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JOHN NORMAN MURRELL
2 March 1932 — 25 January 2016
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Elected FRS 1991

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John Murrell was a theoretical chemist who made important contributions to the understanding of the spectra of organic molecules, to the theory of intermolecular forces and to the construction of potential energy surfaces. He established the University of Sussex as a major centre for research and teaching in theoretical chemistry. He was also a successful writer of textbooks for undergraduate and graduate students on chemical bonding and related topics.

EARLY LIFE

John Murrell was born on 2 March 1932 in Brixton, London. At the age of four he moved to Wandsworth. His extended family was colourful and with strong musical interests. His father, who was the first of the family to have a formal education beyond the age of 14, worked for a bakery firm, first as a roundsman and eventually as a senior supervisor. John was an only child. At the start of the Second World War in 1939 the family went to live in Reigate, Surrey, and he started at Reigate Grammar School in 1943. John recalled being very keen on sport at school, and he had vivid memories of the V1 and V2 rockets flying over

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Reigate during the war. In 1947 he took the School Certificate Examination and achieved good grades in mathematics and chemistry, so in the sixth form he studied chemistry, physics, pure mathematics and applied mathematics. A broken arm playing rugby turned his attention to his studies at a crucial time. His Higher Certificates went well and he obtained a pass in physics, credits in chemistry and applied mathematics and a distinction in pure mathematics. He was chosen as Head Boy and he stayed on for a third year in the sixth form to apply to Cambridge University. He applied to Pembroke College, but was informed that they would only consider him for a place after National Service, which was a compulsory 18 months in the military forces. He was then offered a place to study chemistry at King’s College London (KCL) in 1950 and this allowed him to defer National Service.

**King’s College London**

As an undergraduate at KCL, John became interested in the physical side of chemistry and his lecturers included Sir Eric Rideal (FRS 1951). He found the lectures on statistical mechanics particularly inspiring. Despite living at home, he was an active participant in student life. Indeed, at a Saturday night dance he met Shirley Read, who was studying medicine. This was a key meeting as John and Shirley were to marry in Farnborough, Hampshire, in 1954.

John achieved First Class Honours in 1953 and saw a notice encouraging students interested in theoretical chemistry to contact Professor Christopher Longuet-Higgins (FRS 1958) in the Physics Department at KCL. In this way John started his PhD in this group. Through an interaction with Michael Dewar (FRS 1960), Longuet-Higgins had become interested in the electronic spectra of aromatic hydrocarbons and this was the subject of John’s research that he continued for the next 10 years. His first publication was a semi-empirical molecular orbital calculation on the electronic spectrum of the cycloheptatrienyl (tropylium) ion C\(_7\)H\(_7^+\) in 1955 (1) and four more papers quickly followed that year on the calculation of the electronic spectra of aromatic molecules (2–5). By this time, semi-empirical molecular orbital theory had replaced Hückel Theory as a more accurate quantum mechanical approach for calculating energy levels and wave functions for conjugated organic molecules. Although the required calculations were not analytical, with a small basis set of \(\pi\) orbitals the molecular orbital computations could still be carried out without the need for large computers, which had not yet become available in the mid 1950s. It was, however, necessary to make some approximations to the integrals arising from the molecular orbital theory. A paper with Longuet-Higgins, which considered the interaction between the orbitals of the two benzene rings in biphenyl, received over 300 citations, partly due to the many industrial applications of this compound (4).

Longuet-Higgins at that time supervised a small but brilliant group of researchers at KCL. This included Peter Higgs (FRS 1983), who shortly after moved into elementary particle theory, which eventually won him the Nobel Prize for Physics, and Michael Fisher (FRS 1971), who made important contributions in statistical mechanics. Not long after John started his PhD research, Longuet-Higgins took up the Chair of Theoretical Chemistry at the University of Cambridge, replacing Sir John Lennard-Jones (FRS 1935). Accordingly, John and Shirley, by now married, transferred also to Cambridge. He became a graduate student at Corpus Christi College, which was also the college of Longuet-Higgins. Shirley took up a house officer post in Wisbech, Cambridgeshire.
CAMBRIDGE AND CHICAGO

