William Moffitt, Theoretical Chemist

In the sudden death of William Moffitt on 19 December 1958, theoretical chemistry lost one of its most brilliant practitioners. The loss is the more acute, occurring as it did when Moffitt was only 33. During the past decade he had been foremost in recognizing and solving a succession of major problems relating to molecular structure. The very consistency of this performance had led to the expectation that we would witness a lifetime of intellectual conquest in keeping with the best traditions of British and American science. This is not to be. However, our grief must be tempered by the richness of what he has left behind. His published works stand as a living monument that will be admired and consulted as long as men seek to understand the molecules of which their world is made. His life as he lived it will remain vivid in the memories of his friends and students, for the boundless joy he found in pure science; for the openness of his personality, which was free of banality; for his adherence to high intellectual standards uncompromised by fashion; for his warmth and charm and wit; and for the way he could make the English language sing.

William Moffitt was born in Berlin of British parents. He entered New College, Oxford, in 1943 and received the B.A. degree in 1946 and the D.Phil. degree in 1948. During work for his doctorate with Professor C. A. Coulson, his interests became channeled into quantum mechanics and its application to molecular structure. His constant concern with making theoretical knowledge meet the test of elucidating or predicting the behavior of real molecules could be seen in his first work, in which he demonstrated that existing quantum mechanical concepts could satisfactorily explain the structure of some free radicals, conjugated hydrocarbons, and dyes, as well as the state of strain existing within certain molecules.

William Moffitt

For four years after leaving Oxford he lived in London, where, as a member of the staff of the British Rubber Producer's Research Association, he pursued with great freedom and independence a number of original lines of theoretical investigation through which he reached scientific maturity. These included modifications of the molecular orbital theory to illuminate the structure of carbon monoxide, carbon dioxide, and certain compounds of phosphorus and sulfur. The culmination of this work was in the development of a new conceptual view of the electronic structure of molecules, known as the "atoms-in-molecules" concept, which has been widely adopted. In the hands of the author it led to his prediction of two new states of the oxygen molecule, which were later confirmed experimentally.

Early in 1953 Moffitt came to Harvard University as assistant professor of chemistry, and he was promoted two years later to associate professor. His first work in his new environment dealt with the quantitative prediction of the absorption of aromatic hydrocarbons. Thereafter his work fell into two general areas. In one he delved into well-worked areas of molecular optics and emerged with new findings that created a renaissance—first in showing how dichroism and optical rotation could be used to solve basic problems in the crystal field theory of inorganic complex ions, then in showing how the dispersion of optical rotativity, the Faraday effect, and the Kerr effect were related to spectroscopic properties. These researches have set in motion experimental investigations all over the world and have been influential in the structural determinations of proteins and, most recently, of steroids. Parallel to this he continued his specific interests in the electronic structure of molecules. In this he found the way in which certain electronic motions can couple with nuclear modes, and by this means he was able to solve several important and puzzling stereochemical and spectroscopic problems.

Moffitt's ability to make significant contributions stemmed from his mastery of mathematics and physics on the one hand and his wide and detailed knowledge of many different areas of modern chemistry on the other. His genius lay in his ability to delineate what could be solved and what could not, and what was worth solving from what was not. This having been determined, he would seek his goal with all the force of his robust personality until the solution was found and formulated with that combination of rigor and simplicity and elegance that was the trademark of all that he did.

Shortly before his death, which resulted from a heart attack that occurred while he was playing squash, he unknowingly wrote his own epitaph. "I am a scientist because I enjoy being one more than anything else. I find nothing so satisfying as trying to form convincing bridges between the elegant and elementary principles of modern physics and the much more complicated and yet empirically well-characterized situations encountered in chemistry. The exercise is not unrewarding, since a successful theory most frequently has fruitful applications. Perhaps because I do no experimental work, I aim to be useful."

Moffitt was a fellow of the American Academy of Arts and Sciences, associate editor of the *Journal of Chemical Physics* and the *Journal of Molecular Physics,* and a member of the American Chemical Society and the American Physical Society.

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