Autobiography of Russell M. Pitzer

Berkeley, California was the scene of my birth on May 10, 1938. My parents, Kenneth S. Pitzer and Jean M. Pitzer, were both from Pomona, California, and had gotten married in 1935 after they both graduated from college. I have an older sister Ann and a younger brother John. My father was then a junior faculty member in the Chemistry Department of the University of California, Berkeley. He had grown up helping his father in citrus growing in southern California, and probably watching various banking and real estate transactions develop and take place.

We lived in Kensington, an area just north of Berkeley in the hills. In November, 1941, we moved to a new house with a view, but to me the important thing was that I got to ride in the cab of the moving van. One of the neighbors was the J. Robert Oppenheimer family. In early 1943, we moved to Bethesda, Maryland, for my father to do weapons development work. We took the train (City of San Francisco to Chicago; Capitol Limited to Washington, DC) and then had the right clearance to obtain one of the few new cars available. In the fall, I started kindergarten, but the most memorable thing was to be allowed to get up in the dark and see a horse-drawn cart deliver milk. In the summer of 1944, we drove home. The war was progressing well enough that it was unlikely that any additional weapons developed could be produced and used before the war ended. Later, the Oppenheimers returned also. My brother, Peter Oppenheimer, and I used the vacant lots between our houses as a playground.

In December, 1948, we drove to Washington, DC again, pulling a trailer with a sailboat. My father had an appointment with the Atomic Energy Commission. We lived in DC near Rock Creek Park, which was great for exploring. We visited the Oppenheimers at Princeton once. In retrospect, there were very serious national decisions being made about building fusion bombs, but I only knew that my father and his associates were very busy. We returned home in 1951.

After junior high school, I went to El Cerrito High School and took up football. By the time I was a senior, I played first-string at guard on offense. I also got to know a lot of fellows who had different academic goals and talents than I had. Among the students I saw a lot of in college-prep classes and sometimes at football, there were a number who called themselves *nisei*, second-generation immigrant Japanese. After getting to know some of them well, they told me about spending the war in internment camps, where they often missed some schooling. By the time I was a senior, I would occasionally see that teachers would make mistakes in something they were explaining so I had to learn how to get things straightened out diplomatically. When my father suggested that I apply for college at his alma mater, Caltech, I did so, partly because I knew I could play a lot of football there.

Caltech meant serious studying, but football (and track in the spring) were a good relief. We had only a moderate number of players with substantial high school experience, so I played first string offense and defense all four years, one on the freshman team and three on the varsity. Because no major university team was using the Rose Bowl as a home stadium then, we were able to play our league home games there on Saturday nights. We were 1−5 there over three years, but it was a great experience. The most famous person that played against us was Jack Kemp, quarterback at Occidental College (our present president's first college, but that was later). In 1956, he was a senior; they had a hard time stopping our fullback to the left, but Kemp made enough long-yardage plays to beat us. The following year, we beat them in the Rose Bowl. The person on our team who would be most well-known in the future was Leroy Hood, in the class after mine. He scored a touchdown for us from 60 yards out in the Rose Bowl in 1958 on a misdirection play to the right, but we had insufficient other success to win the game.

We all chose majors at the end of our freshman year. Nuclear physics was very competitive, but I preferred something that was at least partly more visible, so I chose chemistry. My advisor was Linus Pauling, who had given many of the freshman lectures, but had not been in charge of the other parts of the course. At the time, he was heavily involved in the anti-nuclear-testing movement. Each quarter, when I needed to get my schedule card signed, I would look for Prof. Pauling, but if he was unavailable, it was not a problem because I was acquainted with other faculty who would take care of the matter. When he was in, he would invite me to sit down and talk about chemistry for a while, and eventually he gave me advice on attending graduate school (Harvard, but look at MIT also). In my senior year, I was able to take two courses with mainly chemistry graduate students: Harden McConnell's, which included quantum mechanics applied to EPR spectroscopy, and Norman Davidson's statistical mechanics course. A few of the graduate students would sometimes have a little better perspective on the significance of certain results, but I could usually do the mathematics more readily. I was also taking the mathematical physics course, of which two quarters were taught by R. P. Feynman. The competition was tougher, but manageable. He would use the Friday lectures for things that he thought were fun to work out about the subject or anything else. He was such a compelling speaker that I would attend any special lecture he gave, such as his repeat of his Nobel prize lecture and his account of being on a state textbook selection committee.

