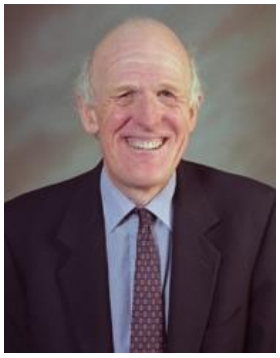
Nicholas Handy 1941-2012



Nicholas Charles Handy was born in Swindon, Wiltshire on 17 June 1941 – at a critical time during World War II. His father was a corn merchant and his maternal grandparents were farmers. He attended Claysmore School in Dorset as a boarder. His mathematical potential was recognised by his teacher, Mr Hilton, who encouraged him to apply to Cambridge. In 1960 he came up to St. Catharine's College to read for the Mathematical Tripos. In his third year he met Carole Gates, whom he married in 1967, and in his fourth year he attended the Part III Mathematics course taught by S F Boys entitled "Quantum Theory of Molecules". He gained a Distinction in the examination and started his PhD with Frank Boys in 1964. His thesis, entitled "Correlated wave functions and energies of atoms and molecules", was approved in 1967 and he was elected to a Research Fellowship at St. Catharine's. In 1968 he was awarded a Harkness Fellowship for a year in the USA and he and Carole went to Baltimore where he worked with Bob Parr at the Johns Hopkins University and published a paper on the asymptotic behaviour of Hartree-Fock orbitals. In 1969 he returned to his Research Fellowship at St. Catharine's and to Frank Boys's research group. When Frank died in 1972, Nick took over the supervision of the research students and became interested in molecular spectroscopy. He was appointed to a University Demonstratorship in 1972 and in 1977 became a University Lecturer. David Clary was one of his research students and worked on explicitly correlated wavefunctions.

In 1978 he went to the University of California in Berkeley on sabbatical leave and worked closely with Bill Miller and Fritz Schaefer. He and Miller wrote an influential paper on how to perform calculations on chemical reactions and he developed "Nick's trick", an algorithm which enabled efficient calculations of the vibrational states of polyatomic molecules. The final quarter of his sabbatical leave was spent in Chapel Hill with Bob Parr, working on bounds for Coulomb integrals. On returning to Cambridge, his research flourished. He and Peter Knowles wrote a general CI program, making it possible to obtain the exact solution, for a particular basis set, of the electronic Schrödinger equation – the so-called Full CI technique. A colleague in the Department, Roger Amos, developed the CADPAC computer code which enabled the efficient computation of analytic gradients of wavefunctions and energies. Nicholas had a long-standing interest in the computation of the vibration–rotation spectra of polyatomic molecules for a given potential energy surface, and collaborated on this topic for many years with Stuart Carter.

In the late 1980s, the density functional theoretical (DFT) approach to the problem of the electronic structure of molecules was rapidly gaining popularity after the introduction of much improved functionals. Handy, and his friend John Pople, entered the field in the early 1990s. In a few months his group had made the modifications to CADPAC that enabled DFT calculations to be carried out routinely. Handy and his group became

almost completely converted to DFT, and much work was done on functional development, calculation of electromagnetic properties and excitation energies.

Handy's distinction in quantum chemistry was recognised by Cambridge University through his appointment in 1989 as a Reader and in 1991 to a personal Professorship. In 1990 he was elected a Fellow of the Royal Society. In 1988 he became a member of the International Academy of Quantum Molecular Science and from 1991-2000 he served as Secretary of the Academy. He retired in 2004 and a conference entitled "Molecular Quantum Mechanics: the no-nonsense path to progress" was held in his honour at St. John's College Cambridge. The conference was attended by more than 300 people. Nicholas and Carole moved to the beautiful location of Thornthwaite in the Lake District in the north of England. His health gradually deteriorated and he died, after a brief battle with pancreatic cancer, on 2 October 2012. He was a loyal, kind and respected colleague and friend. He is survived by Carole, their two sons and six grandchildren.

David Buckingham