Autobiography of William Hase

I was born March 22, 1945, in Washington, Missouri, the oldest of four boys. At the time, my father was in the Army, serving in the Pacific Theater of World War II, and my mother and I moved in with her parents who lived on a farm near Holstein, Missouri, across the Missouri River from Washington. Before the War, my father had worked for the aircraft manufacturer Curtis-Wright in St. Louis. When he returned home after the War, we moved to St. Charles, Missouri, and he attempted to return to his previous job at Curtis-Wright. However, he had been affected by the fighting in the Pacific and his doctor advised him it would be best if he renewed farming as he had done in his youth. We then lived on farms near St. Louis, as tenant farmers, paying rent from the crops and livestock we raised.

In 1949, we moved to Treloar, Missouri, where my mother and father had been raised. Beginning in the 1830s, German immigrants had settled along the Missouri River from St. Louis to Herman, an area that includes Treloar and Holstein. My great, great grandfather and family immigrated from Rehme, Germany, in 1843 and settled in the Missouri River valley near Treloar. The Treloar/Holstein German community, with its scenic hills, streams, and valleys, was idyllic for a young boy, and I have many fond memories of the short time I lived there. The German tradition was strong, and a number of people in the community could speak fluent German. If I have any place I call "home", it is this community.

One of the traits of rivers is that they flood. We were in the Missouri River flood of 1951. All our resources had been invested in planting the year's crop, and all were lost. My mother and father decided it would be better to own their own farm, instead of tenant farming, and in the winter of 1952, they purchased a farm near Batchelor, Missouri, with a population of about 25. I had started the first grade in a three-room school in Holstein, but when we moved to Batchelor, I went to a one-room school, called Scott School.

Scott School had eight grades and one teacher. When we left the farm in Batchelor in 1957, there were only nine students in the school, with three from my family! Scott School closed 4 years later in 1961, when it was consolidated with other rural one-room schools. Studies have shown that the quality of the education one receives from a one-room school depends on the abilities of the teacher. I certainly concur with this assessment. The two teachers I had were outstanding, and I am much beholden to their interest in me.

Life on the farm included taking care of the livestock, tending to the crops planted in the fields, and cutting wood for the stove we used to heat our house. I was a member of the 4-H club and still have my 4-H pins. I enjoyed life on the farm, but there were also hardships and tragedy. My father found a job to help pay expenses. In the winter of 1953, I became very sick, with what we thought was a serious case of the flu. My father had just been laid off from work, and we no longer had health insurance. Going to a doctor without health insurance would be expensive, and I thought I would get better. Finally, one day, the pain was so severe that I said I could not take it anymore, and my parents laid me down in the back seat of the car and drove toward the hospital in the nearby town of Fulton. Somewhere along the way, my appendix broke. Only because of penicillin am I alive today. I stayed in the hospital for quite some time and initially was given a penicillin shot every 3 hours. There was another experience in my life that had a profound effect on me. I had a neighbor and very close friend who shot himself in the head in front of his two sisters. The reason(s) for and circumstances of this suicide are unclear, but it was tragic and bothered me very much. In 1957, after I finished the sixth grade, we moved to Mexico, Missouri, where my father had gained permanent employment as manager of a concrete plant. This was a sad time, for we were leaving our friends and neighbors and sold all our livestock at a public auction. Leaving the farm was a transition to another type of life.

The education I received at Scott School was outstanding, and when I started the seventh grade in the junior high school in Mexico, I discovered I was ahead of the other students. My parents stressed the importance of acquiring an education to improve one's social condition, and they had a believer in me! I had very little science as part of my education at Scott School, and once in junior and senior high school, I took science classes at every opportunity. My interest in chemistry began as a high school junior, when I took chemistry from George Craddock, an outstanding teacher, who inspired me and made the topic interesting. I particularly liked using mathematics to interpret the various concepts.

When we moved to Mexico, it was necessary for me to have a job. My first job was as a caddy at a country club, where I worked from the summer of the sixth grade to the summer after my junior year. During this time, I learned how to play golf and was on the golf team my sophomore through junior years. In the summer after my senior year, I had a job as a laborer at a refractory brick plant in Mexico, where I also worked in the summers after my first 3 years in college.

