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Introduction of Klaus Ruedenberg*

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I am honored to have been asked to introduce Klaus Ruedenberg, a longtime companion in the search.

The first time I introduced Klaus was thirty-seven or thirty-eight years ago, when he was about to deliver a seminar on exchange integrals to my research group beginning at eleven one Monday morning. Fortunately I had had a hunch and had warned him: I should have to attend a committee meeting at two in the afternoon. At two o'clock Klaus was still going on, having covered four blackboards with formulas; I quietly slipped out the door. Tonight we may have the same problem: I have a commitment at 8:30 sharp tomorrow morning. Klaus, please leave me a little time to sleep!

Briefly, then, who is our speaker this evening?

Born in Bielefeld, Germany in 1920, Klaus Ruedenberg received his early education there. In 1938, Klaus was able to move to Switzerland and thereby escape the persecution to which his father fell victim. Until 1948 he resided in Switzerland, studying first chemistry and then physics. He ultimately received his Ph.D in physics from the University of Zürich in 1950, after he had already moved to the University of Chicago with his thesis supervisor Gregor Wentzel. He worked fruitfully in the laboratory of Robert Mulliken from 1950 until 1955, when he joined Iowa State University as Assistant Professor of Chemistry. Except for two years elsewhere he has been here ever since, becoming Distinguished Professor in 1978. In 1975 Klaus received an honorary degree from the University of Basel; this very year he will be receiving another honorary degree from the University of Bielefeld. He has received the Midwest Award of the American Chemical Society and is a member of the International Academy of Quantum Molecular Science. He is, of course, the valiant Editor-in-Chief of Theoretica Chimica Acta.

Up to the present moment, Klaus has worked with thirty graduate students and postdoctorals, about half of whom are participating in this symposium. He

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and his associates have published more than one hundred and fifty scientific papers; these are listed below. These contributions are penetrating and varied, clearly in total constituting a major accomplishment – some of the best theoretical chemistry of our time.

In a few minutes it is impossible to adequately describe Klaus Ruedenberg's achievements. I will venture just a few words, about just a few of his papers.

Klaus' first publication was his doctoral research with Gregor Wentzel. You see what his background was when, in 1950 at the age of thirty, he joined Robert Mulliken, John Platt, and Clemens Roothaan in that great LMSS at the University of Chicago. These four persons influenced Klaus greatly, I believe, particularly John Platt, somebody whom the chemical physics community has much missed since he left us for the career of a futurist.

The second publication of Klaus Ruedenberg, his first in quantum chemistry, was in fact coauthored with me. [Forgive me, Klaus, I hope that this does not embarrass you.] This paper resulted from a month that he spent at Carnegie Tech in the fall of 1950. His technical prowess and physical soundness were immediately evident to me, and I have been his admirer through the decades since then.

The third paper by Klaus is the first of his wonderful series on molecular integrals. Some of you may not realize what a feat this and the subsequent papers constitute. Try, yourself, just to evaluate the exchange integral between two equivalent $1s$ orbitals a distance R apart. Heitler couldn't do it; London couldn't do it. Suguira did it, but to retrace his steps requires a week of work. Introducing powerful new techniques, Ruedenberg did it and went far beyond, to nonequivalent s orbitals, p and d orbitals, and (subsequently) to three- and four-center integrals.

This level of difficulty, this level of success; that is what separates the men from the boys. No wonder Klaus spoke on the subject for three hours as I have already described! And somebody at this symposium yesterday had the gall to say, in effect, that modern quantum chemistry began in the 1970's!

The fourth paper I remark on is Klaus' Publication 8. This is a *tour de force* in which Klaus succeeded in establishing an isomorphism between the free-electron network model for conjugated *pi*-electron systems, including a beautiful representation of electron repulsion within that model, with the LCAO theory of the so-called PPP form. The term "zero differential overlap" was coined by Klaus, incidentally.

Klaus' 1962 Publication 20 and his 1963 Publication 23 are famous, the first for carefully expounding the interplay between kinetic and potential energies during chemical bond formation, the second for establishing the viability of defining localized orbitals as those Hartree–Fock orbitals that maximize the self-coulomb repulsion or minimize the interorbital exchange.

It was just at this point in his career, in 1962, that Klaus for a short time took up a professorship at Johns Hopkins University. [These were days when the quality of one's publications counted for more than their number, it may be noted in passing.] But he preferred Iowa State, most particularly the advantages of being on a faculty that included Robert Rundle, and he quickly returned to Ames.

In my opinion six of Klaus' papers over the next twenty years are particularly important. These are his Publication 33 (electron pair wavefunction for Be), Publication 46 (vibrational spectroscopic constants), Publication A22 (even-tempered orbitals), Publication 83 (relation between total energy and sum of

orbital energies), Publication 87 (MCSCF optimization), and Publication 98 (electron difference densities). Each of these papers is definitive, each is breaking into new territory, and each has led to many later developments. As for Klaus Ruedenberg's contributions from 1985 on, most of you here at this conference are intimately familiar with his succession of fine contributions to the understanding of potential energy surfaces, the latest of which he will be telling us about.

Ladies and gentlemen, here then is a consummate professional; here is a world leader in quantum chemistry. I give you Klaus Ruedenberg. In his person will be found soft-spoken confidence, staying power, guts, zest; that is to say, a certain class. In his writing will be found clarity, thoroughness, elegance; that is to say, a certain style. In his works will be found depth, great scope; jewels; that is to say, bits sculpted for the years. I present to you Klaus Ruedenberg: exemplary physicist, exemplary chemist, supreme expositor, teacher, and friend. One of the men, not one of the boys.

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