Theor Chem Acc (2005) 114: 2–3
DOI 10.1007/s00214-005-0637-0

LAUDATIO

Thomas Bredow · Joachim Heidberg

Karl Jug's 65th birthday

Published online: 31 August 2005

Karl Jug was born on September 12th, 1939 in Essen, at that time a prosperous industrial center with coal mines and heavy steel industry not far from the Rhine river. Working in this field since the late 1960s, Karl Jug belongs to the post-war generation of pioneers in modern quantum chemistry. In 1959 Karl moved to Frankfurt to study physics, mathematics and chemistry at the Johann Wolfgang Goethe-University. Even in his first semester he attended the physical chemistry course given by Hermann Hartmann. The course strongly attracted Karl, as it did many other students, since Hartmann presented such fascinating topics as the calculation of the energy of gases using the residual theorem of function theory. It was around the seventh term when Karl began to think about how to continue. He learned a great deal of nuclear and theoretical physics, and actually participated in all the practical classes offered in physics more than was required, only to finally conclude that all this was not so exciting. When he heard that one could work also with Hartmann for a diploma thesis in physics in the chemistry department, covering molecular theory, he decided to go there. Hartmann offered a choice of two fields: in statistics the Ising model, and in molecular physics the ligand field theory. Others had already warned him against the first field, so Karl decided to work in ligand field theory. And this turned out to be quite right. In those days the time spent on a diploma thesis in physics was formally not limited and there were odd students who needed years for their diploma. Karl was lucky. He completed his thesis entitled "A quantum chemical model of an octahedral titanium complex" within one year. At that time the value of the ligand field theory for understanding the properties of most of the transition metal compounds was already well established. Therefore Karl could focus his efforts on the advanced problem of electron correlation. The work is an excellent example for solving a problem in the precomputer era. He had to find a physically sensible model with simple mathematical structure which preferably could be solved analytically. He chose a spherical shell model. Unfortunately it soon turned out that he had to perform a double integration over products of four Bessel functions. The significance of the work was more the choice of the model, the insight into its fundamentals, and its wide applicability than the quantitative agreement with experiment. Nevertheless, in order to limit the time for his diploma thesis, he had to proceed on numerical mathematics. Fortunately, a ZUSE computer was in operation at the institute, the only calculation machine which existed at the University of Frankfurt. (Hartmann was always quite foresighted). To finish his diploma thesis, Karl finally had to employ an IBM machine located in nearby Mainz. There he could carry out his calculations only at night when nobody else needed the machine.

While he was still working on his diploma thesis in 1963, Karl conducted exercises on π-electron systems at Hartmann's summer school in Konstanz. In the early 1960s Hartmann had already begun to hold his summer schools in Konstanz the first covering ligand field theory. The lectures on fundamentals and advanced topics as well as exercises, given for three weeks, were attended by graduate students, postdocs, professors, altogether around 200 participants. Karl participated three times. In 1963 also Parr, McWeeny and Fukui presented courses. Yet Karl did not perceive the implications of Fukui's work at that time, mainly because he could not understand his English.

Karl also took part in the 1965 school devoted to kinetics, where D. Herschbach, R. Marcus, M. Eigen, and E. Nikitin gave lectures. In the same year Karl finished the work on his dissertation entitled "Application of a one-center method on the π-electron systems of five-membered heterocycles". Hartmann referred to this work on the first symposium on Theoretical Chemistry, which he inaugurated in Frankfurt 1965. Thirty years later Karl himself organized the very successful thirty first symposium in cloister Loccum near Hannover devoted to the Electronic Structure of Large Systems. There were than 200 participants, only about ten left from those who had participated in 1965. In his thesis Karl had chosen a basis of orthogonal one-electron functions in spher-

T. Bredow · J. Heidberg (✉)
Universität Hannover, FB Chemie,
Institut für Physikalische Chemie und Elektrochemie,
Callinstr 313A, 30167 Hannover, Germany
E-mail: nhcibred@rrzn-user.uni-hannover.de

ical coordinates which extend over the whole molecule centered in the middle of the five-membered rings like furan or pyrrol. Slater functions had been taken as radial functions, Legendre functions as angle functions, Mathieu functions as angle functions considering heteroatoms. The energy of the ground-state was minimized with respect to index l of Legendre functions and the parameter q of Mathieu functions.

