Masson Memorial Scholarship in 1952 and its Rennie Memorial Medal in 1958. His lectures and personal contact during his regular visits to Australia influenced generations of young Australian scientists. Many of them were PhD-student, postdoctoral and/or sabbatical-leave members of his research groups in Bristol and Cambridge. David was welcomed warmly in numerous Australian research centres and at scientific conferences. He had a particularly strong affinity with Professors David Craig and Noel Hush—his counterpart leaders in theoretical chemistry at the Australian National

⁷¹ Klemperer (1982).

⁷² Buckingham and Fowler (1985); Legon (1997).

⁷³ Baiocchi, Reiher and Klemperer (1983).

⁷⁴ Ren and others (2012).

⁷⁵ Buckingham and Urland (1975).

⁷⁶ Buckingham and Hentschel (1980).

⁷⁷ White, Lipson and Higgins (2010).

⁷⁸ Buckingham, Del Bene and McDowell (2008).

⁷⁹ Buckingham (2004).

⁸⁰ Buckingham (2017).



Fig. 8. David Buckingham presenting a keynote lecture on ‘Intermolecular Forces’ at the fiftieth anniversary celebratory meeting of the Sydney University Chemical Society in March 1979.

University and University of Sydney, respectively—and their research colleagues. [Figure 8](#) shows David lecturing in 1979 in the School of Chemistry from which he had originally graduated.

During his several-months’ stay in Australia in 1979, David revisited his family home in hilly Pymble, introduced himself to the current owner and searched under the house to retrieve his school-days chemistry set, still intact after at least twenty-five years’ storage: a relic that had set him on his career path. More remarkably, at Sydney Airport a few days later with his family looking on, David persuaded airline staff to accept the large cardboard box containing his chemistry set as hand luggage for the return flight to England—thanks to his characteristic blend of winning charm, irrepressible logic and dogged determination!

Honours and awards

In 1997, David was appointed CBE by the Queen. He was elected Fellow of the Royal Society in 1975. In 2008, he was elected as Corresponding Member of the Australian Academy of Science. Other recent major awards include: Foreign Associate of the National Academy of Sciences (USA, 1992); Foreign Honorary Member of the American Academy of Arts and Sciences (1992); Harrie Massey Medal and Prize of the Institute of Physics (1995); Foreign Membership of the Royal Swedish Academy of Sciences (1996); Hughes Medal of the Royal Society (1996); Faraday Lectureship and Prize of the Royal Society of Chemistry (1998); C. H. Townes Award of the Optical Society of America (2001); Ahmed Zewail Prize in Molecular Sciences (inaugural recipient, 2007).

Other interests

Following David’s achievements in cricket at school and university in Australia, he was 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 ([Fig. 9](#)). He was an opening batsman and occasional off-break bowler. He also played first class cricket while a don at Oxford and was treasurer of the Oxford University Cricket Club. On his return to Cambridge as Professor of Chemistry, he became treasurer of the Cambridge University Cricket Club and in 1990 was elected its president, a position he held for nineteen years.

David greatly valued his family life ([Fig. 10](#)). Jill and David’s children (Lucy, Mark and Alice) recall David as a playful father when they were young: reading and inventing stories, playing board games, helping them to develop ball skills and, more importantly, to learn sportsmanship. He would promote conversation about current affairs over breakfast and encourage them with their maths school-work; he repaired the family bicycles and showed the children how to fix their own. During 1981–93, David and Jill found a new pastime: renovating a sixteenth-century house on a fifteen-acre farm in Suffolk. David was able to relax there, working physically rather than mentally, using his carpentry skills, restoring features that had been hidden over the centuries, and connecting with his teenagers. Other lovely homes followed, large enough to accommodate the expanding family’s eight grandchildren. Jill and David provided memorable hospitality for many students, colleagues, academic visitors and friends in their homes in Bristol, Cambridge and Newmarket.

David Buckingham was an exceptionally talented person who always sought excellence. His intellectual and athletic agility served him well in science, sport and daily life. He was quick to speak up for his beliefs and encouraged others to do likewise. His formidable scientific legacy is complemented by the enduring example of his dynamic personality.