My parents were unable to pay for my college education, so I needed to find some way to find the money to go to college. I applied for scholarships and was awarded a Naval Reserve Officer Training Corps (NROTC) scholarship. I happily accepted and enrolled in the University of Missouri, Columbia, in the fall of 1963. It turned out that I did not have the aptitude to be a naval officer, and during my first cruise, in the summer of my freshman year, I disenrolled from the program. Giving up my NROTC scholarship meant I needed to find another source of income. My first job was with the Chemistry Department, and then, during my junior and senior years, I worked for the Agriculture Experimental Station as part of a team analyzing samples from commercial bags of fertilizer to ensure the reported percents of nitrogen, potassium, and phosphate were correct.

I really enjoyed my 4 years at the University of Missouri. Because of the chemistry course I had in high school, which I liked very much, and the sense that I needed to obtain a professional degree, I enrolled as a chemical engineering major. However, during my freshman year, I changed my major to chemistry. It was when I took Physical Chemistry I, Thermodynamics, from Lloyd Thomas in the fall semester of my junior year that I knew I was a chemist. I enjoyed the logical structure of thermo, which is somewhat like the organization of philosophy that I also enjoy, and I found it particularly appealing to use this structure to explain experimental observations. During my senior year, I took the graduate thermodynamics course from Lloyd Thomas, so if there is anything I know in chemistry, it is thermo.

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I graduated from the University of Missouri, Columbia, in the spring of 1967 with a B.S. degree in chemistry. During my junior year, I met and fell in love with Betty Criscuolo, from Kansas City, and we were married in June of 1967. Though I liked chemistry, it was not clear to me that I actually wanted to pursue graduate studies in chemistry. I was aware that a graduate teaching assistantship would provide financial support so I could decide what I really wanted to do. I had always been drawn to the West, though I had never been west of Kansas City, so I applied to nearly every university in the western United States. New Mexico State University was the first school to offer me an assistantship, which arrived by telegram. Betty and I had a close friend who had been to Las Cruces, New Mexico, and she said it was a wonderful place to live. We decided to accept their offer.

My roots were in rural Missouri and life on the farm, and the decision to go to graduate school meant that I would leave this way of life. This was particularly difficult, since I was very close to my grandfather. His farm, near Holstein, was set back in a "hollow", and with the hills, caves, clear streams, and swimming holes, it was a wonderful place for a young boy. The farm was sufficiently remote that it did not have electricity until 1952. We used lanterns and candles for light. I learned to hunt there and helped with the farm work. The farm had been owned by my grandfather's father, and when my grandparents decided to sell the farm in 1967, it would leave the family. However, my decision was to go to graduate school and not stay on the farm. Shortly before my wedding, my grandfather and I went fishing together for the last time.

The afternoon of our wedding, Betty and I left Kansas City for Las Cruces. The New Mexico State Chemistry Department promised me employment when we arrived in the early summer of 1967. I found it in the laboratory of John W. Simons, who had done his Ph.D. research with Seymour Rabinovitch. When school began in the fall, I officially chose John as my advisor. He was great, providing me direction but also giving me the independence I needed. Under his tutelage, I decided I wanted to pursue a career in chemistry. In hindsight, the supportive environment of the Chemistry Department at New Mexico State University was what I needed. I have many fond memories of the time I spent in Las Cruces. Betty and I fell in love with New Mexico, and it is one of my "homes". Our daughter Heidi was born in Las Cruces, the first baby to arrive in the newly constructed hospital.

I received my Ph.D. degree in 1970, after 3 years of graduate studies. My Ph.D. research was experimental and included relative $^1CH_2$ insertion rate studies and measurements of unimolecular rate constants for the decomposition of chemically activated alkane and alkylsilane molecules. These rate constants were in accord with RRKM theory and, along with work by Seymour Rabinovitch, Don Setser, and others, helped establish RRKM theory as an important model for interpreting unimolecular kinetics. The RRKM analyses of the alkane decompositions led to A-factors for alkane decomposition much larger than those expected from the alkyl radical recombination rate constants.