Theoretical chemistry at Cambridge in 1955 was thriving with lecturers such as John Pople (FRS 1961), a subsequent Nobel Prize winner in 1998 for his research on computational chemistry, Frank Boys (FRS 1972), a pioneer in \textit{ab initio} electronic structure theory, George Hall, who made one of the first formulations of self-consistent field molecular orbital theory, and Leslie Orgel (FRS 1962), who made important theoretical contributions to inorganic chemistry and subsequently to biophysics. There were also students such as David Buckingham (FRS 1975) and Lionel Salem, and distinguished visitors including Bob Parr, one of the pioneers first of semi-empirical molecular orbital methodology and then density functional theory. John published several papers as a sole author during this period (something that would be rare for a student nowadays) and also published with Pople on the intensities of the symmetry-forbidden electronic bands of benzene (6) and with Orgel on the sign of the electron spin density on methyl protons in aromatic molecules (7). His research at this time had the distinctive mark of the Longuet-Higgins school of theoretical chemistry—the detailed application of theory to explain experimental results rather than the development of fundamental theory or new computational algorithms.

John finished his PhD in 1956 and he was examined by Charles Coulson (FRS 1950) from Oxford University. With encouragement from Longuet-Higgins, he won a Commonwealth Fund Fellowship to work in the group of Robert Mulliken (ForMemRS 1967) at the University of Chicago. Mulliken was a pioneer in molecular orbital theory, for which he won the Nobel Prize in 1966. At Chicago, John wrote an influential paper on molecular charge transfer in donor–acceptor pairs such as benzene–iodine (8). His calculations suggested that if charge transfer bands appeared, their intensity was related to borrowing from the excited states of the donor molecule.

John then returned to Cambridge to an Assistant in Research post in theoretical chemistry (figure 1) and a Research Fellowship at Corpus Christi College. Shirley had a position in the radiotherapy department at Addenbrooke’s Hospital. They were now able to buy their first house, and their first child, Catharine, was born. By this time, National Service, which he had deferred due to his research activities, had been abolished. He branched out into applications of molecular orbital theory to a variety of topical problems and started new collaborations. An organic chemist from Zurich, Edgar Heilbronner, was a visitor and this allowed a fruitful collaboration to be started on interpreting the spectra of aromatic hydrocarbons (9) that continued for many years with several joint publications. During this period John also became interested in the expanding data becoming available from NMR and ESR experiments on molecules, properties which were becoming readily understood from molecular orbital theory. This enabled him to publish joint papers with leading experimentalists in this field such as Alan Katritzky (FRS 1980) and Norman Sheppard (FRS 1966) (10).

UNIVERSITY OF SHEFFIELD

John was developing a reputation as a theoretician who could interact productively with experimentalists and this caught the eye of George Porter (FRS 1960, PRS 1985), who wanted to lure a top theoretician to his department at the University of Sheffield. So, in 1960 John moved there to take up his first tenured post as a university lecturer. Not long after moving to
Figure 1. The theoretical chemistry group at Cambridge University in 1959. In the centre of the front row is Christopher Longuet-Higgins, to his left are John Pople and John Murrell, to his right are Frank Boys and Leslie Orgel. (Copyright © Shirley Murrell)

Figure 2. The Murrell research group at the University of Sheffield in 1964. John is third from the right on the back row with Stuart Carter on his immediate right. (Copyright © Shirley Murrell)

Sheffield, Shirley had Luke, their second child. The Department of Chemistry at Sheffield at that time was very active and several other new faculty were also appointed, including Richard Dixon (FRS 1986), Neil Atherton and Brian Brocklehurst. John now started to build his own research group and by the start of his second year at Sheffield had five PhD students and two
postdoctoral associates (figure 2). Several further papers on NMR, ESR and charge transfer resulted.

An important new direction, which subsequently became his major interest, was on intermolecular forces. With Randic and Williams he formulated a double perturbation series for the intermolecular potential involving orbital interaction and overlap terms and their paper on this topic became one of John's most highly cited (16). He also published with Godfrey a series of three papers in the Proceedings of the Royal Society on inductive and mesomeric effects on spectral line shifts of aromatic hydrocarbons explained by a localized orbital model (13–15). Furthermore, he showed with Herbert Fischer that Valence Bond Theory could be effectively used to explain why C$_5$H$_5^+$ is stable whereas C$_5$H$_5^-$ is not (11).