After heart failure, David died on 4 February 2021. His COVID-limited funeral on 1 March 2021 (St David’s Day, appropriately) in Pembroke College’s seventeenth-century chapel was attended by one of us (DCC) and broadcast online. His coffin was draped in the Union Jack and the Australian flag. Jill’s floral arrangement comprised eucalyptus foliage and seasonal daffodils—a green-and-gold theme that would have appealed to David’s ‘Aussie’ instincts. The final tribute, presented by Pembroke Emeritus Fellow Michael Kuczynski, described David as ‘unfailingly courteous’ and quoted Robert Louis Stevenson:

That man is a success who has lived well, laughed often, and loved much; who has gained the respect of intelligent men and the love of children; who has filled his niche and accomplished his task; who leaves the world better than he found it ...; who looked for the best in others and gave the best he had.

Conflicts of interest

The authors declare no conflicts of interest. We have each benefited by having David Buckingham as a supportive mentor through much of our respective academic careers.

Declaration of funding

This research did not receive any specific funding.



Fig. 9. Former England cricket captain Ted Dexter with David Buckingham in 1998.



Fig. 10. David and Jill Buckingham in 1993.

Data availability statement

The data used to generate this paper are available on request to the Corresponding Author at brian.orr@mq.edu.au. All illustrations

have been provided with permission by Mrs Jill Buckingham and her family.

Acknowledgements

The authors appreciate much assistance from Mrs Jill Buckingham and her family for providing material used here. 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. Leo Radom has kindly facilitated production of this article on behalf of the AAS.

References

- Amos, R. D., Gaw, J. F., Handy, N. C., and Carter, S. (1988) The accurate calculation of molecular properties by *ab initio* methods, *Journal of the Chemical Society. Faraday Transactions II*, **84**, 1247–1261. doi:[10.1039/F29888401247](https://doi.org/10.1039/F29888401247)
- Aroney, M. J., and Buckingham, A. D. (1988) Raymond James Wood Le Fèvre, *Biographical Memoirs of Fellows of the Royal Society. Royal Society (Great Britain)*, **34**, 373–403. doi:[10.1098/RSBM.1988.0014](https://doi.org/10.1098/RSBM.1988.0014)
- Baiocchi, F. A., Reiher, W., and Klemperer, W. (1983) Do electrostatic interactions predict structures of van der Waals molecules?, *The Journal of Chemical Physics*, **79**, 6428–6429. doi:[10.1063/1.445722](https://doi.org/10.1063/1.445722)
- Bancewicz, T., Nowicka, K., Godet, J. L., and Le Duff, Y. (2004) Multipolar polarizations of methane from isotropic and anisotropic collision-induced light scattering, *Physical Review A*, **69**, 062704. doi:[10.1103/PHYSREVA.69.062704](https://doi.org/10.1103/PHYSREVA.69.062704)
- Barron, L. D. (1997) ‘Vibrational optical activity’, chap. 10 in *Optical, Electric and Magnetic Properties of Molecules—A Review of the Work of A.D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 283–289.

