Biography of Fritz Schaefer

Henry F. ("Fritz") Schaefer III was born in Grand Rapids, MI, on June 8, 1944. His father, a 1933 civil engineering graduate of the University of Michigan moved the family to Syracuse, NY, when Fritz was one. Seven years later, they moved to Menlo Park, CA, and to a home adjacent to Stanford University's campus, something that probably had an influence on Fritz years later. A major promotion for his father brought the family back to Grand Rapids when Fritz was 13. In 1962, Fritz graduated from East Grand Rapids High School and soon embarked on a career in theoretical chemistry by way of MIT for undergraduate work and Stanford for his Ph.D. The path was not entirely direct.

Karen Schaefer: At East Grand Rapids High School, Fritz dreamed of becoming a basketball star. After a traumatic cut from the freshman team, he redirected his life and focused on his other strengths: math and science. For college he chose MIT, over Stanford, to please his father. He entered with the goal of becoming a high school math teacher. That changed when he found mathematical proofs too "dry". He made a brief switch to chemical engineering but then found the problems too "messy". Finally, he decided to be a chemistry major. During his sophomore year in an organic chemisty lab taught by Professor George Whitesides, Fritz nearly blew the place up with an aniline experiment that started putting out a terrible smell and proceeded to produce tremendous heat. He got it under the hood just before it exploded. It seems about then that he was on course to make theory the focus of his pursuits in chemistry.

Fritz Schaefer's senior undergraduate research project with Walter Thorsen at MIT spurred his interest in theoretical chemistry. When he received his BS degree in chemical physics in 1966, he wanted to go to California for graduate school. He had narrowed his choices to Cal Tech and Stanford. Fritz had communicated with Frank Harris, then at Stanford, and had gotten interested in Harris's line of theoretical chemistry work. With Stanford being a place where both he and his bride-to-be could continue their studies, the decision was made in favor of Palo Alto. In September 1966, he and Karen Rasmussen were married, and they made the cross-country trip to Stanford into their honeymoon.

Fritz got working with Frank Harris quickly after he arrived in Palo Alto. In *less* than three years, he published 12 papers with Harris, and did his thesis defense to boot. He had mastered ab initio methodology as it existed, and he had cultivated a taste for being fast, first, and prolific in doing science.

Fritz joined the faculty at the University of California at Berkeley in 1969, starting his faculty career together with another theoretician, William H. Miller, who had just arrived from being a Junior Fellow at Harvard. They were placed in Hildebrand Hall in adjacent 2nd floor offices, each of which had a glass door opening to a private balcony that overlooked the woods around Berkeley's faculty club. It was a very pleasant setting for an aggressive operation, and the stack of computer output completely blocking Fritz's balcony door made the priorities clear to his students.

Fritz and Bill built their research groups alongside one another. They had very different approaches and yet there was a remarkably cooperative style and atmosphere. This carried over to the students, who, while first identifying themselves as "Miller students" or as "Schaefer students," would readily organize events as simply the "Miller−Schaefer group".

William H. Miller: Fritz was always dreaming up grand plans and schemes during our early years at Berkeley. One I remember, which was probably put forth in jest—but maybe also somewhat seriously—was the year that Sandy Koufax and Don Drysdale, then the ace pitchers for the LA Dodgers, held out together for a larger salary package. Fritz suggested that we try this on the Chemistry Department! As usual, I took a more conservative line, suggesting that the department might very well decide that it did not need either of us!

In his early methods work at Berkeley, Schaefer focused on the iterative natural orbital (INO) approach. The codes he wrote did the integrals for diatomic molecules with Slater orbitals. The intrinsic compactness of these basis sets helped achieve high accuracy when electron correlation was included fully, and INO was a means to push the correlation treatment a long way even when computers were very limited. The correlation techniques Fritz was working on in these early days had the power to be used for excited electronic states, ionization, and even curve crossings. From numerous studies on diatomics, Fritz added a wealth of information about the fundamental role of electron correlation in molecules. His first book, *The Electronic Structure of Atoms and Molecules. A Survey of Rigorous Quantum Mechanical Results* (Addison-Welsey, Reading, MA, 1972), collected this understanding plus information on polyatomics on a molecule-by-molecule tour of calculational results. The monograph became widely referenced as *the* source of information on the applicability of various levels of ab initio treatment.

The simple molecule of carbon and two hydrogens, CH_2, has a very notable place in Fritz Schaefer's career. Quite simply, Fritz dared to challenge the spectroscopic determination that the $^3B_1$ state was linear. The 1970 Bender−Schaefer calculation involved 408 configurations in a CI wave function, and from that, they found the equilibrium structure to be bent with an H−C−H angle of 135°. That potential surface is shown on the cover of this issue. Schaefer, Bender, and D. R. McLaughlin refined that value to 134° by using a larger basis set and an INO−CI treatment and then argued that "the bond angle should be very reliable." And, indeed, it was, once the subtle spectral features associated with unusual predissociation were taken into account by the spectroscopists. In 1992, the impact of this work still was of note when Schaefer was awarded the Centenary Medal of the Royal Society of Chemistry (London) as "the first theoretical chemist successfully to challenge the accepted conclusions of a distinguished experimental group for a polyatomic molecule, namely methylene."