I saw J. Robert Oppenheimer for the last time while I was at Caltech. There was a distinguished visitor program for such people to visit the campus for a week and attend several events. He seemed unusually quiet and gaunt. At one of the receptions I went up and introduced myself and asked about his son Peter, but he did not seem to want to talk at length.

When I was a freshman and at home for Christmas, my sister brought along a fellow that she had been dating at the University of California, Davis. He was from Pasadena, said he had a younger sister, and suggested that I call her or meet her at his family's Rose Parade party. A friend and I went to the parade and the party and met her, Martha Ann Seares. I had to admit that I had taken many pictures of the parade but had neglected to put any film in the camera. I asked her out later. Our relationship grew and we were married in September, 1959, after we had both graduated.

We then set off for Harvard University, where I enrolled in the chemical physics program. One of the basic courses was quantum mechanics in the physics department, taught by Prof. Julian Schwinger in a quite esoteric way, starting with quantities he called measurement symbols. He said that the course was

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not intended for "chemists or metallurgists", but it was required for me so I persevered.

In the spring of 1960, it was time to pick a research advisor, and I chose W. N. Lipscomb, who had told me that he thought that there was sufficient recent progress in using computers to study molecules that it should be possible to compute the barrier to internal rotation in ethane, a property that my father had first obtained the year before I was born using heat capacity data, vibrational frequencies, statistical thermodynamics, and the quantum mechanics of internal rotation. A third-year student, Bill Kern, was my guide to learning the quantum mechanics of electronic motion in molecules and the applicable computer methods. The other theoretical chemists in the group then were Roald Hoffmann and Larry Lohr. MIT had an IBM 704 (vacuum tube) computer available for use. Michael P. Barnett, a faculty member in J. C. Slater's Solid State and Molecular Theory group had students working on writing programs in Fortran II for the needed integrals over Slater atomic orbitals. They were very helpful, and within a year or so, I was far enough along to help them occasionally in return. I made up a list of all the symmetry-unique electron-repulsion integrals for staggered ethane and the same for eclipsed ethane. I needed to find or write programs to evaluate all off these and write a program to do the self-consistent-field (SCF) calculations based on these symmetry-reduced lists. We learned that I. (Shi) Shavitt and Martin Karplus, at Columbia University and IBM Watson Lab, were working on programs to evaluate these integrals by other methods. After a couple of trips to discuss things with them, we agreed on a cooperative plan that included checking the methods against each other. In early 1963, I completed the project and obtained a result of 3.3 kcal/mol, slightly higher than the experimental value of 2.9 kcal/mol. With this and some other work, I had a thesis and went down to MIT to be a research fellow in the SSMTG group before starting a job at Caltech as a Noyes Research Instructor.

We moved to Pasadena in 1963, and I started to organize the software to facilitate future calculations in cooperation with some younger Lipscomb students and working on ways to understand such calculations better. At that time, only a few such calculations had been done, all on smaller molecules, and it was known that a number of these contained errors, so there was reluctance to believe calculations on a larger molecule. Caltech was bringing in other theoretical people. Andrew McLachlan came for a year but then returned to Cambridge. I helped a student that he had worked with, Glen Hultgren, finish his degree. B. Vincent McKoy came from Sinanoglu's group at Yale, and Bill Goddard came from the Duwez group in engineering at Caltech. Sunney Chan asked me to coadvise one of his students, Soe Aung, who wished to do some theoretical work. Bill Palke, from the Lipscomb group, came as a postdoctoral fellow to work with the whole group, and we did some calculations on the internal rotational barrier in hydrogen peroxide.

In 1968, I left to take a faculty job at The Ohio State University. Both Battelle Memorial Institute and Ohio State were building their effort in theoretical chemistry, and Bill Kern was the principal coordinator. Rafael Levine (part-time with Hebrew University in Jerusalem) and I joined Bill Taylor at Ohio State; Shi Shavitt and Bill Kern had joint appointments with their principal base at Battelle. New graduate students Gloria Du and Michael Bowers worked with me for a while and then left to do other things. Jim Power was a postdoctoral fellow who worked on NMR spin−spin coupling and other things with me for three years.