- Barron, L. D. (2015) The development of biomolecular Raman optical activity spectroscopy, *Biomedical Spectroscopy and Imaging*, **4**, 223–253. doi:10.3233/BSI-150113
- Barron, L. D., and Buckingham, A. D. (1971) Rayleigh and Raman scattering from optically active molecules, *Molecular Physics*, **20**, 1111–1119. doi:10.1080/00268977100101091
- Barron, L. D., and Buckingham, A. D. (1972) Rayleigh and Raman scattering by molecules in magnetic fields, *Molecular Physics*, **23**, 145–150. doi:10.1080/00268977200100121
- Barron, L. D., and Buckingham, A. D. (1975) Rayleigh and Raman optical activity, *Annual Review of Physical Chemistry*, **26**, 381–396. doi:10.1146/ANNUREV.PC.26.100175.002121
- Barron, L. D., and Buckingham, A. D. (2010) Vibrational optical activity, *Chemical Physics Letters*, **492**, 199–213. doi:10.1016/J.CPLETT.2010.03.090
- Barron, L. D., Bogaard, M. P., and Buckingham, A. D. (1973a) Raman scattering of circularly polarized light by optically active molecules, *Journal of the American Chemical Society*, **95**, 603–605. doi:10.1021/JA00783A058
- Barron, L. D., Bogaard, M. P., and Buckingham, A. D. (1973b) Raman scattering of right and left circularly polarized light by asymmetric molecules, *Nature*, **241**, 113–114. doi:10.1038/241113A0
- Bishop, D. M. (1994) 'Aspects of non-linear-optical calculations', in *Advances in Quantum Chemistry*, ed. P.-O. Löwdin, San Diego, vol. 25, pp. 1–45. doi:10.1016/S0065-3276(08)60017-9
- Bogaard, M. P. (1997) 'Rayleigh and Raman scattering', chap. 3 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 97–104.
- Bogaard, M. P., and Orr, B. J. (1975) 'Electric dipole polarisabilities of atoms and molecules', chap. 5 in *International Review of Science: Physical Chemistry*, ser. II, vol. 2, ed. A. D. Buckingham, London, pp. 149–194.
- Bogaard, M. P., Buckingham, A. D., and Orr, B. J. (1967) Kerr dispersion of atomic sodium and lithium, *Molecular Physics*, **13**, 533–545. doi:10.1080/00268976700101461
- Bogaard, M. P., Buckingham, A. D., Pierens, R. K., and White, A. H. (1978) Rayleigh scattering depolarization ratio and molecular polarizability anisotropy for gases, *Journal of the Chemical Society, Faraday Transactions I*, **74**, 3008–3015. doi:10.1039/F19787403008
- Bridge, N. J., and Buckingham, A. D. (1964) Polarization of laser light scattered by gases, *The Journal of Chemical Physics*, **40**, 2733–2734. doi:10.1063/1.1725590
- Bridge, N. J., and Buckingham, A. D. (1966) The polarization of laser light scattered by gases, *Proceedings of the Royal Society of London. Series A*, **295**, 334–349. doi:10.1098/RSPA.1966.0244
- Brown, J. M., Buckingham, A. D., and Ramsay, D. A. (1971) Studies of the Kerr effect in high resolution spectroscopy, *Canadian Journal of Physics*, **49**, 914–931. doi:10.1139/P71-110
- Brown, J. M., Buckingham, A. D., and Ramsay, D. A. (1976) High resolution studies of magnetic optical activity in the $^3A_2-^1A_1$ system of formaldehyde, *Canadian Journal of Physics*, **54**, 895–906. doi:10.1139/P76-105
- Buckingham, A. D. (1953) The dielectric constant of a liquid, *Australian Journal of Chemistry*, **6**, 93–103. doi:10.1071/CH9530093
- Buckingham, A. D. (1956) Birefringence resulting from the application of an intense beam of light to an isotropic medium, *Proceedings of the Physical Society. Section B*, **69**, 344–349. doi:10.1088/0370-1301/69/3/309
- Buckingham, A. D. (1959a) Direct method of measuring molecular quadrupole moments, *The Journal of Chemical Physics*, **30**, 1580–1585. doi:10.1063/1.1730242
- Buckingham, A. D. (1959b) Molecular quadrupole moments, *Quarterly Reviews (Chemical Society, London)*, **13**, 183–214. doi:10.1039/QR9591300183
