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Tribute to Max Wolfsberg

This special issue of *The Journal of Physical Chemistry A* honors the many and wide-ranging contributions of Max Wolfsberg to theoretical chemistry. Max's contributions have spanned the scope of theoretical chemistry from early work on electronic structure theory and chemical dynamics to his prodigious work in the area of isotope effects on chemical reactions. His graduate work was among the first applications of the molecular orbital theory approach to electronic structure calculations. That work led to the Wolfsberg−Helmholtz approximation, which was widely used in early calculations of molecular electronic energy levels. While Max has contributed broadly to topics in theoretical chemistry, it has been his fundamental descriptions of isotope effects on chemical reactions that have brought very many experimentalists to him for advice, council, and collaboration. The enthusiastic response to our call for contributions to this issue reflects the high esteem Max enjoys in the theoretical chemistry community worldwide and the profound and lasting impact that his work has had on this field.

My (L.X.D.) graduate career at the University of California, Irvine, working with Max was one of the exciting periods in my life, and I treasured it very much. Max was a wonderful advisor to me, both academically as well as personally. Max was very considerate to my needs as a student. In particular, he likes to give plenty of freedom to students and often encouraged me to explore new ideas and practice independent thinking, from which I benefited tremendously in my later career. Max likes to share every moment of joy with students whenever some new progress has been made, for which I truly appreciated being his student. Of course, what I learned and benefited from the most is Max's scientific insight and vision. Max was and is a consummate teacher. In addition to mentoring a number of graduate students, postdoctoral fellows, and collaborators throughout his career, Max was a guiding influence on a number of undergraduate students who, due to his counsel, went on to graduate schools and successful scientific careers.

My personal friendship and professional collaboration (J.B.) with Max Wolfsberg go back to the summer of 1951 when Max

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joined the scientific staff of the Chemistry Department of Brookhaven National Laboratory. Max had already established himself as an outstanding quantum chemist. His prime interest at the time was quantum chemistry. However, Max had already developed catholic interests in science. One day, he spoke with me about the recent publication by Wesley M. Jones on the tritium isotope effect in the reaction of diatomic hydrogen molecules with chlorine atoms. Although Max is a theorist, he recognized that Jones's measurements were careful and thorough. There was a major disagreement between Jones's experiments and the theory of this reaction which used the Eyring−Polanyi method for the calculation of the transition state. Jones called attention to the suggestion by John Magee that the transition state of H_2Cl might be bent and that this could be the cause for the disagreement between theory and experiment. Max worked on this problem as a side line, but after a number of discussions, we came to the conclusion that a bent geometry was leading nowhere. We came then to realize that the question as to whether the transition state was linear or bent was moot. The answer lay in the force field for the transition state. By the mid 1950s, digital computers became available. Max started to write his computer programs to calculate the vibrational frequencies of isotopic molecules and equilibrium and kinetic isotope effects. Max made his programs available to all and instructed many colleagues in the use of his programs. He was the pioneer in the use of computers in the calculation of isotope effects. He also carried out what he called "computer experiments" to probe different aspects of equilibrium isotope effects. Finally, in this area, Max was the first to make an ab initio calculation of a kinetic isotope effect. Throughout his career, Max has consistently demonstrated his interests in the works of colleagues, so much so that he would, with their permission, work on theoretical aspects of the research, which resulted in his many joint publications. All of us who have had the privilege of collaborating with Max have enjoyed and benefited from the experience.

It is our great pleasure to dedicate this issue of *The Journal of Physical Chemistry A* to Max.

Liem X. Dang
Pacific Northwest National Laboratory

John C. Hemminger
University of California, Irvine

F. Sherwood Rowland
University of California, Irvine

Jacob Bigeleisen

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