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HARRISON SHULL
1923–2003

A Biographical Memoir by

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BY DONALD S. MCCLURE AND MICHAEL KASHA

HARRISON SHULL BUILT AN influential scientific career in research, specializing in the quantum mechanics of small-molecule electronic spectra. He later showed a gift for administration as a chief academic officer of several major educational institutions. He was born into a family of highly achieving scholars and scientists; a hefty book titled *Shull Genealogy* was a proud part of his early personal library. It was clear that this background contributed strongly to his self-confidence and growth, and it can also be stated that he added much luster to the already illustrious Shull name.

Harrison Shull made early, seminal contributions to the theory of molecular energy levels, taking advantage of the growing capabilities of large-scale computers in the decades of the 1950s and 1960s. As his career developed, he found ways to promote the use of computers in chemistry, increasingly using his administrative talents to the great benefit of his colleagues in acquiring access to these facilities

Harrison Shull was born in Princeton, New Jersey, where his father, George Harrison Shull, was a professor of botany at Princeton University. George Shull had become famous for his part in the development of hybrid corn, which had

an enormous impact on the practice of agriculture worldwide. The four brothers and two sisters in the Shull family grew up in a house on Jefferson Street with a special tree their father designated for each one to look after. As a child, Harrison was often hampered by allergies and illness and, being confined to the house, he did a lot of reading. In the summers, however, young Harrison aided his father's genetic research by picking up stones and removing insects for penny wages in the primrose research fields. He worked through grade school and Princeton High School at the top of every class. His high school principal wrote a recommendation for him to go to Princeton University, saying in part, "Harrison Shull is in my opinion the strongest student scholastically that has ever enrolled in Princeton High School." He ranked number one in his high school class and was not yet 17. He entered Princeton University in September 1940 and, repeating his high school performance, graduated number one (in a tie) within three years in the accelerated wartime program. He presented the traditional salutatorian address in Latin at the graduation ceremonies.

Upon entering Princeton he had no firm idea of a major subject, but seeing his three older brothers enroll in Princeton as biology majors (taking their father's course), he decided to do something different. He thought he was better at chemistry than physics, so chemistry was his choice.

His career began as a civilian in the chemistry division of the Naval Research Laboratory in Washington, D.C., during World War II. It wasn't long before every coworker under the age of 26 was drafted. They added basic training to their work schedule, and emerged with the rank of ensign. His association with the Navy continued in various ways throughout his lifetime, and finally, after a long career, ended as the chief administrative officer (provost) of the Naval Postgraduate School in Monterey, California.

Harrison was always certain that he would go to graduate school. He decided that at this time in his life he should see what California was like and so applied to Caltech, Stanford, UCLA, and UC Berkeley. Berkeley won because they sent him a telegram of his acceptance while the others relied on air mail. He also had advice from Henry Eyring, who often walked down Jefferson Street (in Princeton) on his way to the university. He said, "Only Caltech and Berkeley are worth consideration, but Linus Pauling is ill so don't go to Caltech, go to Berkeley and work with Gilbert Lewis, he'll last longer." So Harry packed up his car and drove to Berkeley and within days, in early November 1945, began to work with G. N. Lewis.

Berkeley was an exciting place then as always: Seaborg and others had been discovering the transuranium elements, and a large nuclear research laboratory was growing on the hills above the campus. William Giauque had developed a world-renowned cryogenic research program; Gilbert Lewis had turned to molecular excited-state researches; and Melvin Calvin was using isotopes to trace biochemical processes in living organisms. Several Nobel prizes would be awarded to UC chemists and physicists in years soon to come. Harrison's work was to follow the discoveries of G. N. Lewis and Michael Kasha on the phosphorescence of organic molecules and the electronic triplet state hypothesis of its origin.

Working in the Lewis lab then were Michael Kasha, who had already completed his Ph.D. (in 1945), and Robert Nauman, who was in his last year of research with Lewis. Donald McClure arrived in February 1946. Then Eyring's predictions went badly wrong: Lewis died in March 1946, while Pauling lived another 48 years! Wendell Latimer, then dean of the College of Chemistry, made the decision to keep the group together and persuaded George Gibson to become its faculty supervisor. Latimer also persuaded Michael

Kasha to remain working as the laboratory spectroscopist until Nauman, Shull, and McClure completed their research and embarked on their own (and as it proved, highly successful) research careers. Later Shull, Kasha, and McClure were each elected to membership in the National Academy of Sciences.