- Buckingham, A. D. (1960) Solvent effects in vibrational spectroscopy, *Transactions of the Faraday Society*, **56**, 753–760. doi:10.1039/TF9605600753
- Buckingham, A. D. (1962) Frequency dependence of the Kerr constant, *Proceedings of the Royal Society of London. Series A*, **267**, 271–282. doi:10.1098/RSPA.1962.0097
- Buckingham, A. D. (1965a) Experiments with oriented molecules (Chemical Society Tilden Lecture), *Chemistry in Britain*, **1**, 54–59.
- Buckingham, A. D. (1965b) Theory of long-range dispersion forces, *Discussions of the Faraday Society*, **40**, 232–238. doi:10.1039/DF9654000232
- Buckingham, A. D. (1967) Permanent and induced molecular moments and long-range intermolecular forces, *Advances in Chemical Physics*, **12**, 107–142. doi:10.1002/9780470143582.CH2
- Buckingham, A. D. (1970) 'Electric moments of molecules', chap. 8 in *Physical Chemistry—an Advanced Treatise*, eds H. Eyring, W. Jost and D. Henderson, New York, pp. 349–386.
- Buckingham, A. D. (1972) 'The Stark effect', chap. 3 in *M. T. P. International Review of Science. Physical Chemistry*, ser. I, vol. 3, ed. D. A. Ramsay, London, pp. 73–117.
- Buckingham, A. D. (1974) Molecular structure determination by NMR spectroscopy, *Pure and Applied Chemistry*, **40**, 1–11. doi:10.1351/PAC197440010001
- Buckingham, A. D. (1994) The theoretical background to vibrational optical activity, *Faraday Discussions*, **99**, 1–12. doi:10.1039/FD9949900001
- Buckingham, A. D. (1998) Molecules in optical, electric, and magnetic fields: a personal perspective, *Annual Review of Physical Chemistry*, **49**, xiii–xxxv. doi:10.1146/ANNUREV.PHYSICHEM.49.1.0
- Buckingham, A. D. (2004) Chirality in NMR spectroscopy, *Chemical Physics Letters*, **398**, 1–5. doi:10.1016/J.CPLETT.2004.08.046
- Buckingham, A. D. (2006) Sir John Anthony Pople, *Biographical Memoirs of Fellows of the Royal Society. Royal Society (Great Britain)*, **52**, 299–314. doi:10.1098/RSBM.2006.0021
- Buckingham, A. D. (2017) Fifty years of *Chemical Physics Letters*, *Chemical Physics Letters*, **684**, 443–445. doi:10.1016/J.CPLETT.2017.02.061
- Buckingham, A. D., and Disch, R. L. (1963) The quadrupole moment of the carbon dioxide molecule, *Proceedings of the Royal Society of London. Series A*, **273**, 275–289. doi:10.1098/RSPA.1963.0088
- Buckingham, A. D., and Dunmur, D. A. (1968) Kerr effect in inert gases and sulphur hexafluoride, *Transactions of the Faraday Society*, **64**, 1776–1783. doi:10.1039/TF9686401776
- Buckingham, A. D., and Fowler, P. W. (1985) A model for the geometries of Van der Waals complexes, *Canadian Journal of Chemistry*, **63**, 2018–2025. doi:10.1139/V85-334
- Buckingham, A. D., and Hentschel, H. G. E. (1980) Partial miscibility of liquid mixtures of protonated and deuterated high polymers, *Journal of Polymer Science. Part B, Polymer Physics*, **18**, 853–861. doi:10.1002/POL.1980.180180416
- Buckingham, A. D., and Longuet-Higgins, H. C. (1968) The quadrupole moments of dipolar molecules, *Molecular Physics*, **14**, 63–72. doi:10.1080/00268976800100051
- Buckingham, A. D., and McLauchlan, K. A. (1963) The absolute sign of the spin-spin coupling constant, *Proceedings of the Chemical Society*, 144. doi:10.1039/PS9630000125
- Buckingham, A. D., and McLauchlan, K. A. (1967) High resolution nuclear magnetic resonance in partially oriented molecules, *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2**, 63–109. doi:10.1016/0079-6565(67)80003-7
- Buckingham, A. D., and Orr, B. J. (1968) Electric birefringence in molecular hydrogen, *Proceedings of the Royal Society of London. Series A*, **305**, 259–269. doi:10.1098/RSPA.1968.0117