In the early days at Berkeley, Schaefer and Miller were collaborators on a number of projects, and in a more general sense, they were partners in doing theoretical chemistry since both groups relied on computer resources. The computers at the Department of Energy's Lawrence Berkeley Laboratory (LBL), up "the hill" from the chemistry department, were initially the sole source of computer resources for both groups. But this was to change in a development that was significant in the history of computational chemistry.

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Peter K. Pearson (PhD with Schaefer 1974): To stretch our computing budget, essentially all of our computations at the LBL computing center were run at "background" priority, meaning they ran only when the computer had nothing better to do, typically in the wee hours of the morning. One seldom achieved more than one turnaround per day this way, but the cost was irresistible: free. In 1972, the computer center announced a pricing change that would raise the cost of "background" work from zero to 50% of full price. Fritz calculated that under these rules, our annual computing budget would be exhausted in one month, and of course protested. Two months later (accounting being done at monthly intervals), we had overrun our annual budget by almost a factor of 2. So, Fritz placed grad students in facilities (LLNL in Livermore, IBM in San Jose, and ISD in Oakland) that could provide computing resources for our research. He also began wondering whether minicomputers had become powerful enough for ab initio calculations.

A little "thinking outside the box" of traditional computer centers led Fritz to approach the National Science Foundation with the idea of funding a minicomputer dedicated exclusively to computational chemistry research. It was to be a minicomputer for the sole use of the Miller and Schaefer groups.

William H. Miller: Fritz did all the research into the various possibilities (finally deciding on a Datacraft, that I'm sure many of the early students remember with mixed feelings!) and wrote the proposal. It is a long story of the battle we had with the university to allow the proposal out the door (computing centers in those days wanted all computing funds to be spent there), and it finally took the support of Glenn Seaborg to make it happen. The minicomputer experiment was a success (Fritz decided that before it actually arrived!), primarily due to his energy and that of many talented graduate students

The minicomputer was a Datacraft 6024/4. It had nearly 0.2 MB of memory and offered 48-bit words in high precision. The 54 MB removable-pack disk drive was the size of a washing machine and sounded like one, too. With the senior graduate students in the Schaefer group being responsible for most system maintenance, the minicomputer was able to run ab initio calculations at roughly one-fifth of the costs that were being levied at LBL. Before long, other theoreticians were following Fritz's lead and acquiring their own dedicated minicomputers. The cycles of computing power available for computational chemistry greatly increased as a result of the minicomputer experiment at Berkeley.

Sharing a minicomputer between two research groups presented Bill Miller and Fritz Schaefer with a micro- (or mini-) version of the problems of running a full-fledged campus computer center. Allocating time between individuals, not to mention between the two groups, and dealing with down time and repairs had all the potential to strain a cooperative relationship. It did not. Fritz and Bill got the most out of their small computer and they remained good friends.

William H. Miller: Once, during the Christmas holidays, I was driving back from the Grand Canyon with my family (including my mother, who had come from Mississippi to meet us and come back to Berkeley for a visit), and we had car trouble on the I-5 highway, about 2 h out of Berkeley. In desperation, I telephoned Fritz, found him at home, and he came out in his Chevy Van to haul us home. My mother remarked that she did not know who this fellow was, but that he must be a *very* good friend, and indeed she was right.

The minicomputer experience ignited a new methods push in Schaefer's group. In 1975, collaborating with Wilfried Meyer, then at Mainz, Germany, Fritz was drawn into the correlation problem from a new angle, that of very large CI expansions with the minimal memory limitations of a minicomputer. The new computational avenues opened by Meyer's self-consistent electron pair (SCEP) theory were well-suited to a minicomputer, and soon, the Datacraft 6024 had done CI's with nearly 20 000 configurations. Following that, and with a series of upgraded minicomputers, Fritz's attention to methodology went to the graphical unitary group approach (GUGA), then energy gradients, and by the late 1980s, the coupled cluster (CC) approach. It is fair to say that Schaefer's goal in methods work has been strategic, to make possible and calculable whatever was needed to tackle real chemical problems. In some cases, the methods work led to bold steps and/or significant demonstrations of the appropriateness (or lack thereof) of certain levels of treatment. Other cases were improved performance that made larger problems doable at some high level.

Schaefer was at Berkeley from 1969 through 1987, with one year away as the inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. In 1987, he accepted an offer from the University of Georgia and moved to Athens, GA, to become the Graham Perdue Professor of Chemistry and Director of the Center for Computational Quantum Chemistry at the University of Georgia. In 1998, construction of a beautiful new facility to house the Center was completed—a most significant and lasting marker of the impact of computational chemistry in science and Schaefer's role in bringing that about.