It was around this time that John put his considerable experience on molecular orbital theory into his first book, appropriately entitled The Theory of Electronic Spectra of Organic Molecules, which was published in 1963 (12). This book sold over 10,000 copies and encouraged him to consider writing books on other topics in theoretical chemistry. In this he showed a considerable gift that he put to good use throughout his career. Molecular orbital theory was now starting to influence many areas of chemistry, but there were few good textbooks at the right level for chemistry undergraduates in the UK and postgraduates in the USA. So, with two Sheffield colleagues, the inorganic chemist, Sid Kettle, and the organic chemist, John Tedder, he published Valence Theory in 1965 (17). This book was distinctive in that it did not omit mathematical difficulties, but still managed to explain the basic concepts so that many chemists could benefit. This book was very timely. There were five printings and over 20,000 copies were sold. Valence Theory did much to make the name of John Murrell known to a broad international audience of chemists.

A sabbatical in 1963 at the University of Tallahassee, Florida, enabled John to renew collaboration with Michael Kasha. During this time John and Shirley’s third child, Ruth, was born and she qualified as an American citizen. A sabbatical in Paris also renewed his collaboration with Edgar Heilbronner and their paper explained how conjugated carbon molecules show bond length alternation (18), a topic which was also of interest to his former colleagues at Cambridge, Longuet-Higgins and Salem. During this period, he was awarded the Meldola Medal of the Chemical Society, the leading award then made to early career chemists in the UK, and he also received the John Jaffe Research Fellowship of the Royal Society.

**University of Sussex**

In the 1960s several new universities were formed in the UK, and the University of Sussex at Falmer, near Brighton, was becoming particularly prominent. It had distinctive red brick architecture, due to Basil Spence, and was attracting some of the most promising students and academics. In addition to this, the rising importance of theoretical chemistry was picked up around this time by several UK universities through new appointments. Cambridge had been most prominent in theoretical chemistry and Charles Coulson at Oxford was well known. Now other universities, including Bristol, Manchester and University College London, were creating chairs in the subject and Sussex was keen to be on the crest of this wave function. John was invited to apply for the new chair there. At his interview panel, chaired by Asa Briggs, soon to become Vice-Chancellor (VC), John was asked: ‘Can you teach quantum mechanics to chemists?’
At that time there was probably no better person in the UK to answer that question. So, in 1965, John and Shirley moved with their family to Rectory Cottage at Newtimber, Sussex, and just a few months later their fourth child, Adrian, was born. In his new role as Professor of Theoretical Chemistry at the University of Sussex, John found that there was much interaction between the different science departments, with several joint courses. Initially, chemistry had been part of a School with physics and mathematics, but when John arrived the School of Molecular Sciences (MOLS) was born. This included not only chemistry, but also parts of biochemistry, chemical physics and materials science—and, later, environmental science. A particularly successful course was Structure and Properties of Matter, which was given to all scientists at the university. John enjoyed giving the lectures on the introduction to quantum mechanics and atomic and molecular structure. Sadly, this pioneering course was eventually dropped when engineers and biologists felt that this type of material was not the most appropriate for them.

John brought Geoff Shaw with him from Sheffield and they continued their influential work on the theory of intermolecular forces, making the region of small orbital overlap more mathematically rigorous (19). He also published with Keith Miller on Franck–Condon factors in aromatic molecules (20) and with Bob Ditchfield on NMR coupling constants (21). Keith Laidler from Ottawa was an academic visitor and this enabled a significant joint paper to be written on the symmetries of transition states and the statistical factors that should be used in transition state theory (22). They proved that a single transition state in a multi-dimensional potential energy surface cannot exist through the intersection of two valleys so that three valleys, for example, will give rise to three separate transition states. This result has not only been useful in calculations of chemical reactions of polyatomic molecules, but has also been employed more recently to interpret the structures of weakly-bound atomic and molecular clusters.

John was instrumental in the appointment of Harry Kroto (FRS 1990) to a lectureship in chemical physics at Sussex in 1967. He had known Kroto at Sheffield, when he was a PhD student working with Richard Dixon, and had played tennis with him on many occasions. Little did John realize then that some 29 years later Kroto would win the Nobel Prize for his co-discovery of the C₆₀ molecule. This would be the second Nobel Prize for Chemistry for Sussex University, with John Cornforth, another keen tennis player, winning the Prize in 1975 for his experimental research on the stereochemistry of enzyme-catalysed reactions. No other chemistry department in the UK can match that Nobel Prize record in the last 50 years.

