PER-OLOV LÖWDIN

28 OCTOBER 1916 · 6 OCTOBER 2000

FAMILY, friends, colleagues, Uppsala, and its university bid farewell to Per-Olov Löwdin in October 2000. A memorial symposium preceded the funeral and featured a variety of tributes to a great scientist and teacher. Uppsala Cathedral framed a solemn ceremony on 26 October that marked the end of the earthly presence of Löwdin.

Per-Olov's parents were residents of Uppsala; the father, Erik Wilhelm, was a musician, and the interest in music remained with the son throughout his life. Schoolmates and teachers saw his mathematical ability develop to excellence, and Per-Olov entered Uppsala University in 1935 in order to specialize in mathematical physics in Ivar Waller's department. The theory of relativity occupied his early years, and he wrote about it in his first publication in *Elementa*, the magazine for teachers and other interested parties in Sweden. He earned the *licentiate* degree in 1942 during the Second World War. Neutral Sweden mobilized its defense and most young men served a substantial time guarding the long border through some of the most severe winters recorded. Löwdin did his share and took part in teaching candidates in the officers' training college at Uppsala. He taught courses in mechanics and mathematical physics at the university as well.

Sweden's isolation ended when Nazi Germany surrendered in 1945; opportunities for international contacts became available to many, and young scientists were eager to establish new networks. Per-Olov Löwdin availed himself of these possibilities and initiated an international career that was to last until the end. He studied with Pauli for half a year at Zürich in 1946. Returning to Uppsala he undertook the work that resulted in the doctoral thesis, "A Theoretical Investigation into Some Properties of Ionic Crystals." This contribution is a remarkable accomplishment in which the author develops techniques for integral evaluations and numerical procedures as well as managing the actual computations. The problem that prompted this investigation was the failure of the Cauchy relations for the elastic constants of ionic crystals. Löwdin showed that the many-atom interactions should be considered beyond the "classical" two-body potentials assumed in the derivation of the relations. The additional terms occur when overlap integrals among atomic orbitals are included. Overlap was to remain an important element of Löwdin's analyses. The doctorate was secured in 1948, accompanied with the docent-honor and position.

Docent Löwdin embarked on the enterprise to establish an international platform where he would be able to realize his ideas for the development of the electronic theory of matter. He spent five months of 1948 in Bristol with Neville Mott, and began a series of visits to the United States in 1950. He spent time at major universities there, most

notably with Hertha Sponer at Duke University, with Robert S. Mulliken at the University of Chicago, and with John C. Slater at the Massachusetts Institute of Technology. His presence at the Shelter Island Conference in 1951 allowed him to be recognized among the prominent young men of quantum chemistry. A trip around the world in conjunction with participation in the Nikko Symposium in 1953 added to the network of friends and collaborators.

Löwdin was a well-established player on the international scene when his docent stipend expired in 1954. This prominence made it possible for him to acquire personal support from King Gustaf VI Adolf's Seventy Years Fund for Swedish Culture, Knut and Alice Wallenberg's Foundation, and the Swedish Natural Sciences Research Council in order to establish in 1955 the Uppsala Quantum Chemistry Group. The first publication with this byline is "Quantum Theory of Cohesive Properties of Solids," in the *Philosophical Magazine* Supplement 5.1 (1956). Rooms for the operation were made available in the Department of Chemistry building. Löwdin at Uppsala and Inga Fischer-Hjalmars at Stockholm arranged a symposium to celebrate this new creation. It was graced by the presence of some seventy scientists, including a representative roster of leaders in the field: Coulson, Libscomb, Matsen, Mulliken, and the Pullmans.

Colleagues in the United States suggested to Löwdin that funding for further expansion of the operation at Uppsala might be available from the armed forces of the U.S. An application led to a contract between the European office of the Air Research and Development Command in Brussels and Uppsala University, and gave the opportunity for a substantial increase in manpower for research and in office space. It also provided the background for financing the first electronic computer at Uppsala, the ALWAC IIIE. It was purchased by a grant from Knut and Alice Wallenberg's Foundation at a favorable price from an Axel Wenner-Gren company, Autronic AB. The contract went into effect in February 1957, and Löwdin put up notices on the bulletin boards of the institutes at Uppsala, inviting applications from persons "interested in numerical calculations." I saw such a notice and, as I was looking for a way to make a living in science, I went for an interview, and was accepted as a junior assistant. Thus started an association that was to last for nearly forty-four years.

Expecting to find a part-time occupation to support myself through graduate school doing numerical computations, I found myself a total experience, immersed in a sea of unfathomable depth and having to learn the strokes of swimming, or timidly drown in the waves of quantum theory. Per-Olov Löwdin conveyed the enthusiasm, the dedication, and the discipline of work that are so essential in any endeavor, but

possibly most acutely needed in the pursuit of scholarly or artistic accomplishment.

My first assignment was to give a seminar on the method of second quantization for many-electron systems from the papers of Born, Jordan, and Fock, in particular. Per knew that there were a number of significant things going on. The papers by Gell-Mann and Brueckner and by Hubbard were new. He wanted to put this into his perspective as formulated in the trilogy from the *Physical Review* in 1955.

Jean-Louis Calais and I were also to project state functions for all atomic configurations from a basis of one *s*- and three *p*-orbitals corresponding to the Condon and Shortley tables. We were also to address the term splittings in the lowest states of neutral carbon, with emphasis on the virial theorem.

