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Foreword

Zdenek Herman – An Ambassador of Science

This special issue of the *International Journal of Mass Spectrometry* honors Professor Zdenek Herman on the occasion of his seventy-fifth birthday, and for his seminal contributions to physical chemistry that span half a century. Through these collected papers, Zdenek's colleagues and friends gratefully acknowledge his pioneering studies in diverse areas of mass spectrometry, including kinetics and dynamics of ion-molecule processes, Penning and associative ionization, and ion-surface interactions.

In recognition of his many scientific accomplishments, Zdenek has been honored by numerous awards, including the Joint Prize of the Czechoslovak Academy of Sciences and German Academy of Sciences for work in reaction dynamics (1980, together with V. Pacák, L. Zülicke, F. Schneider and U. Havemann), the Ioannes Marcus Marci Medal of the Czechoslovak Spectroscopic Society (1989), the Alexander von Humboldt Research Award (Germany, 1992), the E. Schrödinger Award of the Symposium on Atomic and Surface Physics (SASP, 1994), the National Prize "Czech Head 2003" for life achievements in science (2003), and the MOLEC Award (2006). He was twice recipient of JILA (Joint Institute for Laboratory Astrophysics, Boulder, CO) Visiting Fellowships (1980, 2001). The Journal of Physical Chemistry published an Honor Issue to celebrate his sixtieth birthday (J. Phys. Chem. 99, No. 42, 1995).

Zdenek was born on March 24, 1934 in Libušín, a small town in central Bohemia, Czech Republic. After graduating from Gymnasium in Kladno (1952), he studied chemistry at the School of Mathematics and Physics, Charles University in Prague, with a specialization in physical chemistry and radiochemistry. After completing his studies in 1957, Zdenek joined the Institute of Physical Chemistry, Czechoslovak Academy of Sciences (now J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic) and he has remained faithful to this institution to the present day. Zdenek began as a research assistant and later became scientist and senior research fellow; he served as Head of the Department of Chemical Physics (1984–1992, 1995–2005), Deputy Director (1990–1992), and Head of the Scientific Council of the institute (1997–1999). Only after the fall of the communist regime (1989) was Zdenek allowed to habilitate (1992), and he became Professor of Chemistry in 1996 at the Institute of Chemical Technology, Prague. Since 1993 he has been Honorary Professor of Ion Physics at Leopold-Franzens University, Innsbruck, Austria. Since 1989 he has also served on many committees of the Academy of Sciences and of the Czech Government.

After a short period of work in radiochemistry and basic mass spectrometry, Zdenek's research concentrated on the chemical reactions of ions. Together with his senior colleague in the institute, Dr. Vladimír Čermák (1920–1980), Zdenek investigated ion-molecule reactions in the ionization chamber of a home-built Nier-type mass spectrometer (Fig. 1).

In their first papers in 1960, they showed that formation of ions such as N_3^+ in $N_2^+ + N_2$ collisions required an excited state of the ion to overcome the endoergicity of the reaction and they assessed the predicted (but yet unobserved) quartet excited state of N_2^+ as the reactant. They later used the ionization chamber of their Nier-type source with modified potentials as a simple perpendicular beam machine (known as the Čermák-Herman experiment) to study products of charge transfer between noble gas ions and polyatomic molecules. They demonstrated that a specific amount of energy was transferred to the polyatomic molecule in the charge transfer process, and this provided a method to experimentally determine the break-down pattern of the molecular ion (1961). For propane, the data were in good agreement with the calculations of absolute rate theory applied to mass spectra of polyatomic molecules by Rosenstock et al. (1952) and they provided one of the early compelling comparisons between theory and experiment. Zdenek's doctoral thesis (1963) examined ion-molecule reactions in mixtures of gases with metal vapors and studied many ion-molecule reactions leading to mercury-containing organometallic ions. It also included studies of associative ionization in metastable excited neutral–neutral collisions. This research led to construction of an ion source with multichannel molecular beam sources and to studies of associative and Penning ionization of polyatomic molecules. A simple model for the competition of associative and Penning ionization was developed. Early experiments on measuring the energy of the electron released in these processes were further developed by Čermák into Penning ionization electron spectroscopy (PIES).

In 1964, Zdenek joined Richard Wolfgang at Yale University as a post-doctoral research associate. He intended to construct a fast neutral beam–surface machine, as a beam analogue to hot atom chemistry, the main interest of Richard Wolfgang at that time.

