THE JOURNAL OF PHYSICAL CHEMISTRY A

 VOLUME 110, NUMBER 2, JANUARY 19, 2006

Autobiographical Notes by Donald G. Truhlar

I was born in Chicago, grew up in Berwyn (a suburb), and went to grade school in Cicero (another suburb) and high school in Chicago. In 1957 Sputnik was launched, and in 1958 I graduated from grade school. As a result of Sputnik, my older brother John was convinced by his teachers to major in physics, and so, two years after he started college, I followed him to St. Mary's College to major in physics. The most exciting science at St. Mary's when I arrived was the carbene research being conducted by Brother Philip Hogan, as a result of which I switched my major to chemistry. The first project Brother Philip gave me was the synthesis of mandelic acid, a project I never finished. I later carried out a more successful experimental project under the guidance of physical chemist Ernest D. Kaufman, involving the reaction of Na with CH_2Cl_2, using methods developed many years earlier by Michael Polanyi. Professor Kaufman was also instrumental in convincing me to remain a chemistry major during my frustrating junior-year analytical chemistry course. Only years later did I discover that part of my difficulty in analytical chemistry was blue-green color blindness. Most of the time, I can distinguish these colors, but sometimes not. Apparently the "not" includes a key blue to blue-green indicator change that played an important role in a titration in my analytical chemistry course; now I have a good excuse for why I passed the end point.

I became very interested in photochemistry and applied to graduate school at Caltech, where George Hammond's work was very fascinating, and at the University of Washington, where B. S. Rabinovitch's work was equally interesting. I had chosen to write my advanced physical chemistry term paper on transition state theory, and the theoretical aspects of Rabinovitch's work were very appealing. I was also still interested in carbenes and also applied to Case Institute of Technology where Harold Shechter had a very interesting project on carbene chemistry. After considerable thought, I decided to accept the offer at Caltech. It would be almost 30 years (until 1997) before I finally coauthored a paper on a carbene, followed by two more in 2002−2003.

On August 28, 1965, I married Jane Teresa Gust, now Jane Truhlar, in her home town of Crookston, Minnesota, and on that same day we started across the country, heading west to Caltech in my almost-new Chevrolet. At that time, most students did not visit far away graduate schools, and this was my first trip west. Upon arrival, I was surprised at how small Caltech was.

My initial discussions with George Hammond were very cordial, but the project he described to me started with an organic synthesis step that did not appeal to me. I elected instead to do physical chemistry photochemical experiments on the

10.1021/jp058265t CCC: $33.50
Published on Web 01/12/2006

reaction H + DI with Aron Kuppermann. I also began to read more theory, and I was very impressed with the trajectory calculations of John Polanyi of Toronto and the phase space calculations of John Light at Chicago. Fortunately Aron Kuppermann had broad and visionary interests, so I was able to switch projects, and by the end of my first year in graduate school, I was a theoretical chemist with a plan to develop methods for calculating the dynamics of chemical reactions. At my preliminary oral exam, George Hammond asked if my theoretical methods could be applied to systems with more than three atoms. I said I hoped that eventually I could do that, but it was to take a while before that happened. My final project as a graduate student at Caltech, in 1969, was an accurate solution of the Schrödinger equation for the collinear reaction of H with H_2, a reaction I have returned to many times in my later work. The IBM computer on which I did that work had 32K of memory.

The idea of pursuing theoretical chemistry without also doing experiments was still rather rare in the 1960s, and I remember Professor Wilse Robinson coming to our "laboratory" (five theorists had desks around the perimeter of a mass spec lab) and kidding us (I supposed he was kidding) about whether purely theoretical chemistry had anything to contribute to the field. Fortunately, there were pure theorists already on the faculty, Russ Pitzer, Vince McKoy, and the newly arrived Bill Goddard; their combined research groups, along with the theorists in Kuppermann's group, had lively lunch meetings, volleyball games, and stimulating interactions in the corridors and at the computer center. In those days, we carried boxes of computer punch cards through the smog to the computer center, without the benefit of a network; I still remember the day that the chemistry department bought an Olivetti desktop electronic calculator, which provided a handy alternative midway between the slide rule or mechanical calculator on one hand and the mainframe computer on the other (hand-held calculators from Texas Instruments and HP were still in the future).

I was fortunate to make many friendships at Caltech, and I particularly remember how much I learned from interactions with fellow students, especially Dave Cartwright, Dennis Diestler, Thom Dunning, Pat O'Keefe, Chris Parr, Merle Riley, Frank Weigert, and Nick Winter. Joel Bowman and George Schatz joined Aron Kuppermannn's group shortly after I left, and this shared experience created a longstanding friendship. At one point the three of us decided to write a book on resonances, which Oxford University Press agreed to publish. Before we had written anything, we were surprised to see the book in an Oxford catalog with a publication date within the year. It seems we will never find the time to actually write this book. The nonexistent book was removed from their catalog years ago.

