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# Early contributions to theoretical chemistry: Inga Fischer-Hjalmars, a founder of the Swedish school

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**ABSTRACT**

Inga Fischer-Hjalmars was one of the pioneers in the creation of the Swedish school of theoretical chemistry. She started her scientific endeavours in pharmacy and biochemistry, but soon sought a deeper understanding of molecules and chemistry. With a genuine experimental background and quantum chemical skills learned from Charles Coulson in the late 1940s, Inga was well prepared to continue her research and to contribute to the establishment of theoretical chemistry as it was later defined by Coulson; the use of quantum mechanics to explain experimental phenomena in all branches of chemistry. During the 1950s and 1960s Inga made important contributions to our understanding of chemical bonding and reactivity. For example, she made key insights into the dissociation of molecular hydrogen, the influence of heteroatoms on dipole moments in organic compounds, the electronic configuration of ozone and on the validity of different approximations in molecular theory. Inga Fischer-Hjalmars and her students developed extensions of the Pariser–Parr–Pople method and during the latter part of her career, she returned to the biomolecules that once had brought her into science, now applying quantum chemical methods to understand bonding and spectral properties of these molecules at greater depth.

## Early career: pharmacy and lab work

Inga Fischer was born in Stockholm in 1918. The family had a tradition of higher education but rather limited finances, so Inga had to get financial support from an uncle in Denmark to be able to go to college. When she wanted to continue to the university, the only option she really had was to choose the shortest education possible in the natural sciences, which was to become a pharmacist. That turned out to be a clever choice though, because it was easy to get a job afterwards and this gave her the possibility to continue with evening classes in chemistry [1,2].

During her chemistry studies Inga Fischer came in contact with the biochemist Hans von Euler-Chelpin, who got the Nobel Prize in 1929 for his work on fermentation. In his lab, Inga participated in rather fundamental studies of differences between normal and cancerous cell nuclei. One issue that they were especially interested in

was under which physico-chemical conditions cell nuclei were stable [3,4].

Von Euler-Chelpin had his lab at the top floor of a massive stone building in central Stockholm up at Odenplan. Down in the basement of the same building, another, then less famous person led some kind of research group, consisting mainly of students and volunteers working together under rudimentary conditions. Nils Löfgren was his name and he was only in his early thirties when Inga joined his work but he was already very determined to make a contribution to the development of pharmaceutics. The group studied inhibition of enzymes and noteworthy the mechanism of action of penicillin on diphtheria was investigated as early as in 1945. Interestingly, they disagreed with Pascal Jordan, who had a theory that similar groups were needed to form enzyme-substrate complexes and achieve what he referred to as 'atomic resonance' [5,6]. In Löfgren's group, Inga had arrived in an environment where one was clearly thinking about the details.

But the big thing in Löfgren's group was that they developed the local anaesthetic Xylocaine, or Lidocaine as it is also known. Nils Löfgren and his close collaborator Bengt Lundquist had already discovered Xylocaine when Inga Fischer joined the group but she had an important role in the early development and evaluation of Xylocaine [2,7]. In order to evaluate the local anaesthetic effect of Xylocaine, something which the colleagues did by injections in their own fingertips, it was necessary to have larger amounts of the compound than Löfgren had before. The synthesis was tricky and there was at the time a lack of the starting material 2,6-xylidine. Löfgren trusted Inga and knew that she was skilled in the lab, and so it came about that Inga Fischer made the first synthesis of Xylocaine on a larger scale. Anyway, Xylocaine did work, Löfgren and Lundquist got a patent, and the rights were sold to Astra. A few years after being released, Xylocaine overtook the world market of local anaesthetics, Nils Löfgren became one of the richest private persons in Sweden for a few years, and the rest is history [8].

For Inga Fischer, it must have been a fantastic experience to take part in all this as a young pharmacist and chemistry student. But although Löfgren wanted her to continue with drug discovery, Inga was more interested in understanding exactly why Xylocaine worked as well as it did. Early on, when the group was synthesising various derivatives of Xylocaine, they had a working hypothesis that the local anaesthetic effect had something to do with the fact that Xylocaine, 2-(diethylamino)-N-(2,6-dimethylphenyl)acetamide, was ortho-substituted on the benzene ring, which in turn affected its dipole moment. In order to test this hypothesis, Inga learned how to construct an apparatus for measuring dielectric constants.