The name Karl Jug is connected above all with the development of semiempirical methods and quantum-chemical concepts for bonding and charge. He began the work as head of the editorial office and referee for Hartmann's then recently founded journal "Theoretica Chimica Acta" from 1965 to 1967. Many of the articles submitted were based on semiempirical procedures. In 1967 Jug went to Peter Lykos in Chicago. There he held a series of seminars on semiempirical methods and his review on that topic made the quantum chemical community take notice of him. Together with Robert Parr he gave a simple explanation of Scheibe's phenomenon of π-electron systems, emphasizing the atomic nature of the effect.

After analyses of the Hückel and of the CNDO method, Jug published in 1973, the first work about the semiempirical method SINDO. In the meantime he had become associate professor at the St. Louis University in Missouri, and developed an expression for the core Hamiltonian integrals over symmetrically orthogonalized orbitals. After its implementation in INDO a clearly higher accuracy was obtained than with the original method of Pople.

In 1975 Jug accepted a professorship in Theoretical Chemistry at the Technical University of Hannover. In order to fill the new area Theoretical Chemistry with contents, lectures on quantum chemistry and mathematical techniques for chemists were prepared. The success of the lectures lead Karl Jug to publish a book, "Mathematik in der Chemie", in 1981, the second edition of which appeared 1993.

Well-known concepts such as bond order, atomic charge and aromaticity, were expediently redefined. The research work reached a first culmination with the suggestion for photosynthesis of anti-aromatics such as cyclobutadiene and pentalene. Together with his student Andreas Köster he showed that aromaticity is characterized by at least two independent criteria, predominantly energetic and magnetic properties. By the end of the 1980s, his activities shifted to the area of clusters. This was initiated by his participation in the research group "adsorbate interaction at ionic crystals", which had been established after the discovery of the laser-induced resonant desorption and the first preparation and characterization of molecular monolayers at ionic single crystals such as NaCl and MgO. A very fruitful co-operation was initiated. Karl used further advanced versions of SINDO with great success for modeling adsorption processes and catalytic reactions. He and his coworkers introduced new concepts. Initially they used stoichiometric crystal cutouts for the simulation of the crystalline surfaces. The important extrapolation from the cluster to the crystalline solid bulk via the average relative co-ordination number k and the quasi-linear dependence of the energy and the bond distances on k opened the way to a reliable simulation of solids. This extrapolation was applied to the crystals NaCl, MgO, later also to TiO_2 (rutile and anatase), V_2O_5, γ-Al_2O_3 as well as to mixed metal crystals.

A substantial improvement could be achieved with the advancement of the cyclic cluster model for ionic crystals. Boundary effects and artificial defect interactions were eliminated. Contributions from the Madelung sum proved essential for anisotropic crystals. New applications concern the miscibility of zinc chalkogenides and their thermodynamic properties. The modeling of the 24-step reaction cycle for the selective catalytic reduction of NO with NH_3 and CO_2 to N_2 and H_2O at V_2O_5–TiO_2 is a highlight in the calculations for adsorption. The successful installation of the Born-Oppenheimer molecular dynamics in MSINDO will lead to further interesting applications not only for adsorption but also for other areas.

A number of visitors, among them N.D. Epiotis, R.A. Evarestov, S.R. Gadre, M.S. Gopinathan, C. Minot, R.F. Nalewajski, and R. Ponec, enriched the Hanover group with their ideas and skills.

For the promotion of Theoretical Chemistry, Karl organized in 1994 the International Workshop on "Electronic Structure Methods for Truly Large Systems: Moving the Frontiers in Quantum Chemistry", in 1995 the Symposium for Theoretical Chemistry in Germany, in 2003 the International Colloquim on the occasion of the 100th birthday of Hans Hellmann, as a chairman of the local section of the German Chemical Society.

The scientific work of Karl Jug is documented in more than 230 original publications, several book contributions and a textbook. He held guest professorships at the Florida State University, the Johns Hopkins University, at the universities in Zürich, Stuttgart, Krakow, Moscow, Paris, at the Nehru Chair in Hyderabad and at the Indian Institute of Technology Madras. He is a corresponding member of the European Academy of Arts, Sciences and Humanities, a member of the Humboldt society, and recipient of the Honor Medal of the Ministry for Education of Hungary.

Karl Jug inspired a large number of students in quantum chemistry. Several became university teachers. The enthusiasm for theoretical chemistry will not permit him setting down to rest. Lectures and research activities, which promise further achievements, are in progress. We, the colleagues, friends and students, cordially wish Karl Jug, his wife Ulrike and the three children all the best for the future.