Gibson's way of running a research project could not have been more different from Lewis's. Whereas Lewis would have twice-daily meetings with each student, giving him ideas to follow up, Gibson just let things happen. But he did have regular meetings to learn group theory and some necessary parts of quantum mechanical theory. He promoted discussion and had interesting ideas. He was a wonderful person and the group flourished under his leadership.

Harrison Shull emulated Gibson's research style more than Lewis's when he later had his own research groups. Harrison enjoyed the considerable independence that the Gibson group offered. So later in his own work in Iowa and Indiana, he particularly arranged for his graduate research group to be somewhat remote from his own office, confiding to some of us that the separation cultivated more independent thinking instead of letting the professor solve each puzzle.

Among the important questions of those days (1945 to the 1950s) was the characterization of excited states of molecules. The first property to learn was the group representation of the state. Harrison Shull's Ph.D. thesis attempted to do this for the triplet electronic states of benzene, and for the lowest triplet state this could be done by an analysis of the vibrational spectrum of the phosphorescence (which Lewis and Kasha had characterized as a triplet-singlet transition). Shull's first paper, published in 1949, was on this analysis. Later, John van der Waals in Holland extended this work, using Harrison Shull's observations.

During his stay in Berkeley, Harrison lived at the Alpha Chi Sigma house, the chemistry fraternity. His leadership qualities, intelligence, and good humor made him a natural choice for president of this local chapter. This was just another example of how he came to the top in the many institutions where he worked.

The urge to see what California was like was expanded into a meandering 20-day trip from Berkeley to Princeton in August 1947. Accompanied by Robert Nauman (who kept a detailed log) and Alan Smith, he traveled 8,000 miles through 19 states and 4 Canadian provinces.

Living in Berkeley as single men with responsibility only for academic work allowed unrestricted concentration on research. Attracting a suitable potential wife was another goal of the young group (all working on triplet states of molecules). As their Ph.D. work came to a conclusion, almost simultaneously each of the three remaining members of the group (Shull, McClure, and Kasha) had succeeded, the laboratory humor resonating with "the triplet state has worked again."

In considering his next move Harrison thought that the postwar climate for financing scientific research might be unfavorable for an experimentalist, who would require expensive equipment. A theoretical capability would be more portable and less expensive. Latimer urged Shull to apply for a National Research Council Fellowship, which he won and which could be used anywhere. He chose to go to the University of Chicago to study molecular orbital electronic theory with the physicist Robert Mulliken. Shull's second paper was on the calculation of transition probabilities in diatomic molecules (1950), the first in a series of his theoretical papers on this subject. It was thought that the theoretical f-numbers (oscillator strengths for band intensity) might be more accurate than measured ones and that the

results would be useful to astrophysicists trying to determine the numbers of molecular species in interstellar gas clouds.

After a year in Chicago, Harrison Shull moved to Iowa State College (later University) at Ames, Iowa, at the urging of Fred Duke. The latter was formerly a professor of analytical chemistry at Princeton and then at Iowa State who had been following Shull's progress for the past six years. There was another connection between Princeton and Iowa State: Harrison's father, George H. Shull, was awarded an honorary degree by the college in 1942 for his part in the development of hybrid corn, which had an enormous effect on Iowa and many other parts of the world.