Thom Dunning came from Caltech to be a postdoctoral fellow at Battelle and pointed out that more definitive studies of Slater orbitals compared to Gaussian atomic orbitals needed to be done. With help from Soe Aung, we did an extensive comparison for water. Slater orbitals had been viewed as the ones to use for 40 years and the bottleneck in doing the integrals until 1960 as the main barrier in the field, but now that we could use them, it turned out that there was a better way to solve such problems. Gaussian orbitals had been considered for 20 years, but it took that long to get the computer power and ideas to learn how to use them effectively. Thom and I helped Wil White, a graduate student of Weldon Mathews in spectroscopy, compute the energy levels of the CF molecule which he had been studying in the laboratory.

With help from postdoctoral fellow Nick Winter and graduate student Wally Ermler from the Kern group, a generalization of the earlier symmetry analysis for molecular integrals was worked out and showed to be general and provide computational efficiency. The permanganate ion was a good example, and use could be made of its full tetrahedral symmetry; this was done by postdoctoral fellows Hsiang-Lin Hsu and Carl Peterson. Ernest Davidson came to Columbus for a sabbatical. He helped us alter our SCF program to calculate deep ionization potentials better, but he spent most of his time at Battelle working with Shi Shavitt on methods of obtaining the lowest eigenvalues of huge, sparse matrices. The method now called the Davidson method was developed at that time. Graduate students John Yates and Dana Grow worked on calculations of the structures of various lithium oxides and transition metal trifluorides, including one of the earliest Jahn−Teller analyses using actual wave functions.

For the summers of 1977 and 1978, I accepted Fritz Schaefer's invitation to help his group improve their basic software at Berkeley. He and Bill Miller had pioneered in the use of minicomputers rather than mainframes. I converted our integral program, which had contributions from the HONDO method of Gaussian integral evaluation together with our symmetry efficiencies, to their Harris computer with its parallel I/O features and then did the same with our SCF program. It was also a good opportunity to work on a number of projects with members of the Schaefer group. The following summer, the Schaefer group needed an integral program adapted to configuration−interaction (CI) calculations, so I ended up doing most of this work at a desk in Michel Dupuis' office at the National Resource in Computational Chemistry at Lawrence Berkeley Lab and learning the features of their CDC 7600 computer. Subsequently, this program was requested by the Shavitt group for the COLUMBUS programs, and then modified for generally contacted orbitals (ARGOS, Argonne−Ohio State), for the Dunning group at Argonne National Lab, where several visitors obtained it for their research groups. In 1980, we spent the spring on sabbatical attending part of Juergen Hinze's year-long program of meetings at Bielefeld University in West Germany. I took along a copy of the atomic SCF program from the Roothaan and Clementi groups, added some features, and brought it up to date. It was used then as now mainly to develop basis sets.

Previous work with biradicals was extended by graduate student Sheila Auster on trimethylenemethane derivatives, collaborating with a new faculty member (now dean) Matt Platz, who had worked on them experimentally. By then, another faculty member, Bill McCurdy, and I were consulting at Lawrence Livermore Lab, so we both gained experience with the new Cray vector supercomputers. My work was with Nick

Winter, who needed quantum chemistry software capable of treating molecules with very heavy atoms (and relativistic effects) and metal ions doped into crystals. There was some software to begin with, but it took some time to modify the older software and write the additional programs needed. When it was working, there were several applications to work on with Livermore people, my students, and Bill McCurdy's students.

In 1985, after the NSF announced their program for funding national supercomputer centers, Bill McCurdy and I, as two of the very few supercomputer-experienced faculty in the state, were included in a group putting a proposal together. We were unsuccessful, but the Ohio Board of Regents expressed interest in having a state center. In 1986, Bill was appointed Acting Director and I was appointed Acting Associate Director. We set about making plans for all aspects of the Ohio Supercomputer Center, including a state computer network for access (Ohio Academic Resources Network). After a year's effort, the center was starting to function, my appointment was up, and it was time for a sabbatical.