She then synthesised a series of aniline derivatives with varying ortho-, meta- and para-substitutions and determined their dipole moments. Since the apparatus was built in-house, and since the available literature values of dipole moments of reference compounds varied due to variations in the way they had been measured, Inga carefully benchmarked her method and re-evaluated the dipole moments of several reference compounds. The scientific rigor of this work was high and she could confirm that ortho-substitution indeed caused a change in the dipole, which was communicated to Nature in 1950 [9,10].

Still, Inga Fischer was aiming at something even more fundamental and together with Lars Ehrenberg, she started to work on hydrogen bonding. In the 1940s, there was a quite lively discussion about the existence and nature of hydrogen bonds, the question was whether they existed as a specific type of interaction and to what extent they could be explained by electrostatics. Inga and Lars contributed to this discussion by studying the solubility of water in different ethers. Using volumetric data and dipole moments, they could estimate the effects of hydrogen bonding versus dipole–dipole interactions on the solubility. They could show that the availability of unshared electrons at the heteroatom affected the solubility of the ether and suggested that the solubility was explained by hydrogen bonding rather than by purely electrostatic dipole–dipole interactions [11,12]. Interestingly, Inga referred to quantum mechanics already in her early experimental papers, in 1948 she wrote [12]:

> Otherwise, the polarizabilities [of the unshared electrons of the heteroatom] might be calculated, if possible, with the aid of quantum mechanics, or the whole problem might be treated through a direct study of the wave functions involved.

## Into the quantum

While working as a chemist, Inga took classes in physics and came in contact with the theoretical physicist Oskar Klein. Klein made many important contributions to the development of quantum mechanics and cosmology, but his only direct contribution to chemistry was that he derived the solutions for the Schrödinger equation of the asymmetric rotor. Inga became good friends with Klein and his family, and Klein was acknowledged in much of Inga's early theoretical work.

Another person that influenced Inga's further scientific development was the Nobel laureate Arne Tiselius, he recognised the talent of the young woman and her unique scientific interests that were only poorly represented in Sweden. Tiselius, who was also a chairman of the Swedish

Research Council, sent Inga to a conference in Paris to find herself a mentor and to learn quantum chemistry [1,13].

The conference *La Liaison Chimique*, held in Paris in 1948, was attended by several of the leading theoreticians of the time, including Robert Mulliken and Linus Pauling, the Pullman couple, Louise de Broglie, V. C. Raman and the Englishman Charles Coulson. Inga and Charles got acquainted during the conference and so it was that Inga spent the following winter at Kings College in London, learning quantum chemistry under his supervision. They only wrote one paper together ever, but this became a landmark paper in the history of quantum chemistry. It is called *Notes on the Molecular Orbital Treatment of the Hydrogen Molecule* and was published in Philosophical Magazine in 1949 [14]. In the introduction, the authors emphasised that the point of this paper was not to make more accurate calculations on $H_2$ than what had been done earlier, but to critically examine the possibilities and limitations of the MO (molecular orbital) method in its simplest form. The MO method had been applied to chemical problems for nearly two decades but without much discussion of its validity except on semi-empirical grounds. Charles and Inga analysed the asymptotic behaviour of the MO wave function, they showed how the MO method fails at large inter-atomic distances and how it overemphasises ionic terms when the hydrogen molecule dissociates into atoms [14]:

…our calculation shows very clearly the dangers inherent in too naïve an application of m.o. theory to interactions across large distances, as, for example, in trying to follow the complete course of a chemical reaction …