This was, however, the era of the first crossed beam studies of reactive scattering of neutrals (Datz, Herschbach, Greene, Ross, Bernstein and others) and the Yale project was soon modified to build a crossed beam scattering machine for studies of ion-molecule reactions (Fig. 2). The instrument known as EVA (originally Evatron, Richard Wolfgang's analogy with the famous Yale Bevatron) combined measurement of angular and translational energy distributions of product ions. It provided unprecedented crossed beam data and detailed characterization of direct and complex formation mechanisms at low collision energies. The productive interactions with Richard Wolfgang continued for several years, despite Zdenek's serious travel limitations under the communist regime. In early 1970 the collaboration was interrupted by the extremely difficult political atmosphere in post-Prague Spring Czechoslovakia; this led to a ban on Zdenek's visits to the United States and western countries. The tragic death of Richard Wolfgang in the

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Fig. 1. Zdenek Herman with Vladimír Čermák in 1962.

Fig. 2. Zdenek Herman with Richard Wolfgang and the Yale EVA machine (1968).

following year ended a close friendship and productive collaboration.

Despite these hardships, Zdenek persevered and continued to excel in his research. In the Prague institute, he designed and constructed an improved version of the crossed-beam scattering machine (EVA II). He also developed a collaboration with theorists in Berlin (Lutz Zülicke and his quantum chemistry group at the German Academy of Sciences) who had computational facilities to carry out trajectory calculations. This collaboration led to one of the first successful joint experimental and theoretical studies of an ion-molecule reaction. Scattering data and quasi-classical trajectory calculations for HeH^+ formation from $H_2^+ + He$ collisions showed good agreement for all reaction dynamics quantities.

Fig. 3. The mass spectrometry group in the J. Heyrovsky Institute of Physical Chemistry, Prague, in 1990. Standing from left: M. Sadílek, M. Fárník, V. Heyrovský, M. Smrčina, L. Hládek, Z. Dolejšek, L. Brabec, Sitting: J. Vančura, V. Hanuš, Z. Herman.

Fig. 4. The Prague group in 1998. Standing from left: L. Mrázek, Z. Herman, Z. Dolejšek, J. Polách. Sitting: J. Žabka, J. Kubišta, P. Španěl, V. Hanuš.

Fortunately, during the limitations on Zdenek's foreign travels in the seventies, many colleagues visited Prague for extended periods to work on the scattering machine (Jean Futrell, Andy Yencha, Michael Henchman, Keith Birkinshaw, Peter Hierl). These projects included scattering studies of ion-molecule reaction dynamics, charge transfer dynamics, investigation of parallel mechanisms in ion-molecule reactions and studies of hydride-ion transfer dynamics.

In the early eighties, together with Břetislav Friedrich and other graduate students, Zdenek investigated dynamics of charge transfer processes involving doubly charged ions. The first studies concerned atomic dication-atom processes and the results led to development of a quasi-classical model (together with E.E. Nikitin's group in Moscow) to describe the angular scattering in dication-neutral electron transfer collisions. Later studies of molecular dication systems resulted in scattering studies of charge transfer and chemical reactions and to the formulation of a potential surface model that describes competition of these processes.

Fig. 5. The Boulder Ion Gang 1980. Standing from left: Steve Leone, Zdenek Herman, Veronica Bierbaum, Barney Ellison, Carl Lineberger; sitting: Chuck DePuy, Eldon Ferguson.

