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Obituary

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Obituary

Professor Nicholas Handy

Quantum chemist and Cambridge professor of world renown who showed how to do accurate calculations on the energies of molecules

In 1929 the theoretical physicist Paul Dirac stated: 'The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that the exact application of these laws leads to equations much too complicated to be soluble.' Nicholas Handy devoted his research career to overcoming these complications and he had considerable success.

Nicholas Charles Handy was born in Swindon, Wiltshire, in 1941. His father was a corn merchant, as was a grandfather. He attended Clayesmore Senior School in Iwerne Minster and his mathematics teacher, Mr Hilton, encouraged him to apply to Cambridge University. So in 1960 he arrived at St Catharine's College to read for the mathematical tripos. In his final undergraduate year he went to a ball with a group of friends, including a young woman called Carole Gates. Their relationship blossomed and they were married in 1967 at Carole's home town, Thornthwaite, in the Lake District.

Handy attended a course of lectures on the quantum theory of molecules given by Frank Boys. He realised that this was a field with a big future and he started his PhD working with Boys in 1964 on quantum chemistry — using quantum mechanics to calculate the electronic structure of molecules. His work went well and he was elected to a research fellowship of St Catharine's. Then, after a Harkness fellowship in the United States, Handy was appointed in 1972 to the post of Demonstrator in the Theoretical Chemistry Group in the Department of Organic and Inorganic Chemistry at Cambridge.

By this time he had also moved up to be Official Fellow at St Catharine's, which he held until his retirement. He took his college supervising in mathematics seriously and generations of students studying the advanced mathematics course for natural scientists benefited from his lucid and precise lecturing style. He was soon asked to become Steward of St

Catharine's, an office which involved overseeing the provision of food and drink for students and fellows in the college. He eventually became President (deputy master) of St Catharine's. He was devoted to the college and continued supervising in mathematics even after his retirement.

Handy's research papers in Cambridge had yet to receive much international attention but this all changed on a sabbatical visit to Berkeley, California, in 1978. There he collaborated with two of the leading theoretical chemists, 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 the efficient calculation of the vibrational states of molecules.

On his return to Cambridge, he and his research group flourished. A major contribution was the development of a method to perform highly accurate calculations on the energies of molecules which could be used to assess the reliability of more approximate approaches. His colleague Roger Amos constructed a widely used computer code which quickly implemented the new methods developed in the Handy group. Handy was now in much demand to give talks at international conferences all round the world. In the late 1980s he lectured at a conference in East Germany at the invitation of Angela Merkel, who was then doing quantum chemistry before she turned to politics.

In the 1960s Walter Kohn, a theoretical physicist in the US, proposed Density Functional Theory, a new way for performing calculations on interacting electrons. This is now a standard technique used by chemists and molecular scientists to confirm or predict the structures and properties of molecules. During the 1990s, Handy's mathematical insight allowed him to make several new advances in the application of this theory. The importance of this field was recognised by the award of the Nobel Prize in Chemistry to Kohn and John Pople in 1998, and Handy's contribution was cited in Pople's Nobel lecture.

In due course many awards rightly came Handy's way. In 1990 he was elected a Fellow of the Royal Society and he was promoted to Professor of Quantum Chemistry in 1991, such promotions being rare at that time in Cambridge. He was also awarded the

Leverhulme Gold Medal of the Royal Society, the American Chemical Society Award in Theoretical Chemistry, the Schrödinger Medal of the World Association of Theoretically Oriented Chemists and, most appropriately, the Boys-Rahman Award of the Royal Society of Chemistry. He was also Secretary of the International Academy of Quantum Molecular Science. This distinguished academy meets every year at Menton in France and Handy took lessons in French so that he could explain quantum chemistry to the local mayor and other dignitaries.

Upon his retirement in 2004 a conference was organised in his honour which was attended by more than 300 quantum chemists. The title of the conference was 'The No-Nonsense Path to Progress', which neatly summarised Handy's style. A book was published which featured his key papers and comments on them from himself and other experts.

He retired to Thornthwaite, near Keswick, where he took up driving a mini-tractor. He built a hydroelectric device and related with pride how this enabled his house to be the only one in the region to

maintain electric power during a major flood. He continued to communicate with his former colleagues in quantum chemistry and his last research paper was published just months before he died.

He is survived by his wife, Carole, and their two sons.

Professor Nicholas Handy, FRS, quantum chemist, was born on June 17, 1941. He died on October 2, 2012, aged 71

This obituary was originally published in the *The Times* on October 12th 2012, and is reprinted here with permission.

This obituary is reproduced here in recognition of Professor Nicholas Handy's contribution to this journal as Editor of the journal from 1994 to 2007, and as a member of the editorial team of *Molecular Physics* for over 35 years. He retired from the Advisory board in December 2010.

David Clary