Björn O. Roos (1937–2010)

Björn Olaf Roos, born June 28, 1937 in Malmö, graduated in 1968 as a student of Inga Fischer-Hjalmars in Stockholm on the "zero differential overlap" approximation, which played a key role in the then dominating semi-empirical quantum chemistry. He spent a year as a postdoc in the group of Enrico Clementi at the IBM Research Institute in San Jose (USA), where he was initiated to the rapidly developing field of numerical ab-initio quantum chemistry.

Roos' first important contribution to quantum chemistry has, in 1972, been the method known now as "direct CI". Unlike to what used to be common in configuration interaction (CI) studies, namely to first construct the CI matrix and to diagonalize it afterwards, in direct CI both steps are combined to one in an iterative way. This reduces the required computer time by one or two orders of magnitude. Early successes were for example the calculation of the water dimer with chemical accuracy (error of the order of 1 kcal mol^{-1}) or the prediction of the rotational spectrum of the experimentally unknown HNC molecule, with an accuracy that allowed to discover this molecule in space.

In 1977 Björn Roos moved to Lund where he became full professor and head of the new Department of Theoretical Chemistry in 1983. Similarly important as direct CI was the CAS-SCF method, published in 1980 together with Peter Taylor and Per Siegbahn. CAS stands for "complete active space". Later Roos understood the acronym CAS as the trade mark of his group, and he chose the name MOLCAS for the powerful quantum chemical program package from Lund that started in 1990 and that has found many users. CAS-SCF has been, together with the program FORS (full optimized reaction space) proposed at about the same time by K. Ruedenberg, the first generally applicable method in the frame of a multi-configurational generalization of SCF theory. It allows the calculation of potential energy surfaces of molecules near bond dissociation, at transition states or near conical intersections and is important for the study of chemical reactions.

While "direct CI" and CAS-SCF are mainly methods for electronic ground states of molecules, B. Roos has, with CAS-PT2, his third mile stone of 1995, introduced another powerful ansatz that has been much used for the calculation of spectra and for photochemistry. CAS-PT2 is a combination of CAS-SCF and MP2 (Møller–Plesset perturbation theory of second order) and allows the approximate treatment of non-dynamic and dynamic electron correlation in a robust way. Another methodologic progress has been the use of ANO (atomic natural orbital) bases of 1995 and very recently (2004) the combination of CAS-SCF with relativistic quantum chemistry (in terms of the Douglas–Kroll–Hess ansatz).

Björn O. Roos

Björn Roos has been one of the most important inventors of methods of ab initio quantum chemistry. The development of methods was, however, never an end in itself. It was mostly motivated by challenges from chemistry. The main topics were from inorganic chemistry, such as the understanding of structure and bonding of molecules built up from compounds of heavy atoms like complexes of actinides, or the problem of multiple bonds in inorganic molecules, with Cr_2 a special challenge.[1] Important biochemical applications, such as the blue copper proteins, also featured amongst his publications.

In some sense Björn Roos has represented within Sweden, and even in the entire Scandinavia a counterpoint to Per Olov Löwdin. Both of them were much concerned with didactics, and became famous for the summer schools, which they have organized. While Löwdin mainly cared for teaching elementary quantum mechanics and the related mathematics, the summer schools initiated by Roos, which are still alive, were meant as an introduction to modern quantum chemical methods and their application to real chemistry. It happens that Roos' former student Roland Lindh now occupies the former Löwdin chair in Uppsala. The first and best-known co-worker of Björn Roos, Per Siegbahn, has become a professor at the University of Stockholm in 1983, and has established there his own group. While Siegbahn has become an adherent of density-functional theory (DFT), which opened him the access to very large molecules such as enzymes, Roos has remained faithful to ab initio theory and to problems that require ab initio reliability.

It was inevitable that Björn Roos received many prestigious awards. Let me just mention that he has been a member of the "International Academy of Quantum Molecular Sciences" (IAQMS, from 1991), has received the Schrödinger Medal of WATOC (World Association of Theoretically Oriented Chemists) in 1999, and that he was a member of the Nobel Committee for Chemistry 1992–2000. I don't pay much attention to Björn's "scientometric parameters", and I think he would not care either.

Björn Roos had a decisive impact on ab-initio quantum chemistry from its beginnings around 1970 until today. He has been a pleasant, extremely modest, unpretentious, intelligent person with a good sense of humor. All those who have known him more closely, will miss him.

Werner Kutzelnigg
Universität Bochum

[1] "Reaching the maximum multiplicity of the covalent chemical bond": B. O. Roos, A. C. Borin, L. Gagliardi, *Angew. Chem.* **2007**, *119*, 1491 – 1494; *Angew. Chem. Int. Ed.* **2007**, *46*, 1469 – 1472.

DOI: 10.1002/anie.201002676