John’s flourishing theoretical chemistry group at Sussex now had a real international flavour with students, postdocs and visitors coming from all over the world (figure 3). He kept up his prolific book writing. With Alan Harget, he published the rather awkwardly titled Semi-Empirical Self-Consistent-Field Molecular Orbital Theory of Molecules (24). The cover was particularly distinctive, showing a computer tape revolving about the O of acronyms such as, CNDO, INDO and MNDO. This was designed by Harry Kroto, whose passion for graphics went all the way through to C₆₀. Valence Theory had been very successful, but had too much mathematics for some students. Thus, Murrell, Kettle and Tedder published The Chemical Bond (30), which was less mathematically demanding and gave the self-consistent field equations only as an appendix.

In the late 1960s larger mainframe computers were starting to be used and their power was beginning to enable more accurate quantum mechanical calculations to be carried out on molecules than had previously been the case. Thus, semi-empirical molecular orbital
calculations were giving way to self-consistent field \textit{ab initio} calculations in which the various integrals required were not approximated and general computer programs were becoming available. One system studied by John and co-workers using this approach was CH$_5^+$, and their conclusion that this important ion can be formed from CH$_3^+$ and H$_2$ without an activation barrier (23) has held up well against subsequent more accurate computations.

The pioneering academic approach at Sussex allowed John and colleagues to initiate a new undergraduate course in theoretical chemistry. This covered the chemistry syllabus, but allowed students to take mathematics courses in the place of laboratory classes. The numbers of students taking this course were small, but some went on to major careers in theoretical chemistry. These included Paul Madden (FRS 2001) and David Clary (FRS 1997) (one of the authors of this memoir).

Danko Bosanac came from Croatia to do his PhD under John’s supervision and this started a close interaction that endured for the rest of their careers. Bosanac started on calculating the bound state of three helium atoms (25). Then he moved on to studying the theory of molecular collisions. Some years later John and Bosanac co-authored a book entitled \textit{Introduction to the Theory of Atomic and Molecular Collisions}, which filled a gap in the market for a monograph on molecular collision theory for graduate students (40). Bosanac started a regular series of conferences on the island of Brioni, Croatia, on chemistry and physics, which were regularly and enthusiastically attended by John and his colleagues (figure 4).

During this period, John and his family took several interesting trips abroad, sometimes to places where it would be difficult to visit in the twenty-first century. One of these was to Iraq during the time of Saddam Hussain. He recalled feasting on a whole stuffed sheep, visiting Basra and Babylon, and seeing belly dancing at the Ali-Baba club in Baghdad. This visit also enabled him to form some close links with academics in Iraq. In particular, Afaf Al Derzi became a PhD student in his group at Sussex and, in collaboration also with Harry
John Murrell is third from the right in the back row. In the front row are his Sussex colleagues, Tony McCaffery (far right) and Harry Kroto, and Danko Bosanac is on the left. (Copyright © Shirley Murrell) (Online version in colour.)

Kroto, calculated that HNSi is more stable than HSiN, a result which was published in the Astrophysical Journal, being of interest for interstellar chemistry (26). Al Derzi was to make regular visits to Sussex and was eventually granted political asylum in the UK as life in Iraq became increasingly untenable for a Christian, female academic.

John realized that reliable potential energy functions were the key to modelling both chemical reactions and the spectroscopy of molecules. He therefore set about putting the representation of these surfaces on a more robust footing. Two key developments were made with his PhD student, Ken Sorbie. The first of these was the development of a new analytic functional form for a diatomic potential curve (27), which extended the standard Morse potential to give a more flexible representation of the interaction of two atoms as a function of their separation. In particular, their new form gave a much better representation of the long-range region of the potential encountered as the molecule moves towards dissociation. This model was later used to make a well-used library of diatomic potential energy curves with a subsequent PhD student, Philip Huxley, for both stable molecules (35) and weakly-bound Van der Waals systems (36).

