

Foreword

Nicholas Charles Handy was born in Swindon in Wiltshire on 17 June 1941, the son of a corn merchant. From 1955 to 1960 he attended Clayesmore School in Dorset, where he was encouraged by his mathematics teacher to apply to Cambridge University. Handy remained attached to Clayesmore School throughout his life and was a long-serving member of its governing body.

Handy was admitted to Cambridge by St Catharine's College in 1960, where he read for the Mathematical Tripos, graduating in 1963. He would remain a member of St Catharine's College until his death, serving as its steward for 17 years and president for 4 years.

During his studies, Handy had been taught by Paul Dirac, John Polkinghorne, and Jeffrey Goldstone, but the strongest influence on Handy would be that of Frank Boys, who taught a fourth year course 'Quantum Theory of Molecules' that Handy attended in 1964. As a result, Handy moved to theoretical chemistry, carrying out PhD research under the supervision of Boys. He defended his thesis 'Correlated Wave Functions and Energies of Atoms and Molecules' in 1967, developing and applying the transcorrelated method for the calculation of molecular electron correlation energies, thereby starting a lifelong preoccupation with the electron correlation problem of quantum chemistry. During his undergraduate years, Handy had met Carole Gates and they married in 1967.

Handy spent the years 1968–1969 at Johns Hopkins University in Baltimore, on a Harkness Fellowship with Bob Parr, working amongst other things on the long-range behaviour of Hartree–Fock orbitals. Handy's first publications appeared in 1969, when he published a total of eight articles on various aspects of electronic structure theory.

Towards the end of 1969, Handy returned to Cambridge, becoming a fellow of St Catharine's College in 1970 and a demonstrator in theoretical chemistry at the Department of Chemistry in 1972. His two sons were born at this time: Paul (1971) and Julian (1973). Handy would remain at the Department of Chemistry until his retirement in 2004, being promoted to university lecturer in 1977, to reader in 1981, and to professor in 1991.

During his career, Handy published 399 papers. None of these are reviews – all are original research papers. In his work, he always looked for simple solutions to important problems. When a conference was held in his honour at St John's College in Cambridge in July 2004, with more than 300 participants, it was titled 'Molecular Quantum Mechanics: The No Nonsense Path to Progress', neatly

summarising his scientific contributions and attitude to science.

Handy's most productive years were from 1979 to 2004, when he published 350 papers. This period falls into two distinct parts, before and after 1992. At first, he attacked the electron correlation problem using wave-function theory, continuing the work initiated with his PhD thesis but with simpler methods. Two important contributions were made in 1984, when he presented the string-based configuration-interaction method and devised a simplified scheme for the calculation of gradients for correlated methods, greatly expanding the applicability of correlated methods in quantum chemistry. Work in this period was strongly influenced by a sabbatical at Berkeley in 1978, where he worked with Bill Miller on the reaction path Hamiltonian and with Fritz Schaefer on derivative theory.

In 1992 an article by Handy on the Kohn–Sham method, inspired by recent work of John Pople and Axel Becke, signalled a complete and unsentimental conversion in Handy's outlook and research, away from the complicated explicit description of electrons offered by wave-function theory towards the simpler implicit description offered by density-functional theory. For the remainder of his career, Handy worked enthusiastically on the development of density-functional theory, making several seminal contributions. It is interesting to note that Handy's most cited paper by far, on the Coulomb attenuated CAM-B3LYP exchange-correlation functional, was published in the year of his retirement, 2004.

In addition to his work on wave-function and density-functional theory, Handy also had a long-standing interest in theoretical spectroscopy, collaborating with Stuart Carter and others for over 20 years, and catalysing the establishment of collaborations between those interested in electronic structure and in dynamics, through European research training networks and beyond.

Handy took great pleasure in teaching, and his style and attitude influenced many. In addition to the PhD and mathematics students he educated at Cambridge, he also played a leading role in several graduate schools, including the Coulson School, the European Summer School in Quantum Chemistry, and in Cambridge. He was a wonderful speaker who required little preparation.

Upon his retirement, Handy moved with his wife to their family farm near Keswick in the Lake District in the north of England. He never regretted his decision to retire early. He enjoyed gardening and travel, and became very

much a part of the local community, maintaining mobility by driving a mini tractor. He died on 2 October 2012, and is survived by Carole, their two sons, and six grandchildren.

Handy was an inspiring individual. He loved to talk science; his first questions were always: ‘What are you working on now? Any new results?’ He had a unique tone and insight that would inspire and strike fear into students at the same time. However, his students soon learned that his loud and frank words were always ones of kindness and inspiration.

Trygve Helgaker, Peter J. Knowles , Timothy J. Lee,
Julia E. Rice and David J. Tozer

ORCID

Peter J. Knowles  <http://orcid.org/0000-0003-4657-6331>