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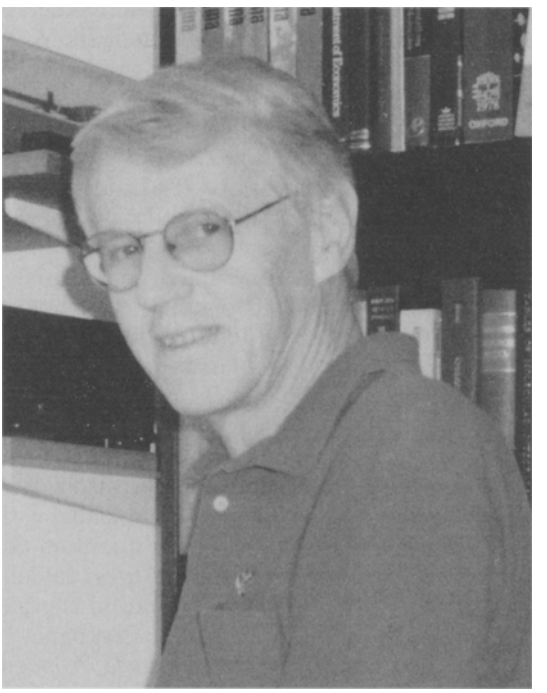

Jan Linderberg

An important event in the annals of the Chemistry Department at Aarhus University took place in the summer of 1966: The wise departmental elders had decided that it was time to introduce quantum chemistry into the research profile of the institute and a young, skinny Swede by the name of Jan Linderberg left a position at the University of Umeå in Northern Sweden to take up the challenge at Denmark's second largest university.

It soon became clear to all parties involved that this had been an excellent choice and, as of July 1, 1968, Jan Linderberg was appointed as ordinary professor of theoretical chemistry. Soon thereafter the first graduate students – among them the undersigned – started under Jan's supervision. In the sequel, we take the liberty of calling him by his first name since it was, and still is characteristic of professor Linderberg to be very informal, much more so than was common at Scandinavian universities in the mid-sixties. Mark Ratner became Jan's first postdoc followed by Rod Bartlett and many others. Erik W. Thulstrup changed his field from molecular spectroscopy to join the theoretical group, and Yngve Öhrn was a visiting professor for nearly two years. Many more exciting and inspiring events in the life of two young graduate students took place and we felt fortunate to be in the truly international group that grew up around Jan. It was obvious to us, already then, that the work of Jan Linderberg was well respected among his peers and that many of the scientists that we knew from the literature enjoyed visiting him in Aarhus.

Since Jan is still very active, this is not the time to draw final conclusions about his contributions to quantum chemistry. Nonetheless, we would like to call attention to some of the fields that have benefited from Jan's sharp analytic mind. We use the plural form on purpose because it has been characteristic of his activities that, once he has solved a problem, he moves on to the next. It is also characteristic that it is the mathematical-physical side of each project that captures his main interest. It is probably not entirely wrong to surmise that theoretical physics has been at least as close to his heart as theoretical chemistry.

More than anything else, the name Linderberg is associated with the development of the Green's function propagator techniques in quantum chemistry. Together with Yngve Öhrn he pioneered a technique for the direct calculation of molecular properties such as ionization potentials and excitation energies, properties that depend on more than one state of the system. The first paper by Linderberg and Öhrn on the subject, entitled *Improved Single-Particle Propagators in the Theory of Conjugated Systems*, appeared in the Proceedings of the Royal Society of London in 1965. Many other important contributions to this subject were published subsequently and the entire development was summarized in what became our "bible", the famous "yellow book" *Propagators in Quantum Chemistry* (Academic Press, London, 1973). By then, Jan Linderberg had become a Danish citizen and Yngve Öhrn a US citizen but, notwithstanding the fact that both enjoyed telling how happy they were to have left socialist Sweden which was nearly as red as the Soviet Union, the front and back covers of their book were yellow and blue respectively, the national colours of Sweden.

Jan has also contributed substantially to various other areas of theoretical chemistry. Suffice it to mention: the $1/Z$ expansion for atomic spectra (early sixties); the cohesive energies of solids (thesis from Uppsala, 1964); a new and consistent expression for the β-parameter in PPP theory (1967); the introduction of the semi-empirical Energy-Weighted Maximum-Overlap Method (with Esper Dalgaard in 1975); a method to simplify the calculation of two-electron integrals by using inherent linear dependencies in the integral lists (with Nelson H. F. Beebe in 1977); and the introduction of the Antisymmetrized Geminal Power (AGP) as a means to avoid the inherent ambiguity in the definition of the reference state in the Random-Phase-Approximation (with Yngve Öhrn in 1977).

In the last 10 years, Jan has turned his attention towards molecular dynamics, once again in collaboration with his long-time friend and co-worker, Yngve Öhrn. The use of hyperspherical coordinates and the finite element method are some of his primary interests in this context.

With his sixtieth birthday on October 27, 1994, approaching, we felt that the best we could do for Jan would be to gather research contributions from all of us who have enjoyed his and his wife Gunnel's friendship and hospitality over the years. It is just a small token of our gratitude to him, also for the reunions that he has arranged in the past in celebration of various anniversaries of the establishment of the Aarhus Division of Theoretical Chemistry on one dark December day 26 years ago.

Even though we were a little late with our invitations for contributions to this issue of Theoretica Chimica Acta and even though we were sending them to colleagues who had many other commitments, the response was overwhelming. Everybody wanted to acknowledge the inspiration and support they had received from Jan and we, therefore, have the great pleasure of being able to present a collection of original papers filling three journal issues and representing the wide span of research interests of Jan Linderberg's friends and associates.

This project would not have been possible without the help and support of Klaus Ruedenberg as well as the staff of the publisher. Foremost, we are however indebted to the long-time secretary of the Division of Theoretical Chemistry at Aarhus University, Hanne Kirkegaard, without whose competent assistance we would not have been able to complete the task.

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