The more significant advance with Sorbie addressed the issue of how to construct reliable potential energy surfaces for systems with many atoms. As the dimensionality of these systems grows rapidly with the number of atoms, the task of constructing and even visualizing reliable potential energy hypersurfaces becomes increasingly difficult. The Murrell–Sorbie approach (28) was to express such potentials as a many-body expansion where the potential energy hypersurface is represented in terms of fragments of the system. Initially they studied systems with three atoms: this approach starts from the constant atomic terms which are independent of the internuclear distances; contributions due to all possible atom–atom pairs (diatomics) are added; and finally a three-body term is added. This form ensured that the dissociation limits were correctly reproduced, and, importantly, the three-body term was generally a smooth
function; the large positive energies that occur at short bond lengths for all potentials were contained in the diatomic terms. For the three-body term, they used the type of function they had developed for diatomic molecules, a tanh function, which was multiplied by a polynomial in the three inter-atomic distances. They based their triatomic function on the three inter-atomic distances because they aimed to derive functions that covered all configurations of the three atoms. In particular, they wanted functions that could be used for both spectroscopic analysis and scattering problems. The dearth of academic openings in the 1970s led to Sorbie taking a position modelling methods for improving the extraction of oil from North Sea fields, before his eventual return to academia where he became a professor in oil technology.

The beauty of the Murrell–Sorbie approach is that the higher-order contributions are usually small and often negligible. This means, for example, that including the diatomic interactions alone often gives a good working approximation for molecules with many atoms and, for many systems, including the three-body terms effectively converged the expansion. As a result, John and his group later extended the approach to represent potentials of larger systems, realizing that usually excellent results could be obtained simply by restricting the representation to two- and three-body terms.

John teamed up with his former PhD student from Sheffield, Stuart Carter, and Ian Mills (FRS 1996), from the University of Reading, to refine his potentials using observed spectroscopic data by using quantum mechanical nuclear motion calculations (32, 33). This approach has been widely adopted by the chemical physics community as the method of choice for generating accurate potential energy surfaces; it is being routinely used by one of us, Jonathan Tennyson (FRS 2009), for this purpose. With Carter, John also extended the Murrell–Sorbie approach to systems comprising multiple, interacting potential energy surfaces by using a matrix representation of the problem (34).

Extensive study of potentials for triatomic and some tetra-atomic molecules using the Murrell–Sorbie approach resulted in some 50 papers. The work on potential energy surfaces was encapsulated in a book published in 1984, *Molecular Potential Energy Functions*, which John co-authored with several of his current and former PhD students: Carter, Antonio Varandas, Stavros Farantos and Huxley (37). Varandas was actually the third generation of students from the ancient University of Coimbra, in Portugal, who had come to the UK to study for a PhD with John following Jorge Veiga (Sheffield) and Jose Texeira-Dias (also Sussex). After Varandas' return to Portugal, the University of Coimbra set up its own PhD programme and, in return, rewarded John with an honorary degree in 1993. At Sussex, Varandas extended the many-body potential approach to systems with many atoms (29). He continued to visit Sussex regularly after completing his PhD. At Coimbra, Varandas has continued to make extensive use and development of this many-body expansion approach to potential energy surfaces, extending the work to treat conical intersections, where two surfaces cross, and significantly increasing the accuracy with which potential energy hypersurfaces can be represented.

One project including John, Varandas and one of us (Tennyson), involved the use of *ab initio* electronic structure calculations to search for a crossing point between potential energy surfaces in the model triatomic molecule LiNaK. The possibility of such a surface crossing for polyatomic molecules had been uncertain given that there is a well-established non-crossing rule for diatomics. However, John’s old supervisor, Longuet-Higgins, a polymath who had moved his Royal Society Research Professorship to the Department of Experimental Psychology at Sussex, had proposed that such crossings should not only occur in polyatomics,
but also leave their signature as a phase change in the wavefunction. Electronic structure calculations were performed on contours round the possible crossing point and change in sign of the wavefunction upon completing a full circuit was used to identify the crossing point. The work was published, in English, with the somewhat whimsical French title ‘Chercher le croisement’ chosen by John (31). The whole topic was subsequently put on a much more rigorous footing by Sir Michael Berry (FRS 1982) and the phase is now known as the Berry or geometric phase. Longuet-Higgins retired while at Sussex, and John and Shirley Murrell became increasingly responsible for his care up until his death at the age of 80 in 2004. John co-authored his Royal Society Biographical Memoir together with Richard Gregory FRS (49).