- Buckingham, A. D., and Orr, B. J. (1969) Kerr effect in methane and its four fluorinated derivatives, *Transactions of the Faraday Society*, **65**, 673–681. doi:10.1039/TF9696500673
- Buckingham, A. D., and Pariseau, M. (1966) Molecular quadrupole moments—quantum corrections to the classical formula, *Transactions of the Faraday Society*, **62**, 1–6. doi:10.1039/TF9666200001
- Buckingham, A. D., and Pople, J. A. (1955a) The statistical mechanics of imperfect polar gases: I second virial coefficients, *Transactions of the Faraday Society*, **51**, 1173–1179. doi:10.1039/TF9555101173
- Buckingham, A. D., and Pople, J. A. (1955b) The statistical mechanics of imperfect polar gases: II dielectric polarization, *Transactions of the Faraday Society*, **51**, 1179–1183. doi:10.1039/TF9555101179
- Buckingham, A. D., and Pople, J. A. (1955c) Theoretical studies of the Kerr effect I: deviations from a linear polarization law, *Proceedings of the Physical Society. Section A*, **68**, 905–909. doi:10.1088/0370-1298/68/10/307
- Buckingham, A. D., and Pople, J. A. (1955d) Theoretical studies of the Kerr effect II: the influence of pressure, *Proceedings of the Physical Society. Section A*, **68**, 910–919. doi:10.1088/0370-1298/68/10/308
- Buckingham, A. D., and Ramsay, D. A. (1965) Stark modulation in electronic spectroscopy, *The Journal of Chemical Physics*, **42**, 3721–3722. doi:10.1063/1.1695786
- Buckingham, A. D., and Stephens, P. J. (1966) Magnetic optical activity, *Annual Review of Physical Chemistry*, **17**, 399–432. doi:10.1146/ANNUREV.PC.17.100166.002151
- Buckingham, A. D., and Tabisz, G. C. (1977) Collision-induced rotational Raman scattering, *Optics Letters*, **1**, 220–222. doi:10.1364/OL.1.000220
- Buckingham, A. D., and Tabisz, G. C. (1978) Collision-induced rotational Raman scattering by tetrahedral and octahedral molecules, *Molecular Physics*, **36**, 583–596. doi:10.1080/00268977800101771
- Buckingham, A. D., and Urland, W. (1975) Isotope effects on molecular properties, *Chemical Reviews*, **75**, 113–117. doi:10.1021/CR60293A005
- Buckingham, A. D., Burnell, E. E., and de Lange, C. A. (1968) N.M.R. spectra of hydrogen in a nematic phase, *Chemical Communications*, **1408–1409**. doi:10.1039/C1968001408B
- Buckingham, A. D., Disch, R. L., and Dunmur, D. A. (1968) The quadrupole moments of some simple molecules, *Journal of the American Chemical Society*, **90**, 3104–3107. doi:10.1021/JA01014A023
- Buckingham, A. D., Orr, B. J., and Sichel, J. M. (1970) Angular distribution and intensity in molecular photoelectron spectroscopy I: general theory for diatomic molecules, *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences*, **268**, 147–157. doi:10.1098/RSTA.1970.0068
- Buckingham, A. D., Ramsay, D. A., and Tyrrell, J. (1970) Electric dipole moment of formaldehyde in the first 3A_2 excited state, *Canadian Journal of Physics*, **48**, 1242–1253. doi:10.1139/P70-156
- Buckingham, A. D., Del Bene, J. E., and McDowell, S. A. C. (2008) The hydrogen bond, *Chemical Physics Letters*, **463**, 1–10. doi:10.1016/J.CPLETT.2008.06.060
- Burnell, E. E. (1997) ‘Anisotropic NMR’, chap. 12 in *Optical, Electric and Magnetic Properties of Molecules—Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 327–334.
- Burnell, E. E., de Lange, C. A., and Snijders, J. G. (1982) Nuclear magnetic resonance study of H₂, HD, and D₂ in nematic solvents, *Physical Review 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., and Barnhoorn, J. B. S. (1997) Tritium nuclear magnetic resonance study of T₂, HT, and DT dissolved in nematic solvents, *Physical Review. E*, **55**, 496–503. doi:10.1103/PHYSREVE.55.496
- Clary, D. C., and Orr, B. J., eds (1997a) *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, Amsterdam.
