Remembrance: John A. Pople (1925–2004)

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Sir John Pople passed away on 15 March 2004 at the age of 78. He will be sorely missed by his many friends and colleagues, and by the greater scientific community. We feel that we speak for a great many in the field when we say that John was our teacher and our scientific inspiration. Throughout our careers, we have all aspired to emulate John's objective, systematic, and insightful approach to science, which we will briefly elaborate on here.

Within quantum chemistry, John Pople distinguished himself by defining and exploring what he termed theoretical model chemistries. In his Nobel address, Professor Pople outlined the quintessential steps in creating a model chemistry: Identify your target accuracy, precisely formulate a general mathematical procedure, implement it as an efficient computational algorithm, thoroughly and systematically test the model, and, finally, apply the model objectively to chemical problems. Clear. Concise. Almost obvious. But, who else but John could have, or would have, articulated such a global vision for quantum chemistry, let alone directed its implementation into a readily accessible, internationally renowned computational program?

John Pople revolutionized the way chemistry is practiced today by making it possible to perform chemistry in the computer as a complement to the conventional chemistry of the laboratory. He was the person most responsible for making computational quantum chemistry usable by the community of chemists at large, and he dominated the scene in this area for the past five decades. It is difficult to imagine any significant chemistry department in the world today that does not make use of one or other of the Pople procedures.

A hallmark of John Pople's career was his tremendous ability to reduce the most complex problems to a simple, logical set of solutions. This applied not only to his own research, but to his interactions with colleagues in both informal and formal settings. His lectures were always the epitome of clarity. It was as if a curtain in a darkened room was opened to reveal the light. Only after the lecture was over, and one thought more about the subject matter, did the depth of the content and the complexities that were being discussed become apparent. That someone could teach the details of quantum mechanics, statistical mechanics, and NMR spectroscopy without ever referring to notes, while, at the same time, making the subject matter clear and compelling, was mind boggling to young graduate students who were just beginning their careers.

John Pople's contributions to science, and his approach to research and teaching, have been an inspiration and a model for generations of theoretical chemists. His passing is a great loss for science and a great personal loss for his many friends and colleagues.