John combined the development of accurate potential functions with classical trajectory studies with a number of people, including Bosanac for over two decades, and with Stavros Farantos, a PhD student and PDRA at Sussex, before Farantos returned to Greece and became a founding academic and subsequently Professor at the University of Crete. John’s work with Farantos studied chemical reactions and inelastic collision processes as well as exploring the boundary between regular and chaotic behaviour in molecules (38). An important feature of this work, as classical trajectories could be used as a probe of unphysical minima in the potential energy surface as the trajectories simply fell down these holes in a way that the quantum mechanical wavefunctions do not.

In 1985 the Murrells went to Chengdu in western China expecting to attend a conference on potential energy functions, but it transpired that John was the only speaker! He duly gave a two-week lecture course to a group of about 30 invited participants from all over China. His interpreter for the lectures was a young scientist called Hua Guo. Guo came to Sussex to do a PhD, where he worked on potential functions and molecular dynamics performing studies of photodissociation of molecules such as water (39). Guo subsequently moved to the USA and now holds a Chair at the University of New Mexico in Albuquerque where he continues to develop potentials and use them to predict molecular spectra and dynamics.

John’s whole career made use of computers, but programs were generally written by members of his group rather than himself. However, he realized the power of electronic computation in pushing forward scientific research, acting as both Academic Director of the Computer Centre at Sussex and chairing the national Science (and Engineering) Research Council (SERC) scientific computing committees. Within SERC he successfully pushed for national investment in both hardware and software for tackling the problems both in electronic structure and in molecular dynamics. In this context, mention should be made of Vic Saunders, who worked at Sussex partly under the direction of Ruth Lynden-Bell (FRS 2006). Saunders chose to work on programs for performing self-consistent field (SCF) electronic calculations using Gaussian basis functions. Saunders plus Martyn Guest (a former PhD student of John’s) moved to the SERC Rutherford and then Daresbury Laboratories, where they developed an early general purpose electronic structure code known as ATMOL, strongly encouraged by John and used extensively by his group. Much of the ATMOL code migrated into the quantum chemistry package GAMESS, which is still widely used.

John was always a keen sportsman. Tennis played an important role among the chemistry staff at Sussex, with about eight active players including the Nobel laureates Cornforth and Kroto, and John played tennis regularly right up until the year he died. Of more direct consequence for his research group was his periodic fishing holidays. He would return from hours of quiet contemplation on the river bank teeming with good ideas for new research projects. On his return, his students were soon tasked with the job of realizing these.
John’s work on potential energy functions, intermolecular forces and the electronic spectroscopy of molecules led to his election as a Fellow of the Royal Society in 1991. Shirley did not have a medical job for the first few years in Sussex. She returned to work part time and studied for the advanced examinations of the Royal College of Physicians. She then returned to radiotherapy and became a consultant. A major achievement of the years before her retirement at 65 was to establish the Martlets hospice, which replaced the two smaller hospices that had served the Brighton area.

An obvious extension of the Murrell–Sorbie potential surface based on the use of two- and three-body molecular systems was the development of a surface suitable for reproducing the properties of bulk elemental solids. This was the last major research project on which John was to embark and was, in fact, initiated through work undertaken by Rachel Mottram during her final year undergraduate project. It was recognized that through a combination of symmetry constraints and a suitable choice of 3-body term, it was possible to reproduce the most stable structures of many cubic solids. This approach to modelling atomic interactions in solids subsequently became known as the Murrell–Mottram potential (41). The work took a significant step forward with the arrival at Sussex of Roy Johnston, who held a Royal Society University Research Fellowship. A difficulty associated with the potential was that of obtaining suitable coefficients for the 3-body polynomial and Johnston showed how these terms could be derived from knowledge of phonon dispersion curves, which could be determined from neutron diffraction experiments (42). These and comparisons with other pieces of experimental data, such as elastic constants and lattice energies, meant that vacancies and the behaviour of surface layers could be modelled for solids with considerable success. Further developments made the potential suitable for studying the diamond lattices found for carbon and silicon, and Hazel Cox, a postdoctoral researcher who went on to hold a Dorothy Hodgkin Fellowship, and who is now a Senior Lecturer at Sussex, also made important contributions (45).

Although the development of potential energy surfaces for solids and clusters dominated much of John’s work towards the end of his career, he continued to cultivate ideas in new areas. A collaboration with Laurence Dunne led to the development of a theory based on orbital symmetry that accounted for electron pairing in high- \( T_c \) cuprate superconductors (44), and a simple charge transfer model based on electrostatic interactions proved successful in the interpretation of stability patterns recorded by Tony Stace (FRS 2002) in experimental studies of multiply charged metal–molecule complexes (46).