Two graduate students (Nora Wallace and Agnes Chang) and another to follow (Frank Kocab) and my wife and I went to the University of California, Berkeley. Nora was trying out our new spin−orbit CI program on the potential curves for CuF and Agnes was attempting to compute the electronic spectrum of uranocene. Frank started studying the spectrum of neptunium hexafluoride.

On returning to Ohio State, a new graduate student, Jean Blaudeau, joined the group and started work on metal complexes with quadruple bonds. A repercussion of my having shown some administrative ability with the supercomputer center was that I was asked to be department chair. Victor Luana from the University of Oviedo, Spain and Michael Dolg from Stuttgart University, Germany, came for extended stays. Two groups in Germany and one in Spain asked for copies of our programs and involved us with some of their projects, particularly cerocene. We continued a series of calculations on beryllium clusters with postdoctoral fellow Robert Ross, (Dean) Bill Kern, and others. Graduate student Ke Zhao (he later walked out of the World Trade Center just before the first airplane struck on 9-11) started work on small fullerenes with 28 C atoms and others and Debbie Tuan from Kent State University came for a sabbatical working in this area also.

Two new graduate students, Zhiyong Zhang and Scott Brozell came and were good at programming projects as well as applications. Zhiyong worked on the well-studied spectrum of the uranyl ion and Scott worked on heavier actinides. On a 1995−1996 postchair sabbatical, my wife and I spent the autumn in Europe with a month in Cambridge with Nick Handy's group and shorter visits with Michael Dolg in Dresden and elsewhere. The winter was spent with the Schaefer group in Georgia and the spring was spent visiting Argonne, Los Alamos, Lawrence Berkeley, and Pacific Northwest National Laboratories. Then graduate student Spiridoula Matsika joined the group, and all of us were able to attend the 1999 ACS meeting in Anaheim and meet Bob Denning, the expert in actinyl spectroscopy. Bob publicly complimented Spiridoula's initial neptunyl work, which impelled Bob's Los Alamos hosts to converge on her and try to interest her in a particular neptunyl spectroscopic problem. The following year, graduate student Qi Wang joined the group, and on a research leave, Spiridoula and Qi joined us in traveling to a conference in Berkeley and several-week visits to Pacific Northwest and Los Alamos National Laboratories. Qi was not able to make the last visit due to the Wen-Ho Lee matter. She subsequently completed her MS degree and switched to biophysics.

Qiang Chang joined us and earned his MS doing calculations on the spectrum of UO_2 to help the Michael Heaven group make assignments. Then he looked into other areas and ended up in astrochemistry. Ilias Sioutis joined and worked on heavy-atom−borane complexes before switching to spectroscopy but using his background to untangle the Jahn−Teller spectra of Ag_3. Next, graduate student Yang Yang and postdoctoral fellow Tianxiao Yang joined the group. Yang Yang worked on the spectrum of Er^{3+} doped into GaN crystals and Tianxiao worked on CUO and EuH and other molecules. Rajni Tyagi switched from another area to quantum chemistry and proved to be quite adept at supplying spectroscopic property values of actinide-containing ions to experimental groups (John Gibson, Oak Ridge and Michael Heaven, Emory) that helped them in their work. Graduate student Michael Mrozik joined us in carrying out similar studies and should finish soon.

In 45 years of teaching a wide range of classes and whether they were composed of 300 freshmen or 100 juniors or a dozen graduate students, it has been intriguing to try to tell them, in an effective way, why certain experiments were done and why certain ideas were developed, as well as assign them problems on these principles to help them understand them. I have been more fortunate than most to have been able to meet many of the pioneers in molecular quantum theory and spectroscopy, so in later years, I have tried to describe these people to students in a useful way. Some students seem to find this information interesting, while others mainly want to know if it will be on the next exam. In the choice of projects in my research group, we often collaborated to various degrees with other groups in one way or another, which I hope has had a broadening effect on all concerned; it certainly has on me.

Now that I am retired, I hope to continue such work in the future for quite a while, but other things change also. Now our younger son feels free to ask me occasionally to help him on weekdays with projects in his home remodeling business. Our daughter and older son live much farther away, so we do not see them as frequently. I have enjoyed working with many people over the years and feel honored to have had the opportunity to do so.

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