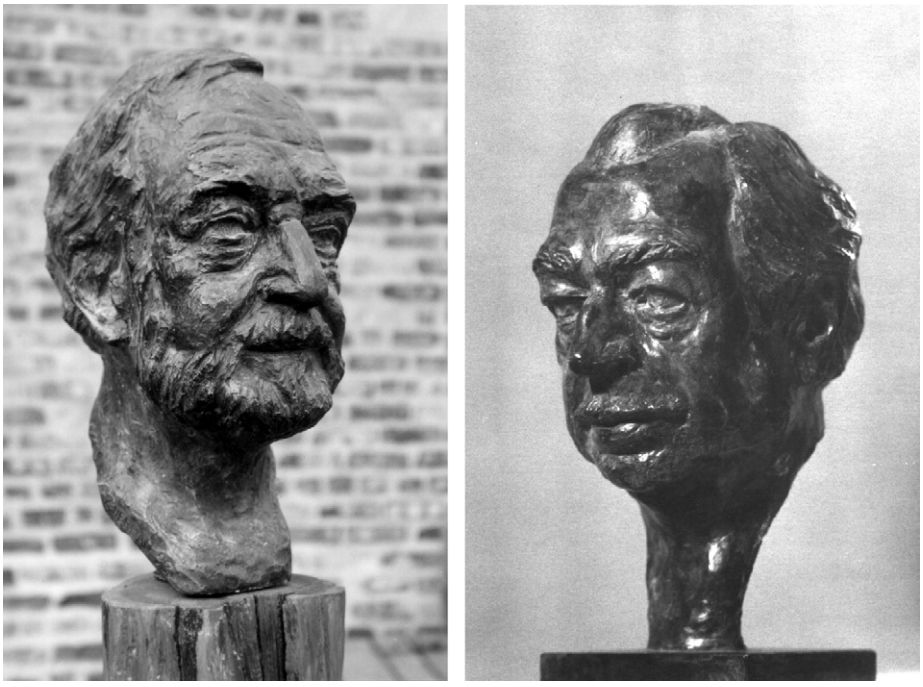

Fig. 6. Steve Berry (1993, left) and John Beynon (1987, right).

During the past decade Zdenek has embarked on an important new area of research; he and his group have been investigating polyatomic and cluster ion-surface interactions using a modified beam scattering apparatus. By combining measurements of mass spectra and angular and translational energy distributions of the product ions from collisions with surfaces (carbon, stainless steel, tungsten, beryllium), they have derived novel information on energy partitioning in surface collisions, fragmentation and chemical reactions of projectile ions, and ion survival probabilities in surface collisions (Figs. 3 and 4).

Over the years, Zdenek has collaborated with many laboratories abroad. His work with Richard Wolfgang brought him a Visiting Professorship at the University of Colorado in Boulder (1968–69) and lasting contacts with the ion research community there. He returned to Boulder twice as a Visiting JILA Fellow (1980, 2001) and collaborated with the research groups of Carl Lineberger, Steve Leone and David Nesbitt, where he was inducted as an official member of the "Boulder Ion Gang" (Fig. 5).

Zdenek's 3-month stay at the Institute for Molecular Science in Okazaki (1984) resulted in studies with Inosuke Koyano on the influence of specific internal excitation of the ion reactant on the kinetics and dynamics of ion-molecule reactions. The first studies of charge transfer with molecular dications (mass spectrometric and translational energy spectroscopy) were initiated during his visit with John Beynon at University College Swansea as a Royal Society Exchange Scientist. During the von Humboldt Prize period (1993-96) in Göttingen (Max-Planck-Institute für Strömungsforschung), he collaborated with Christoph Ottinger (spectroscopy of reaction products) and Peter Toennies (high-resolution beam experiments); this research led to the detailed description of energy partitioning in dication-neutral charge transfer. Since 1989 he has been involved in extensive collaborations with Leopold-Franzens University of Innsbruck (with the late Werner Lindinger on ion-molecule gas-phase collisions, and especially with Tilmann Märk on collisions of ions and cluster ions with surfaces). Zdenek has also enjoyed productive collaborations with Marie Durup and Odile Dutuit at Université Paris-Sud, with Steve Berry at the University of Chicago, and with Steve Price at the University College London.

After the political and social changes in Czechoslovakia at the end of 1989, Zdenek was temporarily involved in science administration in the Academy of Sciences; he was a co-founder of the first grant agency in the country in 1989–1990, and in 1989–1991 he chaired the Collegium of Chemistry, a committee that awarded scientific titles in chemistry. However, in 1992 he returned fully to his laboratory where he continues to actively pursue research.

I first met Zdenek during his JILA Visiting Fellowship in 1980. These wonderful months were filled with exciting research, exhilarating ski trips, and memorable discussions; I grew to know Zdenek as a brilliant scientist, talented artist, and dear friend. He left behind some treasured artwork of the people and places of Boulder, which now adorn the offices and halls of JILA. In addition to his legendary drawings, Zdenek has immortalized several close friends in his handsome sculptures, as depicted in the busts of Steve Berry and John Beynon in Fig. 6.

Zdenek's career embodies many enviable qualities: his remarkable insights, his passion for science, his exceptional craftsmanship, his indomitable spirit, his sincere fellowship with an international community of chemists and physicists. As colleagues and friends, we are pleased to dedicate this Honor Issue to Zdenek Herman, a gifted scientist and extraordinary person. Zdenek, may this landmark birthday be the beginning of an even more rewarding era!

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