John’s enthusiasm for travel made him a keen supporter of international links with other universities and from these came important collaborations and quite often the opportunity to recruit research students and postdoctoral assistants. A visit to Uppsala led to Tom Brobjer joining the group, where he worked on electrostatic interactions—an experience that may possibly have precipitated a career switch to philosophy. Through the Erasmus programme, Bernd Eggen was eventually taken on as a postgraduate student, having arrived as an undergraduate with no formal degree qualification. Sussex has always been flexible with regard to qualifications and Bernd was accepted on the grounds that his work was deemed first class—he went on to make important contributions to the modelling of cluster structures. Of the Russian visitors, the most prominent was Fedor Naumkin, whose experience of the Diatomics in Molecules method led to publications on the structures and stabilities of rare gas cluster ions, such as \( \text{ArHe}_n^+ \) (47). Fedor left to take up a position with John Polanyi (FRS 1971, Nobel Prize for Chemistry 1986) in Toronto. Peter Knowles, an expert on \textit{ab initio}
quantum chemistry, was recruited to a lectureship in theoretical chemistry at Sussex and published several papers with John on the structures of helium cluster ions (43).

John retired to become an emeritus professor in 1997, but, with both Dunne and Bosanac, he continued to publish on superconductors and problems in scattering theory. However, his thoughts become increasingly more reflective and he began to examine some of the historical aspects of chemistry and physics. Most notable in this respect were two articles; one was on Avogadro's constant, where the history behind the concept that a fixed number of atoms or molecules could be present in a mole of a substance was examined (48). The discussion ranged from early ideas proposed by Gay-Lussac following experiments with gases through to modern X-ray measurements on silicon where the constant can be determined to an accuracy of six decimal places. In his last published paper, John developed a time line that mapped out the important contributions scientists such as Mulliken, Condon and Lennard-Jones made to the development of molecular orbital theory (51). In these days of fast computers, it is often difficult to appreciate just how hard those early calculations on, for example, H₂ were to undertake.

During John’s time at Sussex the organization of science administration underwent several transformations. Under the guidance of John and Colin Eaborn (FRS 1970), the then Chair of Chemistry and later Dean, the School of Molecular Sciences proved to be an extremely successful venture, which in part benefited from the early popularity of some of the ‘new’ universities and so was able to attract outstanding undergraduates. In addition to Kroto and Cornforth, Archer Martin (FRS 1950) was also a Nobel Prize winner who came to work in the School of Molecular Sciences, having won the prize for partition chromatography in 1952. A total of 12 staff members of Chemistry and the associated Unit of Nitrogen Fixation were Fellows of the Royal Society (those listed in the above text together with Joseph Chatt (FRS 1961), Alan Johnson (FRS 1965), Ronald Mason (FRS 1975), Michael Lappert (FRS 1979), John Nixon (FRS 1994), Geoff Cloke (FRS 2007) and Steven Armes (FRS 2014 after moving to Sheffield)) (see also figure 5).

John had two periods as Dean of MOLS; the first occasion coincided with a time of student unrest, and Sussex, along with a number of other universities, experienced its fair share of ‘sit ins’. John was a charismatic Dean, but found this experience quite demanding of time and patience. After a second period as Dean, John took on the role of academic director of the computing centre. Since his group required good computing facilities, John was keen to ensure that the service was run for the benefit of users rather than staff. At the same time, he was involved with the organization of computing within SERC. He was able to facilitate the implementation of software packages for national use, including codes for ab initio molecular structure calculations and atomic and molecular scattering, through the Collaborative Computational Projects, some of which have survived to the present day. At around the same period, the then VC of Sussex, Denys Wilkinson, managed to persuade John to become pro-Vice-Chancellor (PVC) for Science, which he did for four years; however, the position ended abruptly with John’s resignation when a new VC, Leslie Fielding, wanted to both reduce the power of PVCs and turn them into full-time administrators.

MOLS as an academic unit was broken up in 1995. In part this was precipitated by declining student numbers, and steps were taken to streamline teaching and research. Material science had already moved in with engineering; maths and physics, which had been known as MAPS, was split into separate subjects with maths becoming a School
in its own right and physics once again becoming associated with chemistry. Before retiring, John became a Dean for the third time, but of a new School (CPES) that combined chemistry, physics, and environmental science. However, despite John’s best efforts to use the opportunity to introduce new innovative teaching programmes, these
were frustrated by the reluctance of students to explore topics away from their main degree.