New offices were available in November 1957 for the Quantum Chemistry Group in a building erected by an insurance company next to the university's main structure in the center of Uppsala. The computer was put in place, complete with a motor-generator transformer in the basement. Löwdin invited sponsors and dignitaries to a formal inauguration on 23 April 1958, which was, as a serendipity, the centennial of Max Planck's birth. Planning was then well under way for the first summer school to be held in a mountain resort in Sweden called Vålådalen in August. My wife and I were fortunate enough to be invited for an Easter week at the place in order to check out the facilities while also taking time for some skiing.

There were no formal teaching obligations for the younger members of the group; we were instead engaged in various administrative duties. Klaus Appel was responsible for the computer operations, Jean-Louis Calais for housing foreign guests, Anders Fröman for the library, and I for keeping the books and preparing the checks for Per-Olov to sign. Responsibility was delegated to us to a degree that I find amazing today, but it provided a stimulus that I have valued throughout the years.

Löwdin's international contacts and outlooks were among the most attractive elements of the quantum chemical family. George Hall seemed to be available for questions and general chatting almost always. It was a wonderful opportunity to be given the charge of showing some Uppsala sights to Art Freeman and to bring Masao Kotani to Marianne and Klaus Appel for a Saturday dinner. Kimio Ohno visited Uppsala from his postdoctoral stay with Roy McWeeny at the same time. Harold McIntosh came to talk about the mapping of the hydrogen quantum problem on the four-dimensional harmonic oscillator. Harrison Shull arrived in early 1958; he came to be an essential role model for my development.

Uppsala University had protracted the process of finding a permanent position for Löwdin, so he initiated an effort that led to his association with the University of Florida. Thus started the Quantum Theory Project as a joint venture between the departments of chemistry and physics in Gainesville in 1960. Linton E. Grinter, dean of the graduate school, Harry H. Sisler, head of chemistry, and Stanley S. Ballard, head of physics, welcomed the Löwdins, the Appels, Calais, and the Linderbergs to establish a new research area that also involved Florida faculty members John S. Faulkner, Charles E. Reid, Darwin W. Smith, and Richard F. Wood. Funding from the National Science Foundation secured the first Winter Institute in Gainesville in December 1960, and on Sanibel Island during the first two weeks of January 1961. Appel, Calais, and I were assigned the practical details and were able to convince Sisler and Ballard that everything proceeded according to plans even when the Löwdins were back in Sweden. Sanibel Symposia evolved into yearly events, but the last one on the island was in 1977. The bankruptcy of the Casa Ybel Hotel and its demolition, which included the Löwdin Hall lecture facility, led to the move to the east coast of Florida. The year 2000 saw the fortieth symposium, in St. Augustine.

Löwdin encouraged travel, and conference contributions were stimulated. It has been my privilege to attend a number of meetings together with Per around the world. Particularly happy memories are associated with a conference at Northwestern University in 1961. Per, the "godfather," took his young protégés to the bars of downtown Chicago as well as to a garden party at the Frosts' house in Skokie. It was fascinating for a young man to be in the presence of so many notable scientists on an informal basis. Good memories remain from a couple of weeks in Hungary in 1967 and Japan in 1976.

Jean-Louis Calais, Osvaldo Goscinski, Yngve Öhrn, and I edited a volume of contributions to Löwdin. It was presented to him at the dedicatory symposium at Dalseter in Norway in 1976. The collection of papers celebrated the various contributions to quantum chemistry that Löwdin could call his own. I believe that he was genuinely surprised. The ready-for-print typescript was prepared at Aarhus.

Aarhus University was almost virgin territory for quantum chemistry in 1966. I was given the opportunity to establish a group there. I infused into it many elements of the operations at Uppsala and Gainesville. Students were sent to the summer schools and, in time, to the Florida events. The years have shown me that we were lucky to be part of the Quantum Chemistry Group and the Quantum Theory Project, where communication was stimulated across age, national, and language barriers, and where the socialization was an important part of the experience.

It has also been important to me to impart to my associates that formal capacity is an indispensable tool when working toward new and ever more complex goals in our science. Linear algebra, as in perturbation theory and in group theory, is a particularly prominent part of Per-Olov's teachings that has meant much to me. He always knew the significant, original papers to consult, and expressed his skepticism toward excessive claims by so-called new theories. These are things I am trying to live up to.

Uppsala University maintains a four-hundred-year-old tradition of celebrating each year the new doctors who have earned their degrees. A special event is the jubilee promotion of doctors who got their honors fifty years earlier. Löwdin was one of four survivors from 1948 at the ceremonies in May 1998. The president of the Uppsala Student Union gave a tribute to them, and Per-Olov returned the honors on behalf of the jubilee doctors. It was one of the best speeches I heard him give, and it turned out to be the crowning accomplishment of a distinguished career. A heart operation in October 1998, when he was eighty-two, presented such strain that a full recovery to previous strength did not take place. Löwdin took part in the Sanibel Symposia that followed, and his last presence was at the fortieth one in February 2000.

Elected 1983

JAN LINDERBERG
Department of Chemistry
Aarhus University

This talk was presented at the Per-Olov Löwdin Memorial Symposium at Uppsala in October 2000, under the title "Quantum Chemistry as a Lifestyle."