- Clary, D. C., and Orr, B. J. (1997b) ‘The career of A. D. Buckingham’, introduction in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 1–15.
- de Lange, C. A. (1997) ‘Towards rotationally resolved photoelectron spectroscopy’, chap. 8 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 231–243.
- Dunmur, D. A. (1997) ‘The electro-optic Kerr effect’, chap. 1 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 41–47.
- Ekundayo, J. M., Rezaee, R., and Fan, C. (2021) Experimental investigation and mathematical modelling of shale gas adsorption and desorption hysteresis, *Journal of Natural Gas Science and Engineering*, **88**, 103761. doi:10.1016/J.JNGSE.2020.103761
- Franken, P. A., and Ward, J. F. (1963) Optical harmonics and nonlinear phenomena, *Reviews of Modern Physics*, **35**, 23–39. doi:10.1103/REVMODPHYS.35.23
- Gray, C. G., and Joslin, C. G. (1997) ‘Solvent effects in vibrational spectra’, chap. 7 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 207–221.
- Gray, C. G., Gubbins, K. E., and Joslin, C. G. (2011) *Theory of Molecular Fluids*, vol. 2, Oxford.
- Hamaguchi, H.-O., Suzuki, I., and Buckingham, A. D. (1981) Determination of derivatives of the polarizability anisotropy in diatomic molecules I: theoretical considerations on vibration-rotation Raman intensities, *Molecular Physics*, **43**, 963–973. doi:10.1080/00268978100101791
- Klemperer, W. (1982) Conference discussion, *Faraday Discussions of the Chemical Society*, **73**, 126.
- Klemperer, W. (1997) ‘Intermolecular forces and molecular moments’, chap. 5 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 149–153.
- Ligon, T. (1997) ‘Van der Waals molecules’, chap. 6 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 191–197.
- Orr, B. J., and Ward, J. F. (1971) Perturbation theory of the non-linear optical polarization of an isolated system, *Molecular Physics*, **20**, 513–526. doi:10.1080/00268977100100481
- Pople, J. A. (1997) ‘... it is hard to imagine a more fortunate start ...’, foreword in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. xiii–xiv.
- Ren, P., Chun, J., Thomas, D. G., Schnieders, M. J., Marucho, M., Zhang, J., and Baker, N. A. (2012) Biomolecular electrostatics and solvation: a computational perspective, *Quarterly Reviews of Biophysics*, **45**, 427–491. doi:10.1017/S003358351200011X
- Ritchie, G. L. D., and Disch, R. L. (1997) ‘Field-gradient induced birefringence: a direct route to molecular quadrupole moments’, chap. 2 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 67–80.
- Saupe, A., and Englert, G. (1963) High-resolution nuclear magnetic resonance spectra of orientated molecules, *Physical Review Letters*, **11**, 462–464. doi:10.1103/PHYSREVLETT.11.462
- Shelton, D. P., and Buckingham, A. D. (1982) Optical second-harmonic generation in gases with a low-power laser, *Physical Review A*, **26**, 2787–2798. doi:10.1103/PHYSREVA.26.2787
- Shelton, D. P., and Rice, J. E. (1994) Measurements and calculations of the hyperpolarizabilities of atoms and small molecules in the gas phase, *Chemical Reviews*, **94**, 3–29. doi:10.1021/CR00025A001

- Snijders, J. G., de Lange, C. A., and Burnell, E. E. (1983) On the orientation mechanism of small molecules in liquid-crystalline environments, *Israel Journal of Chemistry*, **23**, 269–281. doi:[10.1002/IJCH.198300040](https://doi.org/10.1002/IJCH.198300040)
- Ward, J. F. (1997) ‘Nonlinear Optics’, chap. 9 in *Optical, Electric and Magnetic Properties of Molecules—a Review of the Work of A. D. Buckingham*, eds D. C. Clary and B. J. Orr, Amsterdam, pp. 257–262.
- White, R. P., Lipson, J. E. G., and 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](https://doi.org/10.1021/MA902707U)