In addition to examining its limitations, they suggested an improvement upon the MO wave function, namely the use of different orbitals for electrons with different spin. By introducing a parameter ($\lambda$) that determined the contribution of atom-centred basis functions to the molecular orbital, and by optimising this parameter variationally, they had constructed a wave function that captured the strengths and avoided the weaknesses of both the MO and VB (valence bond) methods. Near equilibrium distance, the Coulson–Fischer (CF) wave function was identical to the MO wave function, but at slightly extended distances the MO method broke down rapidly and the CF wave function converged toward the VB wave function at large distance (Figure 1). One should realise that this was five years before the Pople–Nesbet equations and the unrestricted Hartree–Fock method, which were essentially built on the same idea [15]. The 1949 paper also contained a discussion of differences and similarities of the MO and VB approaches and their formal relation to the more general method of configuration interaction (CI).
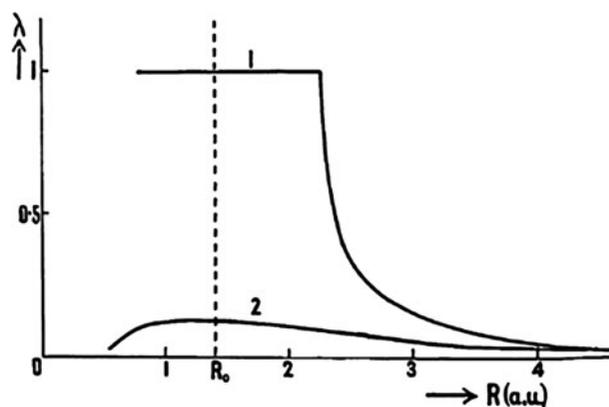


**Figure 1.** Diagram illustrating the optimal value of the variational parameter $\lambda$ in the Coulson–Fischer wave functions with (2) and without (1) exchange.

An in-depth analysis was made of the combined effects of screening and CI for the potential energy surface of $H_2$, and ends with the following statement [14]:

…some of the difficulties already found in interpreting the u.v. spectra of large condensed molecules arise from its [CI] neglect.

This shows that Inga was early aware of the importance of accounting for multiple configurations in certain cases, and she would continue to apply small CI calculations in much of her early work. By 2016, the CF paper, which was Inga Fischer's first publication in quantum chemistry, had been cited nearly 500 times.

## Home with new skills

Inga returned home from London with new skills and did what theoreticians typically do if they have any experimental experience before they turn to theory; she applied her new tools to her old questions. The first problem she took on was the hydrogen bonding between ethers and water. By doing MO calculations within the $\pi$-electron approximation, Inga could show that the purely electrostatic interaction was too weak (only 2 kcal/mol) to account for the complexation observed experimentally, and that a delocalisation of the oxygen 2p electrons occurred in the ether–water complex. These results confirmed her earlier experimental findings suggesting that the hydrogen bond was not purely electrostatic in origin. The paper is interesting because it contains several considerations of how the limitations of the MO method affect the interpretation of the results. Also, the results sensitivity to the choice of parameters was examined critically, once again showing how well aware she was of the methodological limitations [16]. This work was initiated while she was still with Coulson in London, and Inga's
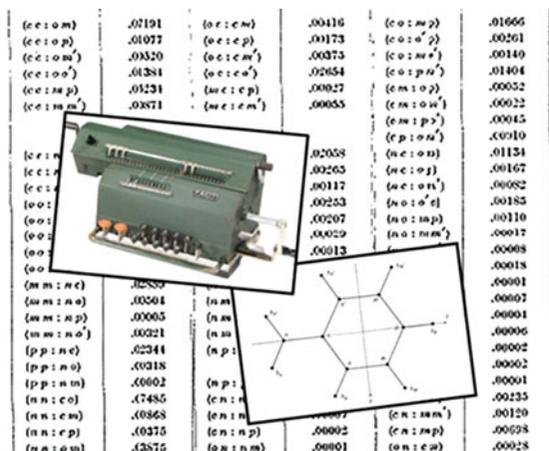
**Figure 2.** A mechanical Facit desk calculator from the 1950s, used by Inga to compute the molecular integrals of aniline [18].



**Figure 3.** Stig Hjalmars and Inga Fischer-Hjalmars looking at a molecule model in 1952.

future work in the field would be much in the same spirit as how Coulson would later define theoretical chemistry; as concerned not only with physical chemistry, but with all branches of chemistry [17].

