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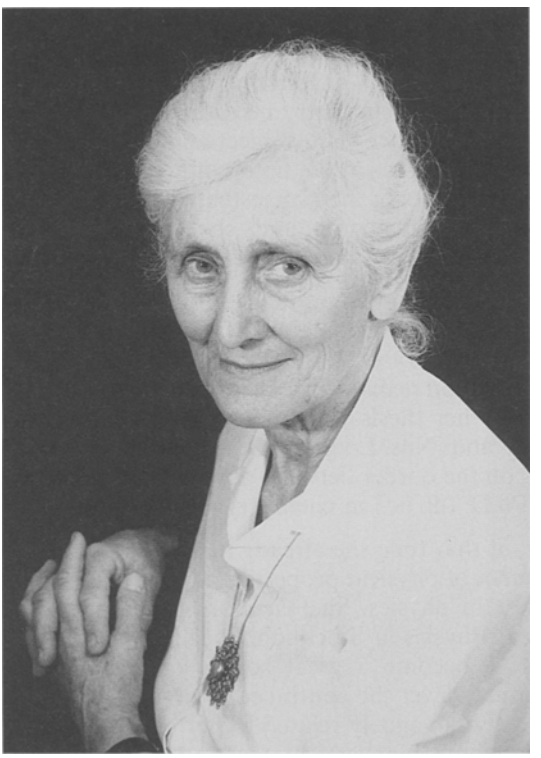

Inga Fischer–Hjalmars

Introduction

Inga Fischer–Hjalmars was born in Stockholm on January 16, 1918. The present issue of Theoretica Chimica Acta is honouring Inga at the occasion of her 75th birthday. She started her scientific career with a bachelors degree in pharmacology in 1939. This education awakened her interest in chemistry and she continued with studies of this subject at the University of Stockholm, where she received a second bachelors degree in 1944. Initially, her intention was to take courses in mathematics, physics and chemistry necessary to become a middle-school teacher. She chose chemistry as her main subject and joined a small research group headed by Nils Löfgren, who was at the time synthesising a series of organic compounds and making simple tests of their anaesthetic strength. Inga carried out several of these syntheses. One of the compounds she prepared turned out to be a most powerful local anaesthetic: *xylocaine.*

After finishing her undergraduate studies, Inga realised that to her research was more fun than teaching at a high-school. She started to work as a research assistant at the Biochemistry Institute headed by the Nobel laureate Hans von Euler-Chelpin, but soon realised that she needed a broader scientific background. To find a subject for her thesis Inga went back to Löfgren's group. Together with Lars Ehrenberg and Nils Löfgren she published a number of papers dealing with problems on the border between physical chemistry and biochemistry. These years led to a Ph.D. (fil. lic.) in chemistry in 1950.

However, at that time she already had a Ph.D. (fil. lic.) in theoretical physics. The measurement of physical properties, in particular dipole moments, had stimulated her interest in physics. She therefore took some courses at the Department of Theoretical Physics in Stockholm, headed at the time by Professor Oskar Klein, who was to become a great source of inspiration for her. After passing the undergraduate level she continued with graduate studies also at this department. The subject was vaguely related to her experimental studies and involved kinetic theory for some biochemical reactions. The thesis in theoretical physics was completed in 1949.

With this background it is maybe not surprising that Inga's main scientific interest was finally to be quantum chemistry. Her first studies in this direction were on the solubility of ethers and other organic substances in water, published together with Lars Ehrenberg in 1948. The hydrogen bond was assumed to be responsible for the difference in the interaction energies and the possibility to compute its strength using quantum mechanics was indicated. In a third paper, published in 1949, such studies were actually performed for some ethers. An important event that took place during the fall of 1948 was a visit to professor C. A. Coulson in Oxford. The visit resulted in a paper discussing the form of the wavefunction for a dissociating hydrogen molecule (*Phil. Mag.* **40**: 386 (1949)). This landmark paper, which is still used as a reference, pointed forward to the development of the unrestricted Hartree–Fock method and multi-configurational self-consistent field methods for the description of the dissociation of the chemical bond.

Inga Fischer–Hjalmars became *Doctor of Philosophy* in 1952 and the same year was appointed *Docent* in mechanics and mathematical physics at the University of Stockholm. She held a "Docent" position at the same university during the years 1953–59 and succeeded Oskar Klein as professor of Theoretical Physics in 1963 after a four-year sojourn at the Royal Institute of Technology in Stockholm.

Her insight into the nature of the chemical bond is maybe best illustrated by the impressive study of the ground and excited states of the ozone molecule, published in the years 1955–1957 (*J. Chem. Phys.* **23**: 411 (1955); *Arkiv Fysik* **11**: 529 (1957)). Approximate *ab initio* SCF calculations were carried out in the LCAO-MO formulation. All this was done on a desk calculator! Different approximations were investigated. Inga realised that some doubly excited states have a low energy and may interact strongly with the SCF configuration. Small CI calculations were performed and showed, for the first time, the multi-configurational nature of the wavefunction of ozone.

Inga's interest focused during the '60s mainly on the zero differential overlap (ZDO) approximation and the Pariser–Parr–Pople method. In a series of papers (*J. Chem. Phys.* **42**: 1962 (1965)) she discussed the theoretical foundation for the ZDO approximation and showed that, if it was based on orthogonalised atomic orbitals, it was correct to the second order in the overlap integral for orbitals on neighbouring atoms. This was an important contribution, which led to a re-parametrization of the PPP method. Inga, together with her students (myself being one of them) determined semi-empirical parameters for many different types of π-electron systems, including heteroatomic molecules containing nitrogen, oxygen, sulphur, and halogens. This led to a series of studies of spectral properties of a number of biologically interesting molecules, like porphyrines and nucleic acid base monomers. She was one of the inventors of the so-called PEEL method, which made it possible to include also metals into the PPP formalism. The approach was used by Inga and her students to study electron structure aspects of metal bonding in biological systems.

For Inga, the line connecting basic theory and advanced applications is short and direct. With her background in pharmacology and biochemistry she early realised the potential possibilities that quantum chemistry offered in answering many of the questions asked by the experimentalists. It is important for her that the theoretical techniques are chosen with this aim in direct sight. Therefore, theory development and application always ran side by side in her research group in Stockholm. Her students learned this lesson and her ideas have had a strong influence on the development of quantum chemistry in Sweden.

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Björn Roos