One advantage of Iowa State was that the government-sponsored Ames Laboratory was located there, and Shull was given a joint appointment in that laboratory and in chemistry as an assistant professor. The Ames Laboratory under Frank Spedding (a G. N. Lewis disciple) was a source for spectroscopic equipment and money for summer salaries. The Ames Laboratory specialized in rare earth (4f-element) chemistry, which was a fundamental basis for the chemistry of uranium-plutonium (5f-elements) in the World War II Manhattan District projects. Spectroscopic research in this field had been nurtured in G. N. Lewis's laboratory, with collaborative work by Frank Spedding, Simon Freed, and Noel S. Bayliss (the last was later prominent in Australian spectroscopy). Harrison Shull's students there included several who later had outstanding careers, especially Lionel Goodman, Stanley Hagstrom, and Frank Ellison. His research topics at Iowa included papers that he wrote on the comparison of transition probability calculations using dipole-length versus dipole-velocity operators, which give different results due to the use of approximate wave functions. An important calculation for that time was the all-electron self-

consistent field treatment of H_2O with Frank Ellison. There were several papers on π-electron systems in organic molecules with Lionel Goodman.

The first international conference on quantum chemistry was held on Shelter Island, New York in September 1951 with Robert Mulliken as one of the organizers. Harrison Shull was invited. At the Shelter Island Conference he roomed with Per-Olov Löwdin, who had just completed his Ph.D. in Sweden. Harrison and Löwdin began an inspired friendship and a lifelong collaboration. Early in 1954 at the urging of Löwdin and Harrison's wife, Jean, Harrison applied for and won a Guggenheim Fellowship, which would support the parents and their four children for a year in Sweden. But the department chairman refused to give Harrison a leave of absence; Harry said he would quit, and did so even when the leave was later granted. The self confidence illustrated by this act was entirely justified by later events.

A year earlier, Iowa had tried to hire Walter Moore (author of a landmark text in physical chemistry and later of a definitive biography of Erwin Schrödinger), but Walter elected to accept an offer from Indiana University instead. Mutual admiration led Harrison and Walter to stay in touch and this led to an invitation for Harrison to give a talk at Indiana before going to Sweden. The Shull family departed for Sweden in September 1954, and for a Christmas present that year Shull got an offer from Indiana, which was quickly accepted.

Shull never returned to Iowa, but having shown the faculty there the value of a chemical theoretician, he made it easier for them to hire Klaus Ruedenberg, saying in a letter to Klaus that "everybody would be gaining by the two moves, each of us two by getting a better job, Indiana University by getting a good theoretical chemist, and Iowa State University by getting a better theoretical chemist."

The collaboration in Sweden with Löwdin in the academic year 1954-1955 resulted in the development of a significant new idea, the concept of natural orbitals. Their papers on this and several other aspects of electronic structure calculations were published in 1955. Taking leave from Indiana in 1958-1959, Shull again spent a year with Löwdin in Uppsala, this time as assistant director of the quantum chemistry group. These visits convinced him to concentrate on *ab initio* quantum theory and to use large-scale computers to solve the equations.

Shull's association with Indiana lasted 24 years, longer than with any other institution. He arrived as associate professor in 1955 and within three years was promoted to the position of full professor; in 1961 he was named research professor. He enthusiastically promoted the use of large electronic computers, and later as director of the Computing Center he established the principle of free use to researchers, paying the operating expenses by separate grants. He founded the Quantum Chemistry Program Exchange (software), which put Indiana on the map for everyone doing quantum chemistry. Ultimately he became dean of the graduate school (1966-1972) and then vice-chancellor for research and development (1972-1976). He was recognized as a brilliant administrator who brought in fresh ideas for handling the tough problems of appointments, tenure, promotion, and salary increases.

The Chemistry Department at Indiana was a vibrant place with Harrison Shull, Walter Moore, Vernon ("Jack") Shiner Jr., Henry Mahler, Frank Gard, Felix Haurowitz, and others there during the period of their tenure. The graduate students in Shull's group were having fun both scientifically and socially. They were often invited to the Shull home for parties with the family or included in faculty gatherings. He was a stimulating person and would bring visitors to

Bloomington with their new ideas. Harrison was very good at debating, and the graduate students jokingly said that the criterion for deciding when it was time to face the world and leave the university was when you could win a scientific argument with Harrison. After they left, he would follow their careers with interest and pride. One, Ralph Christoffersen, shared Harrison's bent for administration and went on to become vice-president of the University of Kansas and then chancellor of Colorado State University at the very time Harrison was chancellor of the University of Colorado.