Next, she turned back to the problem of dipole moments of Xylocaine and related compounds. The hypothesis was that ortho-substituents forced the amino group out of the molecular plane, so that any $\pi$-electronic interaction between the nitrogen lone-pair and the delocalised system was switched off. If this assumption was correct, it would mean that the dipole moment would be caused mainly by polarisation of the $\pi$-electron cloud. Equipped with a mechanical calculator (Figure 2) and an assistant, Inga aimed to calculate the $\pi$-electron dipole moment of aniline. This was an ambitious task to do without a computer, since even an eight-electron problem requires tedious evaluation and bookkeeping of a large number of integrals. An unsolved problem was how to treat the heteroatom lone-pair; as an $sp^3$ lone-pair or as a 2p atomic orbital? Anyhow, Inga took on the aniline molecule using Roothan's equations (restricted Hartree–Fock) and calculated its $\pi$-electron dipole moment to be 0.5 D, which was in quite satisfactory agreement with the experimental value of 0.7 D [18].

In 1952 Inga Fischer defended her doctoral thesis: *Studies of the hydrogen bond and the ortho-effect.* Later that year she added Hjalmars to her name when she married Stig Hjalmars, who actually made his proposal as the final question at the dissertation ceremony (Figure 3) [2].

Worth to mention is also a study of LiH and BeH$^+$, communicated to Nature and published in its full length in Arkiv för Fysik in 1952. In this work Inga examined carefully how different approaches, e.g. MO, VB, all-electron, valence-only and orthogonal atomic orbitals, performed in the determination of potential energy surfaces for these simple heteronuclear bonds [19,20]. From

these studies and her earlier work on H$_2$ together with Coulson, Inga had now achieved the deepest understanding of both homonuclear and heteronuclear chemical bonds as contemporary methods of quantum chemistry admitted. She was now prepared to approach much more complex systems.

## Recognised early

This is a good point to pause and ask: who was Inga Fischer-Hjalmars in the theoretical chemistry community in the 1950s? A 1955 review by Parr and Elison can give us an idea. The authors cited three of Inga's papers before 1955 explicitly, of which the most telling reference might be this one [21]:

> Perhaps the most interesting SCF calculation on an unsaturated molecule to date is the calculation of Fischer of the dipole moment of aniline; this professional work clearly shows the nature of the problems met in any such calculation on a large molecule containing heteroatoms.

They also mentioned that Inga had suggested an alternative method for asserting the degree of hybridisation, *the condition of maximum penetration*, which was an alternative to the maximum overlap criteria proposed by

Linus Pauling, and which in opposite to Pauling's criteria would work equally well for homonuclear and heteronuclear bonds [22].

Another interesting source is John Slater's book from 1963, *Quantum theory of molecules and solids, Vol. I* [23]. Slater referred to nine of Inga's then around 20 theoretical papers, he wrote a two pages review of the 1949 $H_2$ paper with Coulson, and he mentioned that Inga was one of the earliest to work on bonding in LiH and $BeH^+$. It seems that Inga Fischer-Hjalmars was recognised by the theoretical chemistry community very early in her career, and that she made several important contributions already during the 1950s.

## Attracted to theory

That Inga, who began her scientific endeavours in pharmacy, became so deeply involved in theory is intriguing. There are, at least, two persons who may have influenced her in this direction. One was Nils Löfgren, the inventor of Xylocaine and one of Inga's first chemistry teachers. Although being pragmatic and goal oriented, Löfgren was also very interested in contemporary theories of electrons in organic chemistry [8]. In his papers one finds a lot of references to things like mesomerism, inductive effects, resonance and so on [6].

Another interesting person was Inga's father, Otto Fischer. He was an engineer, who began his career in railway construction in Canada and then moved to Sweden where he started his own parquetry factory in Stockholm. Otto Fischer had a great interest in theoretical physics, as later told by Inga [1]:

> Each morning he spent one to two hours at his desk, before going to the office, and these early hours were mainly devoted to mathematical physics. He followed the development of relativity and quantum theory with great interest …

And in the same source she says [1]:

> When I was about sixteen he started to tell me about his work. On long Sunday walks in the woods, he told me about his attempts to bring the whole of physics within a single frame of reference. In those days I was not able to understand the details of his research, but I became fascinated by the general scientific perspective.

Otto Fischer never became an academic researcher, but he was progressive in his thoughts and achieved a deep scientific knowledge. When he retired he published two advanced books on developments he had made in the field of quaternions and Hamiltonian mechanics [24,25]. It seems that Otto had a great influence on his daughter's interests for science in general and theory in particular.

