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Biography of Jan Erik Almlöf

Jan Erik Almlöf was born in Malung, Sweden on 1 April 1945. He received his Fil. Kand. degree at the University of Uppsala in 1967. He started his research career the same year in the Department of Inorganic Chemistry at the same university with Professor Ivar Olavsson as his mentor. Jan started as an experimental chemist. The task given to him was to study, using X-ray diffraction techniques, the structure of crystals containing hydrogen bonds. The Fil. Lic. degree that he received in 1971 was based on a thesis on the crystal structure of three different hydrates of perchloric acid. Jan realized early that a deeper understanding of the hydrogen bond would have to involve theoretical studies. His earliest attempts were based on simple semi-empirical calculations, but it was soon clear to him that such an approach would not be adequate. In 1968 he therefore contacted the quantum chemistry group at the Department of Theoretical Physics, University of Stockholm. He found there a small group of people (Björn Roos, Per Siegbahn, and Ulf Wahlgren) who were trying, for the first time in Sweden, to implement ab initio quantum chemical methods. At the time the group was working with the IBMOL program, and Jan soon realized that this code was not capable of attacking the problems in which he was interested. He found an effective way to speed up the calculation of integrals by using both the local (atomic) symmetry of the basis functions and the molecular symmetry. Based on these ideas he wrote a new integral code – MOLECULE. This program represented a breakthrough for both Hartree-Fock and correlated methods, since it enabled calculations with considerably larger basis sets than the previous generation of integral codes. The novelty and insight that coloured all of Jan's work is already manifest in this work.

In May 1974 he presented his doctoral thesis "Studies of Hydrogen Bonding by Quantum-Mechanical Calculations and X-ray Diffraction Methods", which included both his experimental and theoretical work. Among the papers included in the thesis was a Hartree-Fock study of the intramolecular hydrogen bonds in the porphin molecule, certainly one of the largest ab initio calculations performed up to that time. Jan's integral code was to become the cornerstone of many of the ab initio codes developed during the 1970s, and his method of embedding symmetry deeply in the code had a profound influence on how symmetry was also exploited in wave function codes developed by the Stockholm group and by others.

After a postdoctoral period with Enrico Clementi at IBM, San Jose (where, among other things, he used MOLECULE to study the interaction between an iron porphyrin and an oxygen molecule), in 1975 Jan accepted a permanent position as "docent' at the University of Oslo. He and his family moved from Uppsala to Nittedal, a small village outside Oslo. He did some of his most important work during his stay in Oslo, work that established his international reputation in the field of theoretical chemistry. For example, it was in Oslo that he developed the direct SCF code DISCO together with his student and collaborators (Knut Fægri, Knut Korsell). Jan always credited the notion of recomputing rather than storing integrals to a chance remark made by Enrico Clementi, years before, but in fact it was entirely an effort of the Oslo group that showed not only that a direct SCF approach was practical but that it could also be made very efficient. For example, the Oslo group were able to perform SCF calculations with more than 500 contracted basis functions on a minicomputer in 1979! In addition, in collaboration with the groups in Lund and Stockholm (Björn Roos and Per Siegbahn) and a student (Anders Heiberg) he made important contributions to the CAS-SCF field. With Svein Sæbø he developed an energy gradient code for Hartree-Fock wave functions, and then with Trygve Helgaker Jan extended his contributions to the field of energy derivatives. With Danish collaborators (Hans Jørgen Jensen and Poul Jørgensen) they developed one of the first practical MCSCF second-order properties programs. Methods for relativistic quantum chemistry, resulting among other things in an important paper, "*A Variational Approach to Relativistic Effects in LCAO Calculations*", together with Knut Fægri and Hans Grelland, were another interest that originated in the Oslo years.

Jan's importance for theoretical chemistry in Norway went beyond his direct scientific contributions. He also played a key role when Norway installed its first super-

computer, a program which has developed into a national computer network serving as the backbone of scientific computing in Norway. In addition, Jan's interest in chemistry stretched far beyond the field of theoretical chemistry. He influenced the chemical society in Norway through this genuine interest in chemistry as a whole. Many experimental chemists enjoyed long and illuminating conversations with Jan about their own research projects and chemistry in general.

In 1984 Jan spent a sabbatical at the Theoretical Chemistry Department at Lund University. During that time he became involved in the rapidly developing field of high-performance computing, writing a new Gaussian integral program that was vectorized for the CRAY-1 computer. On his return to Oslo Jan became a full professor in the chemistry department.

In 1985, Jan left Oslo to assume a position as Professor of Chemistry and Fellow of the Minnesota Supercomputer Institute at the University of Minnesota, Minneapolis. Here, Jan had a full program of teaching, service, and research. He taught courses in general chemistry, physical chemistry, quantum chemistry, computational chemistry, electronic structure theory, and mathematical methods of chemistry at the university and was in great demand as lecturer at workshops and summer school. He was elected a member of the Commission of Charge Density of the International Union of Crystallography in 1993, he served on the Chemistry Focus Group Advisory Board of the Maui High-Performance Computing Center, and he served on the UniChem Scientific Advisory Board of Cray Research, Inc. He served the entire theoretical chemistry community by accepting positions on the advisory editorial boards of *Theoretica Chimica Acta* and the *International Journal of Quantum Chemistry*.

While Jan was in the United States, he maintained his contacts in Europe through visiting professorships at the University of Lund, the University of Tromsø, the ETH (Zürich), and the University of Strasbourg. He maintained especially close relationships with friends and colleagues in Norway and served in many respects as a bridge-builder to scientific culture in the United States both for established colleagues and, probably more importantly, for younger scientists. This close collaboration over the years was strengthened further when he assumed a joint professorship in Tromsø in 1994, where for many years he had come regularly to work with students and staff on the development of relativistic theory and the theoretical study of heterogeneous catalysis and clusters (with Odd Gropen, Merethe Sjøvoll, Trond Saue).

Scientific collaboration with researchers in the United States was not neglected either. For example, he continued an association with Peter Taylor at NASA in Ames and later in San Diego that had begun when Jan was in Oslo and Peter in Melbourne – a long-range interaction indeed in the days before e-mail. this association led to the development of basis sets for accurate correlated calculations, work that influenced a number of other workers in this field.

Jan's research in Minneapolis was funded by Control Data Corporation, the Strategic Defense Initiative, the National Science Foundation, the Petroleum Research Fund of the American Chemical Society, NASA, IBM, Cray Research, and the U.S. Department of Energy. His research interests continued to be varied, including nonlinear optics and synthetic optical materials, proton transfer, electron detachment, molecular structure, bond energies, van der Waals molecules and intermolecular interactions, porphyrins, organometallic compounds, parallel computing, density functional theory, and improved algorithms for perturbation theory calculations. He continued to carry out influential work on avoiding the molecular integral storage bottleneck, including an original algorithm (with Hans-Peter Luethi at ETH Zürich) for direct SCF calculations over a network of distributed computers, and several studies on what would now be called "linear scaling" methods for calculation of Hartree-Fock and density functional theory energies. The one topic to which the devoted most of his attention was probably a continuing series of large-scale calculations on the molecular structure of small carbon clusters.

Jan was awarded the Schroedinger Medal of the World Association of Theoretical Organic Chemistry in 1993, fitting recognition of his many influential contributions to chemistry as a whole, not only quantum chemistry.

Jan died on 16 January 1996, and is buried at Malung, Sweden, his birthplace.

Students and Colleagues of Jan Erik Almlöf

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- Visiting Scientists at Minnesota
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