Indiana University is famous for its Music Department. Harrison's interest in music was evident during his Berkeley days, when he and McClure would go to hear the Thursday night performance of the San Francisco Symphony orchestra. In all his later university positions he encouraged musical performances and attended many.

During his tenure at Indiana and especially after his election to the National Academy of Sciences in 1969, Harry accepted many invitations to join committees and boards. He was very effective, and in many cases he became the chairman after several meetings. It seemed especially appropriate that he joined the Advisory Council to the Chemistry Department at Princeton University and eventually became its chairman. He became well known nationally and met many people who would become important in his life. One of the scientists important in Harrison's life was George Low, a brilliant engineer and manager who among many other things had been chairman of the Manned Lunar Program Planning Group, which provided the technical background for President Kennedy's decision in May 1961 to commit the U.S. government to landing a man on the Moon before the end of the decade. Subsequently, Low held major positions in NASA. In 1976 George Low accepted the

offer of the presidency of Rensselaer Polytechnic Institute, his alma mater. Low soon found that he needed a provost and made the offer to Shull. Low's idea was to make Rensselaer into a major research university, and the new position seemed to be an attractive challenge, which Harry quickly accepted in the fall of 1979.

Harrison spent only three years at Rennselaer but was influential in wisely and gently nudging its faculty members toward a higher level of academic achievement and in rewarding them with a better scheme of salary increases. His colleagues in administration and on the faculty recognized him as a warm and supportive person who always acted with high and strongly held academic principles. While at Rennselaer, Shull was aggressively pursued by the University of Colorado, which was seeking a chancellor for its large Boulder campus. Harrison and his second wife, Wil, had spent a summer there while he lectured on quantum chemistry in 1963, and they loved it there. Shull refused the offer at first, persuaded to remain at Rensselaer by George Low, but he was finally persuaded to make the move.

In the Colorado University system there was a president over all branches and a chancellor for each campus. Harrison's term as chancellor of the Boulder campus was from the spring of 1982 to the summer of 1986. Harry got along well with the president, Arnold Weber, and began some bold initiatives. He invested about $1 million in a chancellor's computer fund to enable the faculty to buy personal computers at about a third of the market price. This had followed some intense negotiations with computer manufacturers in which he was able to persuade the companies that it was good business even if they didn't make money on the deal in the first year. The scientists, of course, loved it, and the rest of the institution rapidly became computer literate. Arnold Weber left to become president of

Northwestern University in 1985, and under the new administration it was difficult for Shull to operate, so he considered moving again. Harrison and Wil had discussed retirement times and places so that these factors entered into the choice for the next move. Providence descended again when Wil noticed an opening for provost at the Naval Postgraduate School in Monterey, California. Harrison Shull was well known in the Navy and once his name came up for this position, the school was ready to do anything to get him.

During the period from 1988 to 1995 he held the positions of provost and vice-president for academic affairs at the Naval Postgraduate School. There he was able to increase significantly the number of faculty members and improve the quality of graduate education. Harrison was very impressed by the education plan and its effect at the Monterey school. The students were Navy personnel of considerable practical experience. As students, they were older than normal college students, often were already head of a family, and dedicated to advanced technical education. Their focus, dedication, and desire to succeed were thrilling to Harrison to see in action. He was inspired by the effectiveness of the students' achievements. No low grades, low aspirations, or failures there. Admiral Ralph West, superintendent of the school, wrote a penetrating evaluation of Shull's performance in these years, and it seems to apply to all of Shull's academic administrative positions, so we quote from it here.

> Harrison was an experienced academic administrator who was very effective in generating change to strengthen the school's educational capabilities. He always approached issues with a long-term view and the patience and ability to achieve his goals. He put in place tenure guidelines that resulted in continuous improvement in the faculty. He ensured departments conducted rigorous recruitment campaigns to provide the selectivity needed to be able to hire only quality faculty. All of these occurred during

a period in which the Navy's size and therefore the school's input was declining. Through Harrison's efforts the school was able to retain top faculty personnel, ensure sufficient openings for hiring strong new talent, and meet the strictures of reduced funding.