## Further contributions to theoretical chemistry

*Back to work*. In the late 1950s Inga worked on ozone. The geometry of ozone had been determined finally in 1953, and both Mulliken and Walsh had made MO calculations and investigated how the orbital energies depended on the angle (remember the Walsh diagrams) [26,27]. Mulliken and Walsh suggested basically the same ground state configuration, except they disagreed on the energetic order of two valence orbitals. Inga Fischer-Hjalmars made a rigorous re-investigation of $O_3$ and accounted for excited states in the $\pi$-approximation by performing CI calculations with respect to the configurations suggested by Mulliken and Walsh. She showed that the ground-state energy could be lowered by several eV if Mulliken's configuration was allowed to interact with a doubly excited configuration, and for the first time, the multi-configurational nature of the ozone wave function was shown [28–30].

In the 1960s they got the first electronic computer in Stockholm, BESK (Binär Elektronisk Sekvens Kalkylator). This opened up for more extensive calculations and Inga continued her earlier work on aniline. This time she examined the performance of some of the state-of-the-art methods of her time, namely Hückel, Pariser–Parr–Pople (PPP) and Hartree–Fock (HF). Although the PPP method had been used for several years, there was at the time very scarce information about how the method compared with both the simpler semi-empirical Hückel method and the purely theoretical HF method. Inga concluded that Hückel performed decently for ground state properties like ionisation potentials, bond orders and dipole moments, but this required that the parameters were chosen with great care. She examined the parameter sensitivity of the PPP method and seemed to be delighted by the finding that it was less sensitive to the choice of parameters than Hückel [31]:

> …it would seem that the Pariser-Parr-Pople method could be used with great confidence for all kinds of calculations involving the electronic properties of complicated molecules.

Starting with this paper, much of Inga's work to come would be advanced applications of the PPP method or modifications thereof. She emphasised though, that good spectra required CI and made calculations with up to seven configurations for the spectrum of aniline and benzene. The diagram in Figure 4 is reproduced from the 1962 paper and shows how the computed spectra for
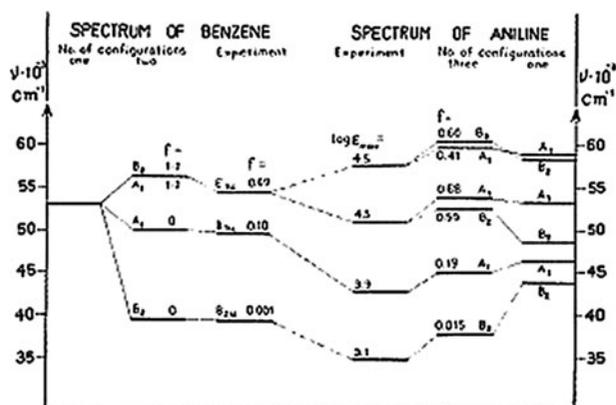
**Figure 4.** Comparison of experimental and computed spectra for benzene and aniline [31].



**Figure 5.** Sanibel Island in 1962. From the left: Lars Hedin, Stig Hjalmars, Anders Fröman, Inga Fischer-Hjalmars (admiring a sea-shell), Per-Olof Löwdin, Stig Flodmark, Yngve Öhrn and Jan Nordling.

aniline converged towards the experimental spectrum when the number of configurations was increased from one to three in the $\pi$-electron space [31].

In the early 1960s, there was an intensive debate on the cause of variations in C–C bond lengths. What especially divided the theoretical chemists was the relative importance of concepts like hybridisation, Van der Waals interactions, conjugation and hyper conjugation. Michael Dewar took a strong position against the concept of conjugation, as Inga wrote (author's translation from Swedish) [32]:

> …he [M. Dewar] has raised a storm against the use of the concept of conjugation whatsoever, except in aromatics. He is of the opinion that all effects, earlier described as conjugation phenomena, may advantageously be attributed to other causes.

In what seems to be an attempt to resolve this conflict within the community, Inga Fischer-Hjalmars took six different empirical potentials for non-bonded interactions, and combined them with computations of conjugation energies using the PPP method. This was done with an IBM 7090 computer at the Swedish Defense Department and a program she got from Robert Nesbet. She concluded that the conformations of butadiene and biphenyl could not be understood from either non-bonded interactions or conjugation alone, only the combined effects led to consistency with the experimental picture. This work was presented at the Sanibel Symposium in 1962 (Figure 5) [33,34].