John Simons took a 1 year sabbatical in 1970, and I remained at New Mexico State University to direct his research group. During this time, we measured the $^1CH_2-^3CH_2$ energy splitting, which we got correct. I applied for several post-doctoral positions and accepted one with Don Bunker at the University of California, Irvine. John met Don at a conference and convinced him that, though I had been trained as an experimentalist, it would be worth the risk to take me on. My 2 years with Don, starting in the summer of 1971, were marvelous. Independent research was expected, and I enjoyed working in such an environment. When I arrived, Don handed me a manual detailing the assembly language I was expected to use to write my chemical dynamics simulation program. The fortran compiler on the university's PDP-10 was so inefficient that it was worth the effort to write the code in assembly. The PDP-10 was a base-eight machine, and I still remember naively asking Don why the manual never identified processors 8 and 9. I still smile when I recall Don's response, that "the computer did not find these two numbers very important". My simulation identified non-RRKM dynamics for CH_3NC isomerization, and Don and I wrote an article describing our findings within the context of the origins of non-RRKM kinetics. During my time at Irvine, Don brought his work, now known as variational RRKM theory, to my attention. In an article published in 1972, I used this model to explain the apparent inconsistency I had found in my Ph.D. research between alkane molecule unimolecular rate constants and alkyl radical recombination rate constants.

The Bunker group at the time included Sally Chapman, Bruce Garrett, Alan Gelb, Trina Valencich, and others. They were great to work with. I also had rewarding interactions with Ed Lee, Sherry Rowland, Max Wolfsberg, and their research groups. Ed became a close friend. It was tragic that he and Don died so young. Gary Loper, a post-doctoral researcher in Ed Lee's group, and I became good friends, and I also had a close relationship with C. C. Chou in Rowland's research group.

After 2 years with Don, it was time to find permanent employment or accept another post-doctoral position. I applied for faculty positions and post-doctorals. Because most faculty positions in physical chemistry were in experimental chemistry and not theoretical chemistry, I applied to experimental post-doctorals. For my family and me, it was a very uncertain time. I was fortunate to receive interview invitations from Syracuse University and Wayne State University. Both interviews went well, and I was offered a position as an assistant professor in experimental physical chemistry at each school. Choosing was a difficult decision. However, physical chemistry was quite strong at Wayne State University. Larry Kevan and Ed Lim were on the faculty, and I decided to accept their offer and joined the Wayne State faculty in the fall of 1973.

Wayne State University was a very supportive environment for developing a research program. I was fortunate to have the opportunity to work with outstanding students and post-doctoral associates. I had been hired as an experimentalist, and I initially maintained both experimental and computational/theoretical research programs. One of our experimental projects addressed the singlet−triplet methylene splitting problem I had studied at New Mexico State. As we were analyzing our results, Carl Lineberger and co-workers published a manuscript which suggested the splitting was much higher than we had reported. This was a rather convincing direct spectroscopic measurement, and Fritz Schaeffer pointed out that there was enough uncertainty in the *ab initio* calculations to explain Lineberger's result. Our experiments were not direct, and a different interpretation, which required "throwing out" many experimental studies, agreed with Lineberger's experiment. We published a manuscript to this effect, but as we now know, Lineberger's experiment was also open to question, because it was contaminated by hot bands. This episode made me more critical of scientific findings.

The first two theses I directed at Wayne were in experimental chemistry. However, my heart was in computational/theoretical chemistry. Some time in the late 1970s, I discontinued my experimental program. In the 1970s and early 1980s, we

performed simulations of the unimolecular and bimolecular dynamics for a number of molecules, including H−C≡C−Cl, C_2H_5F, and model HCC. This work addressed non-RRKM dynamics and product energy partitioning and was done with Christine Sloane (a Professor at Oakland University), Ralph Wolf, K. C. Bhalla, Kandadai N. Swamy, and others. Our HCC → H + CC studies led us to semiclassical theory, resonances, the concepts of mode specific and statistical state specific decomposition and intrinsically unassignable states, and a deeper understanding of the classical and quantum dynamics of unimolecular dissociation and their relation to RRKM theory. This work was a harbinger of the outstanding work on unimolecular resonances by investigators such as Reinhard Schinke and Joel Bowman. Our additional work in unimolecular rate theory included the importance of anharmonicity in calculating accurate RRKM rate constants, very nice work by Ling Zhu of adiabatic and active treatments of the *K*-rotation quantum number in RRKM theory, connecting state specific resonance rate constants to the Lindemann−Hinshelwood thermal unimolecular rate constant $k(T,P)$, and Gilles Peslherbe's treatment of the multiple minima of fluxional molecules in RRKM theory.