While Harrison outwardly appeared to be a kindly grandfather figure, his incisive method of leadership ensured a detailed knowledge of and impact on all issues associated with instruction, faculty and educational support. He had unusual strengths in the area of informational technology and was able to ensure smart decisions were made concerning computer services and equipment as well as library support. At the personal computer level, Harrison showed an uncommon ability to use various software for combining multiple data sources to compare performance, reveal problems, and evaluate solutions. Harrison was the perfect person to have in the academic leadership position at the school during a time of change and the need to strengthen the school's capabilities. The results of his efforts played a major role in justifying the retention of the school during the reviews of the early 1990s to close military bases.

Harrison and Wil built their dream house on a hill overlooking Monterey Bay and lived there after retirement in 1995. There was enough room in it for the many visiting children and grandchildren and for the many friends made in different parts of the world during a long and highly visible career.

CONTRIBUTIONS TO SCIENCE

The following four paragraphs were contributed by Professor Ernest R. Davidson, formerly a Shull student at Indiana.

During the 1950s Shull produced his most lasting contributions to the theory of electronic structure of atoms and molecules. Several of these papers are still frequently cited 50 years after they were written. Before this time, mixing of "configurations" was generally limited to configurations that had a clear physical significance as nearly-degenerate zero'th order approximations to electronic states of the system. Also, perturbation theory used a formal expansion in eigen-functions of operators with both a discrete and continuous spectrum. With the access to digital computers in the 1950s it quickly became clear that the Hartree-Fock method would not

produce results of sufficient accuracy. Description of the correlation energy (defined as the error in the Hartree-Fock energy) using digital computers required a new approach.

Working with Löwdin, Shull approached this as a problem in numerical analysis rather than a problem in chemistry. They showed that the continuum problem could be avoided by simply expanding in a complete discrete basis set with no physical significance [1955]. They then used this approach to generate an accurate wave function for the helium atom. Factorization of this function into its expansion into Natural Orbitals led to a very compact and easily interpreted result even though the individual terms had no relation to any zero'th order model problem [1955, 1959]. Shull extended this approach to the hydrogen molecule [1959] and then showed how the results could be simply interpreted [1960].

Shull and Löwdin extended the helium atom results to the ground and first excited triplet state of the iso-electronic two-electron atomic ion series, H^-, He, Li^+, etc. [1956]. They were the first to note that the correlation energy of the ground state of these ions is nearly independent of the atomic number, Z. This led Shull to two additional papers. In one, he examined other iso-electronic atomic ion sequences and showed that those which became degenerate in the high-Z limit had correlation energy which was linear in Z, while those that remained non-degenerate had a correlation energy that was nearly independent of Z [1960]. This has been a key paper in constructing accurate tables of atomic energies. In the second, he showed that direct variational calculation of the excited state energy as a higher root of a secular equation could lead to the exact wave function without convergence of the lower states [1958]. Before this it had been assumed that the lower roots would have to be converged in order to get an accurate wave function for the higher state.

This flurry of key papers profoundly changed the way people approached the electronic structure problem. Before these papers, the problem had been approached using qualitative reasoning or semi-empirical explanations for spectra and bonding. After these papers, the problem was viewed more as a problem in numerical analysis and construction of rapidly converging sequences of approximations. Other research groups around the world with access to digital computers soon adopted this viewpoint.

Shull's publication list of about 80 papers contains work on several other subjects, some of them already mentioned

earlier in this account. In his later years he published articles and editorials on the social aspects of the educational process.

PUBLIC SERVICE

Shull's ability to work with people was expressed both in his university administrative positions and in being a member or chair of committees. Especially during the Indiana years he may have had as many as 10 such obligations at once.

The Naval Studies Board was created by the National Academy of Sciences at the request of the Navy Department in 1974 to be a source of independent, long-range scientific and technical planning advice for the Navy and Marine Corps. Shull was one of several people who worked with Admiral Zumwalt, chief of Naval Operations, and Philip Handler, president of the National Academy of Sciences to organize the Naval Studies Board and then served on it for six years, and again for six years after his retirement in 1995. While still at Colorado, he was a member of the Advisory Committee on Chemistry for the Office of Naval Research and during his tenure at the Naval Postgraduate School was a member of the workshop on Navy intelligence technology.