In 1963, Inga Fischer-Hjalmars succeeded her mentor Oskar Klein and thus became the first woman in Sweden to become professor of theoretical physics. In light of her recognition in the field of quantum chemistry, the choice of Inga might seem natural. But it was a quite remarkable appointment, remembering that Inga's background was in pharmacy, that her main research interests were of

chemical significance rather than physical, and of course the fact that she was a woman.

In the late 1960s, Inga penetrated further into the contemporary $\pi$-electron theories. In a series of papers she explored the formal validity and connection between different methods, such as Hückel, the $\omega$-technique (a self-consistent Hückel method), and the PPP method, which she had used frequently in her own work [35–37]. A fundamental brick in the PPP method was a set of conditions commonly referred to as *the approximation of zero differential overlap* (ZDO), and Inga intuitively felt that there was a need to critically examine the rigidness of this approximation. In a quite famous paper with the title *Deduction of the Zero Differential Overlap Approximation from an Orthogonal Atomic Orbital Basis*, she carried out a systematic analysis of the validity of the ZDO approximation by using an expansion of different matrix elements and energy integrals in terms of the overlap integral ($S_{ij}$) [35]. In this way she could compare the various terms that arose in the energy expressions of different $\pi$-electron theories, with each other and with the Fock operator. She concluded that if an orthogonalised atomic orbital basis was used, such as had been proposed by Per-Olof Löwdin in 1947, then the ZDO conditions were correct to second order in $S_{ij}$ for most type of integrals. However, the so-called penetration integral ($W_{\mu}$), first introduced in molecular theory by Maria Goeppert-Mayer in 1938, was correct only to the first order. This revealed an imbalance inherent in the PPP method, since it meant that this integral was non-local and thus not strictly transferable between different molecules. The paper was cited frequently during the 1960s and 1970s and this was what Björn Roos (who was a doctoral student with Inga) said in 1994 [30]:

This was an important contribution, which led to a re-parametrization of the PPP method [ … ] the so-called Peel method, which made it possible to include also metals into the PPP formalism.

## Late career: back to biology and further into the details

During the late 1960s and early 1970's, Inga and her students extended the modified PPP or *Peel* method, by determining parameters for Cu, Fe and several main group elements [30,38–40]. This led to a series of studies of spectral properties and bonding in biologically interesting molecules, for example DNA bases and small metal complexes. A sub-set of this work on bio-molecules is a series of papers on the topic of metals in biology. During the 1980s, most work was done with either the self-developed *Peel* method or by HF and Gaussian basis sets. There are two papers especially worth to be noted. *Metals in biology: an attempt at classification*; started with a review of the knowledge of metal-body interactions in the context of contact allergy, followed by a systematic study of bonding in small four-coordinated metal complexes with N, O, and S donor atoms in different oxidation states [41]. *Oxidation state and the chemical bond in metal-organic complexes*, from 1992, was Inga's very last scientific paper and concerned the chemical concept of oxidation state and its meaning from a quantum chemical point of view [42]. Although appearing scientifically sound, Inga's papers from this period are not cited very much. Possibly, because the theoretical chemistry community was already turning to either post-HF methods or later even density functional theory, so that semi-empirical or pure HF calculations were perhaps not any longer considered as being *state-of-the-art*.

There are two series of papers that deserves to be mentioned, although they are a bit remote from the rest. In a series of four papers, Inga studied quasi-classical approaches to scattering problems with chemical applications. This was done during the 1970s together with Vladimir Dubrovskiy and Aleksander Bogdanov at Leningrad State University [43]. In another series of eight papers published in the 1980s, Inga, sometimes together with her husband Stig Hjalmars, explored the continuum description of crystals and its formal validity [44].

Inga Fischer-Hjalmars was one of the key founders of the Swedish school of theoretical chemistry. She died in 2008 at the age of 90 but her scientific spirit lives still, through the influence she and her students had on the development of theoretical chemistry, in Sweden and internationally.

## Disclosure statement

No potential conflict of interest was reported by the author.

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