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Preface

Björn's top ten

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1 Introduction

On 1 July 2002 Björn Olof Roos was promoted to professor emeritus. To celebrate this transition we wanted to honor his contributions to chemistry by dedicating a special issue of Theoretical Chemistry Accounts. The editor liked the idea, and here is – finally – the result. Many thanks to those who contributed, and with an apology for the many difficulties along the road.

2 History

Björn Roos started his academic career at the beginning of the 1960s as a Ph.D. student of Inga Fischer-Hjalmars at the Institute of Theoretical Physics at the University of Stockholm. Originally working in pharmacology, she changed to studies in chemistry and theoretical physics, and graduated in both. She worked with, for example, Per-Olof Löwdin, Charles Coulson, and Oskar Klein (whom she had just replaced after his retirement), and was determined to refine the predictive power of semiempirical methods for computing properties of compounds such as the local anaestetic Xylocain (Lidocain in USA). Her emphasis on the importance of close contact between theory and experiment was also adopted by Björn and his fellow students. His work consisted of the refinement of semiempirical methods to extend their applicability to, for example, transition-metal compounds. Figure 1 shows Björn at a contemporary piece of equipment, the Swedish BESK (''Binär Elektronisk Sekvens-Kalkylator'') computer.

Following his Ph.D. exam in 1968, Björn went for a post-doc stay at the IBM Research Laboratory (later Almaden Research Center), San Jose, with Enrico Clementi. A self-consistent field (SCF) program (originally by Roothaan and Bagus) was extended and modified. The resulting program (ATOM-SCF) could use either Gaussian or Slater basis functions, and also optimized the exponents. He returned to his alma mater as a convinced ab initio quantum chemist. The application of ab initio methods to, for example, hydrogen-bonded systems was studied, Gaussian basis sets were extended to second- and third-row atoms, and molecules as large as copper porphin and phthalocyanine were studied. He now formed a group of his own with his students Per. E. M. Siegbahn, Jan Almlöf, and Ulf Wahlgren, who would later become distinguished scientific leaders themselves.

With this group began a period of achievements which would alter the face of computational quantum chemistry. Calculation of four-index integrals, and their transformation to a molecular orbital basis for use with correlated methods, had been practical only for rather small systems. New storage techniques, use of point-group symmetry, and the systematic development of good Gaussian basis sets led to more ambitious application calculations. These involved small species treated with high accuracy, as well as larger systems, like the azabenzenes, with an emphasis on the correlation effects necessary to get, for example, spectroscopic data and reaction barriers right.

In 1977 he moved from Stockholm to the University of Lund, and in 1983 the Department of Theoretical Chemistry was formed, with Björn as the leader. Under his leadership the new group has continued to make significant contributions to the field. Some of the methodological advances involved collaborators from Björn's extensive network of friends and colleagues, but the well-known ''direct configuration interaction'' and complete-active-space SCF (CASSCF) methods are rather the fruit of his ability to see and exploit the potential of a combination of technical advances, such as the use of Shavitt's graphical unitary group approach technique, Davidson's eigenvalue solver, and the swiftly increasing power of digital computers. By this time, P. R. Taylor had also joined the group.

While the first CAS second-order perturbation theory (CASPT2) article did not appear until 1990, experiments with this type of approximation were made as early as

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Fig. 1. An early swedish computer

1982. That work was reassumed following a collaboration with K. Wolinsky, who had worked on this approach with P. Pulay.

In 1989, a number of programs were integrated into a software package, and the MOLCAS group was formed in order to ensure a continuous process of developing top-quality software, niched towards our own use as well as that of a growing circle of what we may call "multiconfiguration ab initio" people. For the last 10 years or so, this work has evolved until it presently (from January 2003) constitutes a formal project sponsored by the Swedish Foundation for Strategic Research.

During the same time period, the biannual European Summer school in Quantum Chemistry (ESQC), given for the first time in 1989 on the initiative and through the continuing leadership of Björn, has given high-class education to approximately 600 quantum chemists, and the contacts forged have been valuable not only to the careers of these young people of all ages, but has also spun off a multitude of cooperative research as well as program development.

Of course, since he seemed to be going full steam ahead with no signs of reducing speed it was commonly expected that Björn would also continue working after retirement. What was not expected was that his new emeritus status would be so short-lived – but more about that in a moment.

3 Björn's top ten

Björn Roos has now produced about 300 scientific articles, and the publishing rate may be on the increase rather than on the decline. People in similar positions – who are rare – are sometimes asked what is their favorite paper in their own production, and the answer is usually along the line that the old papers are quite boring compared to the present and future work.

Instead of asking him, we made a shortlist of those papers that others had found most interesting, defined simply, if nonscientifically, as the ten currently most cited papers from his career. In the reference list at the end, they are given in top-down rating order.

The four most cited papers are the first CASSCF paper [1], the atomic natural orbital basis set [2], a CASPT2 paper [3], and an early compilation of basis sets for the first- and second-row atoms [4]. While this neatly summarizes his interest in method development, it fails to underline that the driving force is not the computational challenges in themselves, but the need for new approaches which might help with specific problems in chemistry and molecular physics.

Of course, this type of list disfavors his most recent work. It would be interesting to sneak a preview, a few years into the future, of a similar list. He is presently working on compounds with very heavy elements, such as actinides, and also on spectroscopy and reactions of large molecules, which demand multiconfigurational treatment combined with very large basis sets. We look forward to the outcome of this work, and of course with this question: Will quantum chemistry then be finished, reduced to the use of a few established methods like an engineer uses his CAD programs? We do not think this will happen yet. There is plenty to do, Björn!

4 Congratulations

As it turned out, owing to two of his greatest achievements – the MOLCAS project, and the ESQC school – Björn would not be able to enjoy his emeritus status for long. Since January of this year, he is again formally employed as professor, as leader of the MOLCAS project. Furthermore, the ESQC school will continue for some time, and it seems unthinkable to have any other hand at the helm.

It thus appears that this issue, rather than giving tribute to a long and distinguished service to quantum chemistry, simply uses a suitable opportunity to celebrate a milestone marker still far from the end of Björn Roos' journey through science. It is noteworthy that he has recently embarked, with customary gusto and enthusiasm, to embrace also density functional theory methods. We are much looking forward to the results.
With gratitude and congratulations,

Roland Lindh

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