Even before this issue of the *Journal of Physical Chemistry A* has appeared, there are over 1000 H. F. Schaefer papers to be found in the scientific literature. The quantity is a measure of the incredible diversity of chemical problems he and his group have tackled. He has been recognized through many awards, with three from the American Chemical Society being representative: the ACS Award in Pure Chemistry (1979), the Leo Hendrik Baekeland Award (1983), and the ACS Award in Theoretical Chemistry (2003).

Fritz has long loved—others might say, endured—extensive travel all over the globe. In his early career, he was known to accept invitations for lectures in such a sequence that he was sure to visit some new, remote place along the way. Some of his travels led to regular collaborations and scientific exchanges, including one with Leo Radom, a long-time member of the Australian National University and more recently at the University of Sydney.

Leo Radom: One of Fritz's favorite pastimes has been to "escape" to Australia during the northern hemisphere winters, which he has now done on 13 occasions. Since Fritz's host for his initial visit to the Research School of Chemistry (RSC) of the Australian National University in 1975 was to have been Keith Roby, who had just moved to Murdoch University in Western Australia, I happily filled the breach. This turned out to be the beginning of an ongoing, long-term academic association and treasured friendship. Fritz was always a popular visitor to the RSC and became immersed both in the science that was going on and in the local "culture". He was a lively contributor to the topics of the day in the RSC tearoom (generally politics and sport), quickly becoming knowledgeable in cricket and other local pasttimes. Fritz especially enjoyed

partaking of the wide variety of ethnic foods available in Canberra, ranging from the *giros* at the Acropolis, to the *laksa* at the Rasa Sayang, to the *dosa* at the Ruchi South Indian restaurant, a discovery made on his most recent trip. For a while, Fritz also heartily enjoyed Australian meat pies, until he discovered how "healthy" they really were!

Fritz Schaefer has trained 70 Ph.D. students so far. They are distributed in faculty positions around the world, in corporate research centers, and in national laboratories. He has been an extraordinary mentor.

Peter Pearson: Fritz was a full-service thesis adviser. On several occasions he invited us all to his house for Thanksgiving dinner, and he once opined that Miss Wright, a bright undergraduate chem major, was a fine young woman whom I should consider dating. For misdirection, I grumbled something about Miss Wright (whom I was, in fact, dating) being rather conservative for a guy like me, but I could not maintain the pretense when we got married about a year later.

Fritz has also supervised numerous undergraduate research projects with the result that a very high percentage of those students went on to complete Ph.D.'s. At Georgia and at Berkeley, he gladly taught large sections of general chemistry, receiving teaching awards and the appreciation of many struggling freshman.

Fritz's work with students is always a positive experience. He is known to be both cheerleader and coach for his team, whether that team means the students in his course or it means his research group. He shares enthusiasm and kindles excitement and drive. Probably not surprising is that he brings these qualities and more to his role as father. He and his wife Karen are loving parents of Charlotte, Pierre (d. 1979), Theodore, Rebecca, and Caleb.

Charlotte Schaefer: Dad's love of and penchant for research permeated our lives and showed up in places we'd least expect it. But nowhere was it more apparent than in his attitude toward the theater. Somewhere around the time I started third grade, my father rediscovered the wonders of Shakespeare. We found a tiny amphitheater in Berkeley, CA, that was home to the Berkeley Shakespeare Festival. There I met Harry Percy and Arial and Macbeth. By the time I entered fifth grade, we were searching for performances that coincided with his scientific conferences. We attended performances in Illinois, Oregon, and Ontario. It was not until we'd moved to Georgia, however, that he brought his skills as a researcher to bear on our Shakespearian experiences. We became semiregular attendees of the Alabama Shakespeare Festival, a four and a half hour drive from our home in Athens. Rather than waste that time, Dad developed the preplay research regimen. First, a summary of the evening's play, from a "tales of Shakespeare" sort of book, taking care to note all character names. Then on to *Shakespeare's Characters* to look up each name from the summary and learn about their importance to our play in particular and theater in general. Next, a scan through the Cliff's Notes to hear about the major themes and historical setting of the play. Finally, a glance at *Bartlett's Familiar Quotations* to be sure we were prepared for any particularly famous lines. By the time we reached the theater, I was certain we knew more about the play than some of the actors.

Fritz can adroitly recount great swaths of science history in engaging and even humorous terms, and he often does so. One readily sees that Fritz deeply values the science on which his work has been built, and he values many scientists, past and present, that he considers to have made a special mark on the world. One can recognize that his favorites include scientists from several centuries, for instance, Blaise Pascal (1623−1662), Michael Faraday (1791−1867), George Stokes (1819−1903), and Charles Coulson (1910−1974). He gladly points to two individuals that have directly impacted his career, the late Kenneth S. Pitzer (Berkeley) and David P. Craig (Australian National University), these two being "great scientists and men of considerable character and wisdom." Fritz Schaefer's inspiration and his motivation for science, something shared with his favorites in the history of science, are no secret.

U.S. News and World Report (December 23, 1991, p 62, quoting H. F. Schaefer): "The significance and joy in my science comes in those occasional moments of discovering something new and saying to myself, 'So that is how God did it.' My goal is to understand a little corner of God's plan."

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