

Roy McWeeny

19 May 1924 - 29 April 2021

Roy started his academic life as a schoolboy in Bradford (a town in the West Riding of Yorkshire) just after the publication of works of Heitler and London, Planck and the wave mechanics of Schrödinger. He was clearly destined for science even then, although his progress was challenged by the advent of the second world war. His university education took place at Leeds University and then to a D. Phil. with Charles Coulson in Oxford. His thesis topic was on the solutions of the Schrödinger equation in momentum space. His first paper was published in 1948 [Quantum mechanics of the anharmonic oscillator, Proc. Cambridge Philos. Soc. 44, 314-422 (1948) (with C. A. Coulson)]. He published some 74 papers in the period 1970-2021 as cited in Web of Science, the last in 2008 on his favourite subject (valence Bond) VB theory.

In 1948 Roy obtained his first academic post at King's College, Newcastle upon Tyne (at that time a college of the University of Durham) where he was to teach mathematics for chemists, quantum chemistry, and statistical mechanics. Roy's scientific output during this time was truly ground breaking, e.g., Gaussian approximations to wave functions, the diamagnetic anisotropy of large aromatic systems, charge densities in conjugated systems, the valence bond theory of molecular structure including cyclobutadiene and benzene, and the density matrix in self-consistent field theory

In the mid-50's Roy visited the group of Slater at MIT where computational quantum chemistry was just beginning. He was also able to visit Mulliken, Roothaan, Ruedenberg, Platt, Fermi, Wentzel, Hirschfelder and many others during this time. It was during this period that he published seminal papers on subjects such as MC-SCF theory that were much more general than the work of Roothaan and would form the basis of computer codes decades later.

In 1957 Roy moved to University College of North Staffordshire (UCNS) in Keele, then an exciting new university in the heart of the Staffordshire Potteries. Here he began with his first post-doctoral students and had, by 1964, developed a group involving students from Poland, Japan, Italy, India and Germany and with its own computational facilities, an IBM 1620. In all this he was wonderfully aided by the charm and hospitality of his first wife, Pat in making his group a happy working environment. He also taught undergraduate courses in mathematics as well as chemistry and managed to teach both Brian Sutcliffe and Brian's future wife!

This was followed by a move to the Chair in Sheffield. This period saw the publication of his book with Brian Sutcliffe. The importance of this book cannot be overstated. Other than the older text by Eyring Walter and Kimball, this was the first ever book on Quantum Chemistry. This period also saw the publication of his Rev. Mod. Phys. paper [Some Recent Advances in Density Matrix Theory, Rev. Mod. Phys. 32, 335-369 (1960)] which unified so many ideas of early quantum chemistry (although now second quantization is more often used). Roy also began to develop a long-term relationship with the University of Pisa.

Then came the crisis in funding in UK universities that lasted from the mid 70's for 20 years (which included the Thatcher era from 1979-1990). During this period everyone over age 50 was asked to consider early retirement or voluntary redundancy. The UK then lost some of its pioneers in quantum theory such as George Hall and Roy McWeeny in this period. Roy moved to Pisa in 1982 with his second wife Virginia. He was by unanimous decision of Faculty invited to the chair in Pisa that had been Professor Scrocco's. There, he remained for the rest of his career. His science continued, particularly in VB theory. Indeed, the last time one of us (MAR) met him he was using his PC to carry out *ab-initio* VB computations.

It is difficult for those who knew Roy and his work not to feel that his innate modesty and economy (he hated to say anything more than once) have not deprived him, in some instances at least, of credit that might well have been his. Thus, as Shavitt so perceptively noticed in a review [Isr. J. Chem. 33, 357 (1993)], to Roy belongs the credit of the first documented proposal to use Gaussian basis functions in molecular structure calculations. It is also the case that the idea of population analysis was invented by Roy and published slightly before Mulliken's first paper on the subject. To continue on these lines would be inappropriate and Roy would not have welcomed it. But to some extent it was recognised in the entertaining paper "Modus Computandi Eigenvectores et Eigenaestimationes Matrice Densitatis," (Lim and Whitehead [Theor. Chim. Acta 7, 1 (1967)]) noted in their opening sentence that "McWeeny erat primus." And so, he was and so he will remain.

Brian Sutcliffe Mike Robb May 2021