I also enjoyed the wide array of courses at Caltech, and I was fortunate enough to take a solid-state physics class from Rudolf Mössbauer, a numerical analysis class from John Todd, a quantum mechanics class from Sunney Chan, and advanced quantum mechanics from Richard Feynman. Professor Todd always told us that "computing center" was etymologically derived from the Latin *putare*, which he translated as "to think"; he contrasted computation to calculation, by which he meant computing without thinking. That some ways of doing calculations were more thoughtful than others made a lasting impression on me. The subject of computational science was not generally recognized as a separate field at that time.

Feynman assigned a term paper instead of traditional exams, and I was eventually satisfied that my paper on adiabatic passage of a particle through a field was good enough to hand in. The semester ended, and I was back at my desk in the mass spec lab doing research when the phone rang: it was Feynman, and he had been thinking about the class. Some of the students had handed in a second term paper for extra credit, and he had decided that maybe he should have assigned two term papers to everybody. Therefore, he was calling anybody who had handed in only the required single term paper; could I come over right now and take an oral examination (since I had handed in only one paper)? I did, and in retrospect, it was very satisfying to have passed an oral exam on time-dependent perturbation theory from Richard Feynman without having had the worry of studying for it.

In December 1969, I returned to Minnesota to take up an assistant professorship at the University of Minnesota. Carl Melius, a native Minnesotan in Goddard's group, gave me a Minnesota map, and Jane and I took the Chevrolet on a reverse trek from Pasadena to Minnesota. When we got to Des Moines, the car, spoiled by a youth in California, would not start because it was too cold. This was a gentle reintroduction to Minnesota winters because the temperature that day was a balmy +40 °F.

I am very grateful to my Minnesota colleagues for having had the confidence to hire me without postdoctoral experience. In fact, I had only one published paper when they made me the offer of a position, primarily I suppose on the basis of my recommendation from Aron; and they must have liked my interview seminar. (At the top of my schedule when I interviewed, I was described as a "molecular beam theoretician," something I had never heard of, and I doubt that my talk even mentioned molecular beams.) I have enjoyed the lively and collegial atmosphere of the Chemistry Department at Minnesota, where I have interacted with many stimulating colleagues, especially a large group of outstanding theoretical chemistry faculty colleagues: Jan Almlöf, Chris Cramer, John Dahler, Ted Davis, David Dixon, Jiali Gao, Alden Mead, Al Moscowitz, Steve Prager, Ilja Siepmann, Fred Van-Catledge, and Darrin York. I have also been fortunate to work with a large number of talented graduate and undergraduate students and postdoctoral associates. Talented, enthusiastic co-workers make the research experience productive, enjoyable, and satisfying. I was fortunate to be able to continue to collaborate with some of my former students and postdoctoral associates long after they were no longer students; others went their separate ways, but I am very proud of all of them. Because these co-workers are listed on a separate page, I will not re-list them here, but simply give a hearty thank you. I have been very lucky to have Flurnia Hadley-Davis as my secretary since 1984; her daily good cheer and extraordinary ability to take on all tasks are irreplaceable. Finally, I wish to single out one person not mentioned yet, my faculty colleague Ron Gentry, whose pioneering molecular beams research was a great stimulation to our local chemical dynamics community for 30 years, even though we never managed to coauthor a paper together. Actually, I take some pride in my small role in recruiting Ron to Minnesota in the following sense. Although I was a very new faculty member, the department chairman Robert Hexter consulted me on the hiring (but it does make sense, since I was the "molecular beam theoretician"). He was very concerned that if the department hired Ron, we would need to wait for him to build a molecular beam apparatus from scratch, whereas the other candidate could begin research almost immediately. I advised him to hire Ron and wait, which he did, and this was the start for me of a friendship that has lasted to this day.

In closing this account, I would like to gratefully acknowledge my many teachers. In addition to research advisers and professors mentioned above, I would like to especially single out Brother Hyacinth Andrew and Brother Linus Paul for their calculus and English composition instruction at St. Mel High School. Being forced to write an essay every week was good preparation for a career that has involved a lot of writing.

I would like to thank Chris Cramer, Bruce Garrett, Dave Thirumalai, and Thanh Truong for their combined efforts in putting together a 60th birthday symposium in 2004 and organizing this special issue of *Journal of Physical Chemistry A* in 2005 as well as for many other enjoyable and productive interactions through the years.

Last, but most important of all, I thank my wife Jane and my daughters, Sara Elizabeth Truhlar and Stephanie Marie Eaton Truhlar, for their love, support, and inspiration, which are essential to all my successes and make it all worthwhile.

Donald G. Truhlar