Harrison Shull made notable contributions to the field of human resources in science and engineering, mainly through the Office of Scientific Personnel of the National Academy of Sciences, which was reorganized in 1974 as the Commission on Human Resources. He was its chairman from 1977 to 1981, but had been a consultant before then on the use of computers to organize large data files on Ph.D.s in science and engineering. The committees meeting under the aegis of the commission had to be chosen, their agendas defined, and their reports monitored. The commission

conducted postdoctoral associate programs for several dozen of the leading scientific organizations of the federal government, such as the National Institute of Standards and Technology, the Naval Research Laboratory, NASA, National Oceanic and Atmospheric Administration, the Air Force, and the Army. Both the quality and the numbers of Ph.D. graduates had to be considered, and this led to studies of the fluctuations in supply and demand for these valuable people. Shull noted that, since it took four to five years to get an advanced degree, what looked like a good employment prospect at the start might not be so good at the end, leading to fluctuations that government programs might be able to damp by granting or withholding grants at the right times. Shull wrote an article on this plan for the 1978 National Research Council annual report.

Some appointments to other National Academy of Sciences endeavors were the Committee on Science and Public Policy (1957-1974), the Stockpile Assessment Panel of the Committee on Demilitarizing Chemical Munitions and Agents (chairman, 1983-1984), the Committee for Joint U.S.-U.S.S.R. Program on Fundamental Science Policy (chairman, 1983-1991), and many others.

FAMILY LIFE

Harrison was the youngest in a family of four boys and two girls and one father and one mother. His own family came to eight children with two wives. Jean, whom he married in 1948, had a son, James, from a previous marriage, and they had a son, George, and two daughters, Kathy and Holly. He and Jean, who did not return from Sweden when Harrison and the boys returned to Indiana, were divorced in 1962. Harrison met and married Willa Bentley in 1962. She had two boys, Jeffrey and Warren, from her previous marriage, and they had a son, Stanley, and a daughter,

Sarah, together. Harrison and Wil made an excellent academic team with Willa cheerfully taking on the role of university first lady as Shull moved up the academic ladder. A Shull reunion was a big, happy gathering with siblings, nephews and nieces, children, and grandchildren. (One special reunion was a surprise seventieth birthday party in Monterey organized by Wil.) The children of these unions got along well with one another. Most obtained university degrees, and there are some with professional degrees and Ph.D.s. Harrison was a central and beloved figure in this expanding group.

Harrison had a great sense of humor. His children and grandchildren remember his twinkling eyes, followed by a joke. We remember locating him in a noisy crowd by hearing his uninhibited laugh. Still he could be disappointingly critical when he thought you could do better.

EPILOGUE

Harrison Shull, Harry to all of his friends and associates, will always be remembered for his great skills, both scientific and administrative. But most of all, we share the warm recollection of his good-humored nature, his wise advice on many occasions, and especially for his fair-mindedness and elegance as a great human being.

MEMBERS OF THE SHULL family were very helpful to the writers of this memoir. Harrison's wife Willa Shull was central in providing details of his life and making contacts for us. His son Stanley gave details of family life and a recording of his conversation with Harrison about his career. Harrison's older sister, Georgia Vandersloot, who helped bring him up, wrote about his early life, and her daughter, Karen Richards, wrote about family relationships.

We thank his former students and university colleagues: Robert Nauman (Berkeley); Lionel Goodman, Klaus Ruedenberg (Iowa); Stanley Hagstrom (Iowa and Indiana); Vernon ("Jack") Shiner, Ernest

Davidson (Indiana); Ralph Christoffersen (Indiana and Colorado); Gary Judd, Van C. Mow, and Don Miller (Rennselaer); Charles Depuy (Colorado); Ron Taylor (Naval Studies Board); William Kelly (Commission on Human Resources); Ralph West (Naval Postgraduate School).

Details of Harrison's father's part in the development of hybrid corn appear in the recently published book *Mendel in the Kitchen* by Nina Fedoroff and Nancy Marie Brown (Joseph Henry Press, Washington, D.C., 2004, pp. 57-62).

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