In the early 1980s, Ron Duchovic developed an analytic potential energy function for H + CH_3 ↔ CH_4. Ron, Xiche Hu, and others used this function to calculate the H + CH_3 association rate constant by both trajectories and variational transition state theory (excellent agreement was found) and to investigate apparent non-RRKM dynamics for CH_4 decomposition. The transition state theory (TST) calculations led to models for calculating variational TST rate constants. In another set of projects, Da-hong Lu collaborated with many investigators to study intramolecular vibrational energy redistribution (IVR) in vibrationally excited molecules. Classical dynamics give the correct overall line widths for C_6H_6 overtone states. However, the ability of classical mechanics to give the detailed structure inside the overtone bands remains an open question.

In the late 1980s, Scott Vande Linde initiated our studies of gas-phase S_N2 reaction dynamics, which became an integral component of our research program. Significant non-RRKM and non-TST dynamics were discovered for these reactions, which have been confirmed by experiments. These studies led to an important extension of the model proposed by John Brauman for S_N2 reactions. Much of this work was first done by Haobin Wang and then by Guosheng Li, Lipeng Sun, and Kihyung Song. I cannot recall why we initiated these studies, but a suspicion that they would have interesting dynamics was suggested by our earlier simulations of ion−molecule association. Da-Fei Feng, Kandadai N. Swamy, and Cindy Darling found that the probability of ion−molecule association strongly depends on the molecule's angular momentum and the collision's impact parameter and relative velocity. Eldon Ferguson had found such effects in his experiments. Our current S_N2 studies address these reactions in solution and the extent to which microscopic solvation is an equilibrium process. Some of these questions were raised by the study of Xiche Hu in which he probed the effect of microscopic solvation on the kinetics of association reactions. It was also in the late 1980s when I established collaborations with scientists at the Ford Research Laboratory. For multiple reasons, I felt this was an important thing to do. I enjoyed working with Bill Kaiser, Ken Hass, and Bill Schneider, and together, we did some very good work on atmospheric kinetics and interfacial science.

An unpublished manuscript by the Y. T. Lee group motivated studies by Sylvie Bosio and Tianying Yan of rare gas atom scattering off hydrocarbon surfaces. This has been an extremely enjoyable research project, which lead to collaborations with John Tully, Steve Sibener, John Morris, Tim Minton, and hopefully others. Classical dynamics gives a quantitative interpretation of the energy transfer dynamics in these experiments. We have also simulated collisions of projectile ions, including protonated peptides, with hydrocarbon surfaces to interpret mass spectrometry experiments of surface-induced dissociation (SID). This work was initiated by Sylvie Bosio and was continued by Samy Meroueh, Yanfei Wang, Kihyung Song, and Jiangping Wang. Our studies of collision-induced dissociation (CID), initiated by Pascal de Sainte Claire, are extensions of this work, as well as our QM/MM studies of $O(^3P)$ reaction with hydrocarbon surfaces.

I spent 30 years at Wayne State, and during this time, I worked to enhance both the Chemistry Department and the University. I developed close friendships with Milt Glick, who as Chair made me feel welcome in the department. Larry Kevan was an exceptional mentor, providing valuable advice and encouraging one of his graduate students, Da-fei Feng, to work with me when I first arrived at Wayne. This helped "jump-start" my research program. Ed Lim was a great colleague, from whom I learned much about time-dependent spectroscopy and photophysics. I value my continued friendship with Dick Lintvedt, who was Chair for many years. Though I have left Wayne, we continue to play golf, which maintains my sanity. I was instrumental in bringing Berny Schlegel, Joe Francisco, Bob Levis, Evi Goldfield, Gang-yu Liu, John Santa Lucia, Ted Goodson, and Mary Rodgers to Wayne. I am particularly happy with the friendship of Gang-yu Liu and the growing research collaboration with Mary Rodgers. A reward of science is the close relationships one develops, and those with Yuan Lee, Bill Miller, Jürgen Troe, Reinhard Schinke, and Tom Baer have been particularly meaningful. When Don Bunker passed away in 1977, I was left as an orphan in the chemical community. I will always remember the support I received from Yuan Lee, Bill Miller, and their research groups. Jürgen and I have shared much in the development of unimolecular rate theory, and if anyone understands the details of Jürgen's work, it is me! In the mid-1990s, Reinhard invited me to Göttingen to work with his group on the calculation of unimolecular resonances and relating them to RRKM theory. This has led to a very warm friendship. Tom brought me in as co-author of the book on unimolecular dynamics he agreed to write, and this gave me the opportunity to get to know Tom, whom I already respected, even better. There are many others, too numerous to name, and with my "adventures" outside the unimolecular domain, I have developed many other friendships.