Soon after John’s retirement, the subjects once again went their separate ways: physics again joined mathematics, but to be known as MPS rather than MAPS, and chemistry and environmental science joined biology to form the School of Life Sciences. However, this latest step in the life of chemistry at Sussex has not been an easy one. A further decline in student numbers and changes in research council and university funding patterns put pressure on the finances of small departments. Some universities, for example, Exeter and Kings College London, had already closed their chemistry departments and the then VC of Sussex, Alasdair Smith, proposed in 2006 that the department at Sussex might also close. Uncertainties in the department’s future had already prompted the loss of several staff members—Stace to Nottingham, Armes to Sheffield and Kosmas Prassides to Durham. Although the remaining
John Norman Murrell

staff came under considerable pressure, they eventually succeeded in keeping the department open. However, the number of chemists at Sussex is now significantly smaller than it was in the days of MOLS and John’s tenure. John had great affection for the spirit of MOLS and, on the fiftieth anniversary of the University of Sussex in 2011, he produced a book which gave an informal reflection on the scientific contributions that were made and the many social events attended by the members of the School.

FAMILY

Outside of science, John was very much a family man (see figure 6). He and Shirley followed very closely the activities of their four children and 11 grandchildren. A main passion at home was his garden (figure 7). John was an active member of the local horticultural society, giving talks and holding the position of Chair for five years. He regularly exhibited vegetables and in 2007 he and Shirley produced a book on how to grow less common fruit and vegetables (50); an activity that was inspired by their many trips abroad.

JOHN MURRELL’S LEGACY

John Murrell played a significant role in enhancing the reputation of theoretical chemistry in the UK during the second half of the twentieth century. He established a major school for teaching and research in his subject at the University of Sussex. His textbooks on many aspects of theoretical chemistry were very timely. He wrote several important papers and his research on potential energy surfaces continues to be particularly influential.

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The frontispiece photograph was taken in 1990 and is copyright Shirley Murrell.

AUTHOR PROFILES

D. C. Clary FRS

David Clary was an undergraduate in theoretical chemistry at Sussex University and published his first paper there with John Murrell. His PhD was from Cambridge and he has been on the faculty at UMIST, Cambridge, UCL and Oxford. He is now President of Magdalen College, Oxford, and directs a research group in the Chemistry Department at Oxford University working on the theory of chemical reactions. He was elected to the Royal Society in 1997 and was knighted by the Queen for services to international science in 2016.
Tony Stace took his first degree and PhD at Essex University at a time when it still had a chemistry department. In 1974 he moved to Sussex University to work with John Murrell on the computer simulation of elementary chemical reactions. Three years later Stace moved to Southampton University where he began developing experimental methods to study gas phase clusters. In 1983 Stace returned to Sussex University, where he stayed for the next 21 years. During that time he continued to collaborate with Murrell on topics ranging from the structure of \( \text{Ar}_3^+ \) to the chemistry of metal dications ions. In 2004, Stace moved to Nottingham University and has recently given away all his apparatus and returned to the (comparatively!) cheaper pleasures of computer simulation. He was elected to the Royal Society in 2002.

Jonathan Tennyson studied Natural Sciences at Cambridge and then moved to Sussex to do a DPhil with John Murrell on the \textit{ab initio} calculations of molecular energies. Following postdoctoral work at the University of Nijmegen, in the Netherlands, and Daresbury Laboratory, he moved to the Department of Physics and Astronomy at University College London. At UCL, Tennyson works on a range of problems involving structure and collisions of small molecules with applications in a variety of areas from astrophysics and atmospheric physics to neutrino mass measurements and plasma processing. He has recently been leading a major project, ExoMol, to compute molecular absorptions in hot atmospheres with a particular emphasis on exoplanets. He has published a textbook on astronomical spectroscopy. Tennyson was elected to the Royal Society in 2009.

**BIBLIOGRAPHY**

The following publications are those referred to directly in the text. A full bibliography is available as electronic supplementary material via http://dx.doi.org/10.1098/rsbm.2016.0026 or via https://dx.doi.org/10.6084/m9.figshare.c.3635066.


