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Photo by Juli Tredwell

Dedication to Fritz Schaefer

It is interesting in these days of widespread, rapid-fire computational studies in chemistry to look back to 1969, the year Henry F. ("Fritz") Schaefer III started as a new faculty member at the University of California at Berkeley. Computing in academic environments back then was limited. IBM mainframes were common enough, but their speeds were so slow by today's standards that it is hard to believe millions of dollars were eagerly spent on single computers that could do little more than one of today's bargain-store laptops. This was the age when programs were kept on punch cards and when FORTRAN II was a new "high-level" language. This was the age when the fastest data transfer rate was achieved by walking from one computer to another carrying a big magnetic tape loaded with perhaps a few megabytes of data.

Theoretical chemistry had already emerged as an identifiable subfield of chemistry, especially with the quantum mechanical revolution several decades earlier. One could say that chemistry had a place in its heart for those few adventurous individuals who could do the integrals and such to give the quantum mechanical workup that would account for what chemists already knew. Fritz Schaefer entered the field with a different vision of theoretical chemistry, one that involved some of the

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most extensive uses of computational capabilities. Others were seeing the promise of computation, too, but Fritz had one further, more ambitious aim. From the start, he sought to engage experimentalists on their own turf and on the very problems that they were attacking. Large-scale computation was the means to push quantum mechanics beyond its role of fitting and accounting for what was already understood. Perhaps sensing how dramatically technology would evolve, Fritz saw large-scale computation as being a first-line weapon in the scientific discovery process for everything having to do with molecules.

What Fritz had in mind was not easy. At the start, methodology was as primitive as the use of punch cards for maintaining codes. Computer time, memory, disk storage, and so much more were minimal. Most of all, the chemical community had a justifiable skepticism. Quantum mechanics was not the problem; it was that the approximations, truncations, and incompleteness of what could be done readily left a lot of room for doubt. Fritz had to tackle a genuine molecular problem, and get it right. That problem was methylene. Fritz and his long-time colleague and friend, Charles F. Bender, calculated a potential energy surface that showed the molecule was bent. This was a molecule of serious experimental interest at the time, and the accepted interpretation of spectroscopic data was that methylene was linear. The story ends with Gerhard Herzberg reexamining his data, concluding that methylene was indeed bent, and thereby giving this new type of theoretical pursuit the boost in credibility it was now ready to take on. From that point, Fritz could concentrate on the underlying essentials of what he did, the methodology and the computing environment, and build and gather whatever was needed to go after chemical problems of an increasingly wider scope.

Fritz Schaefer did not make computational quantum chemistry what it is today alone. Pioneers before him and alongside him developed methods and ideas that later proved essential in the wide range of computational chemistry approaches. Collaborators as well as competing groups kept the activity level high, soaking up unused computer cycles wherever they could be found. That drew the attention of the chemical community and it built a wider base than any one individual could build. But in all this, Fritz had, and continues to have, an uncanny ability to recognize molecular problems where computational attack yields significant new understanding. We, the organizers of this special issue honoring Fritz on the occasion of his 60th birthday, know that firsthand. We have each seen him lead his group into problems that jump from one area of chemistry to another. Somehow, every jump lands him in the just the spot where computational chemistry can unravel or resolve something genuinely chemical. In many cases in Fritz's list of investigations, theoretical−calculational work has given the deciding piece of evidence.

Fritz has produced an enormous number of published reports, trained many students, and received many awards. That is all listed in this volume for those not already aware of it. Not expressed in such lists is that Fritz has been a gracious scientist, a generous mentor, and a fair and objective colleague to all. He is known for several running competitions with experimentalists to arrive at some answer first, and the outcome always seems to be raising up the significance of the experiment every bit as much as it highlights the role of computational quantum chemistry.

We take special pleasure in helping bring about this issue of the *Journal of Physical Chemistry A*. Three of us are among the first 10 graduate students to work with Fritz, and all of us have an immense appreciation for what he added to our growth and development as theoreticians and computational chemists. We take this opportunity to record in the literature our heartiest wishes for a happy 60th birthday to you, Fritz Schaefer.

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