In 1999, I chose a new companion. Betty and I had become successful in our individual careers and had raised a lovely daughter, Heidi, but had grown apart. We separated amicably, and I fell in love with a wonderful woman, Alice Young, who agreed to marry me. Her father is also a physical chemist, with a Ph.D. degree from Brown University. For many years, he headed the research laboratories of the Eastman Corporation in Kingsport, Tennessee. With Alice as a partner, I left Wayne State in January of 2004 to join the faculty at Texas Tech University as the Robert A. Welch Professor of Chemistry. It is a great position, and we plan to spend many wonderful years at Texas Tech. Dick Bartsch, Chair of Chemistry at Texas Tech, was very persuasive in convincing me to move. Alice has a highly recognized research program in behavioral pharmacology and biopsychology and holds a joint appointment in the departments of psychology and of pharmacology and neuro-

science. The Texas Tech faculty have welcomed Alice and me with the warmth of West Texas and the tradition of Buddy Holly and Waylon Jennings, and we are excited about our new opportunities.

During my last years at Wayne, I led an effort to develop an interdisciplinary program in scientific computing, which I feel is very important for the future health of science in the United States. Computer simulation, and its use of theoretical models, is highly interdisciplinary, and tying it to individual departments hinders its development. However, the emergence of this discipline requires support from the university administration as well as the faculty, and though there was initial support from the former at Wayne, with changes in administrative structure, it waned. The universities that are able to surmount the barriers that hinder the development of interdisciplinary programs will be the most successful. While at Wayne, I became the Director of the Institute for Scientific Computing and when there were leadership problems in the Department of Computer Science I was asked to lead the Department as Interim Chair. My 3 years as Chair were successful, and I left the department in good hands with Farshad Fotouhi as Chair. With the experiences I acquired at Wayne, clear support from the administration at Texas Tech, and help from many others, including Philip Smith, the Director of High-Performance Computing, we are steadily building a Scientific Computing Program at Texas Tech University.

I am excited about our current research projects. We are developing algorithms and writing software for direct dynamics simulations, with the help of Yu Zhuang of the computer science department at TTU. The applications include the dynamics of complex gas-phase reactions such as those between $O(^3P)$ and hydrocarbon molecules, reactive collisions of radicals and ions with surfaces, and post-transition state dynamics. The latter refers to the complex chemical dynamics which may occur, after passing a transition state that leads to multiple reaction paths, potential minima, barriers, and products. Kim Bolton and David Mann initiated these studies. An interesting question, for these dynamics, is how fast equilibration occurs and when may one consider a free energy profile. Our studies of intramolecular energy transfer were extended to heat transfer and friction at the interfaces of sliding surfaces by David Mann and Hongwei Xie, and we plan to use direct dynamics to study reactions at these interfaces. We have always tried to make our software available to others and feel that a website is the best way to provide these resources to the scientific community. To distribute chemical dynamics software, documentation, and simulation models, we are developing the chemical dynamics software and simulation (CDSSIM) website cdssim.chem.ttu.edu. It is currently in a rudimentary form, but keep checking! I am very happy with my current research group of Srirangam Addepalli, Navdeep Chawla, Bipasha Deb, Jose Lopez, U. Lourderaj, Jason McAfee, Oleg Mazyar, Rajkumar Murthy, Asif Rahaman, Kihyung Song, Uros Tasic, Grigoriy Vayner, Jiangping Wang, and Mingying Xue.

In looking back, my life has been quite a journey. Many of the people who have provided the love and support for my success are included above, and there are more. I wish to thank each of you! Each time I thought every thing was settled, there was something new around the corner. My sense is that there will be a number of exciting developments in nonequilibrium dynamics, and I hope to be part of them!

William Hase