



Werner Kutzelnigg

Curriculum vitae – Werner Kutzelnigg

Born 10 September 1933 in Vienna.

Student in Bonn (1952–1954) and Freiburg im Breisgau (1954–1960). Thesis (*summa cum laude*) with R. Mecke on experimental IR spectroscopy. Postdoc in Paris (1960–1963) with B. Pullman and G. Berthier, then in Uppsala (1963–1964) with P.O. Löwdin. 1964–1970 in Göttingen (*Habilitation* in 1967). Associate professor in Karlsruhe 1970–1973, full professor at RUB (Ruhr-Universität Bochum) since 1973.

Received the Carl-Duisberg memorial price of the German Chemical Society in 1971. Visits to various European countries, especially to France, the United States, Canada, and Japan.

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A personal view

I first met Werner Kutzelnigg when he joined Bingel's group in Göttingen in 1964. At that time I was a student. He arrived just in time to help me formulate a Diploma Thesis: "The direct determination of natural orbitals" (NO). This was a turning point in my life; it was decisive for my scientific career.

Werner Kutzelnigg studied chemistry in Bonn and Freiburg, where he wrote his Ph.D. thesis (1960) with R. Mecke on IR spectroscopy. He then worked as a postdoc with B. Pullman and G. Berthier, Paris, and P.O. Löwdin, Uppsala. I was fascinated by his impressive command of chemistry (I still envy him for this), physics and mathematics – not to mention other fields such as linguistics, biology, etc. This was not only important for my training as a young scientist, it also shaped the way I try to set standards for myself (and others).

The Göttingen years (up to 1970) were fascinating. A group of promising students and postdocs, especially Volker Staemmler and Martin Jungen, was directed by him to tackle the correlation problem by a CI expansion based on NO. Our success was based on Werner Kutzelnigg's unquestioned ability. It was equally important that he treated us as coworkers, which we all appreciated since this could not be taken for granted in Germany at that time. It was the best apprenticeship I could think of.

After my time as a postdoc in Chicago I did not hesitate to join Werner Kutzelnigg in Karlsruhe, where he held the position of associate professor (1970). He attracted very able postdocs and students, e.g. Frank Driessler, Hans Lischka and Volker Staemmler, and was able to complete previous NO work which culminated in the Karlsruhe PNO-CI and PNO-CFPA programs. Although these methods had been foreshadowed by work in Göttingen, they were first formulated and implemented in a general form by Wilfried Meyer. I firmly believe that the healthy competition among us contributed to the progress in molecular electronic structure theory. Among the numerous applications, the Li^+H_2 paper became a citation classic.

The time we spent in Karlsruhe may prove to be happiest of our lives for some of us: we were all good friends, we did good work – and we were not yet subjected to the stress that was to come with more responsibilities. We really owe much of that to

Werner Kutzelnigg's personality. He was an understanding and very generous boss – he paid for the first fancy dinners and wines in my life (!); he let every one of us have his own way and gave us his never-ending support.

In 1973 he accepted an offer to become full professor in Bochum and his best work was still to come. Assisted by Herbert Kollmar and Volker Staemmler, Werner Kutzelnigg quickly established Bochum as a leading center for quantum chemistry. Nearly 20 students have finished their Ph.D. theses and many postdocs have worked with him since this time. Among a wide variety of activities – which cover such important matters as the continuation of PNO-CEPA work (with Ralph Jaquet), pseudo potentials, Fock space theory, and the treatment of relativistic effects – I consider three topics to be outstanding.

The first of these is the work on the nature of the chemical bond, together with Frank Driessler and Holger Wallmeier, which is nicely described in Werner Kutzelnigg's book *Theorie der Chemischen Bindung*. In typical Kutzelnigg style – starting from the first principles and approaching the goal in a well-thought-through individualistic and lucid way – it is an extremely valuable guide for every student who wants to learn about quantum chemistry and bonding.

The next topic concerns the treatment of NMR chemical shifts, the famous IGLO method, developed with Michael Schindler, Ulrich Fleischer, and Christoph van Wüllen. This method and its impressive applications – partly together with Paul v. Rague Schleyer – finally convinced many a chemist of the usefulness and necessity of quantum chemistry.

Finally, I would like to mention the work on an r_{12} -dependent Ansatz for correlated wavefunctions performed mainly together with Wim Klopper. This has already led to impressive results and the method may very well revolutionize computational quantum chemistry.

There may be a very personal reason behind the success of the Bochum years: the marriage of Irmgard and Werner Kutzelnigg. He surprised many of his friends by turning into a caring and loving husband. Her charming personality, her genuine friendliness and constant support must have been vital for his scientific work.

I am sure I speak for all of his friends and colleagues: chemistry as well as quantum chemistry owe a lot to Werner Kutzelnigg. With our best wishes for the future – we are sure that there is more to come!

Reinhart Ahlrichs