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In memoriam: Pavel Rosmus

Dne 13. října zemřel ve Frankfurtu po těžké nemoci profesor teoretické chemie Pavel Rosmus. Odešla světově uznávaná vědecká osobnost, která zanechala v oblasti teoretické chemie nesmazatelnou stopu svým příspěvkem k obecné racionalizaci a interpretaci vlastností molekul v termínech elektronové struktury. P. Rosmus se narodil 11. 8. 1938 v Přerově na Moravě v rodině tragicky poznamenané druhou světovou válkou. Jeho otec byl za aktivní účast v odboji proti německé okupaci odsouzen k několikaletému vězení, což otce těžce zdravotně poznamenalo, i nepříznivě ovlivnilo celou rodinu. V roce 1957 maturoval P. Rosmus na Průmyslové škole chemické v Přerově a zahájil svá vysokoškolská studia na Vysoké škole chemicko-technologické v Praze. Jako vynikající student byl v roce 1960 doporučen ke studiu na Technische Universität Dresden, kde v roce 1964 obhájil titul Diplom Chemiker. Na Ústavu organické chemie Drážďanské univerzity vypracoval doktorskou práci specializovanou na siriné sloučeniny a její úspěšnou obhajobou získal v roce 1968 titul Dr. rer. nat. V roce 1968 se v Drážďanech oženil, ale také prožil velmi dramatické události spojené s koncem Pražského jara. Po svých protestních vystoupeních proti okupaci Československa spojeneckými vojsky Varšavské smlouvy byl východoněmeckými úřady donucen NDR opustit. Odešel s celou rodinou do Prahy, kde získal místo ve skupině prof. R. Zahradníka v tehdejší Ústavu fyzikální chemie ČSAV, což znamenalo počátek jeho přeměny z organického na kvantového chemika. Po dvou letech pobytu v Praze se rozhodl se ženou a dvěma dcerami k odchodu do Spolkové republiky Německo. Později byl soudem v Praze odsouzen k jednomu roku vězení a propadnutí veškerého majetku za ilegální opuštění republiky.

Prvním exilovým azylem P. Rosmuse byl Frankfurt nad Mohanem, kde se mu dostalo podpory od prof. H. Hartmanna na Johann Wolfgang Goethe-Universität Frankfurt (JWGUF). Rok 1973 prožil jako post-doc na University of Sheffield u prof. R. McWeenyho. Významným milníkem pro jeho celou vědeckou kariéru se stal rok 1974, kdy přišel do skupiny prof. W. Meyera na Johannes-Gutenberg-Universität Mainz. Jako „research associate“ se zde začal věnovat svému nejvýraznějšímu oboru vědecké činnosti, a sice aplikaci pokročilých kvantově-chemických metod v oboru molekulové spektroskopie. V roce 1974 také zahájil teoretické studium a počítačové simulace foto-elektronových spekter molekul ve spolupráci s prof. Bockem z JWGUF a získal na této univerzitě nabídku „definitivy“. Nabídku přijal a v roce 1978 se navrátil do Frankfurtu. V roce 1982 se na JWGUF habilitoval v oboru teoretická chemie a získal stálou pozici profesora. Během následujících 15 let v této pozici působil na chemické fakultě JWGUF. V těsné spolupráci s prof. E. A. Reinschem a prof. H.-J. Wernerem (spoluautory jednoho z dnes nejpo-užívanějších souborů kvantově-mechanických programů MOLPRO) otevřel nové možnosti teorie pro racionalizaci molekulových spekter v termínech vysoce přesných povrchů molekulových vlastností (potenciální energie, elektrické dipólové a přechodové momenty) a výrazně tak rozšířil poznávací potenciál experimentální molekulové spektroskopie. V roce 1993 byly zásluhy P. Rosmuse oceněny jmenováním nejprve do pozice Professeur de Pre-mière Classe a později do vysoce prestižní pozice Professeur de la Classe Exceptionel na Université de Marne la Vallée ve Francii s pověřením zde vytvořit novou skupinu v oboru teoretické chemie. Tohoto úkolu se zhostil s naprostým úspěchem a společně s prof. G. Chambaudovou opublikoval řadu zásadních příspěvků umožňujících interpretaci vibronických spekter iontových molekul, komplexů iontů a neutrálních molekul, Rennerových-Tellerových systémů, monomolekulárních procesů a molekulových fotodisociací, tedy výsledků obecného fyzikálně-chemického a astrofyzikálního významu. Dosažené výsledky byly oceněny jak v laboratořích, tak i oficiálními prestižními poctami. V roce 2000 byl P. Rosmus nominován na Mem-bre Senior Institut Universitaire de France, v roce 2007 na Gauss-Professor na Königliche Gesellschaft der Wissenschaften v Göttingen a, konečně, v roce 2008 ho francouzská vláda jmenovala Chevalier dans l'ordre des Palmes Académiques za zásluhy o francouzskou kulturu.

Díky hlubokému porozumění teorii i experimentu, schopnosti správně vidět a popsat nevyřešené problémy a neméně i schopnosti tvořivě spolupracovat, patřil P. Rosmus mezi nejvyhledávanější partnery celé komunity teoretické chemie. Pro ilustraci: v roce 1984 spolupracoval jako Visiting Professor na Manne Siegbahnlaboratoriet ve Stockholmu s prof. Larssonem při studiu pravděpodobností zářivých přechodů v molekulách; v roce 1985, jako Visiting Fellow proslulého ústavu JILA v Coloradu, navázal dlouholetou a vysoce produktivní spolupráci s Dr. S. V. O'Neilem věnovanou Rosmusovu oblíbenému tématu pravděpodobností zářivých přechodů a také studiu negativních iontů a

procesů spojených s přenosem náboje; v roce 1987, jako Overseas Fellow of Churchill College v anglické Cambridge, zahájil letitou spolupráci s prof. N. Handym směřovanou k teoretické interpretaci intenzit rotačně-vibračních přechodů v termínech povrchů elektrických dipólů; v letech 1997 a 2000 byl pozván do superpo-čítačového Conzorzio Interuniversitario CINECA v Bologni spolupracovat s prof. Palmieri na problematice spin-orbitálního spřažení a dob života molekulárních iontů; studium nabitých molekulárních útvarů bylo rovněž námětem i jeho dlouhodobé spolupráce s prof. J. P. Maierem z Universität Basel.

Vedle intenzivní vlastní vědecké práce byl P. Rosmus velmi aktivní i v organizaci evropské mezinárodní spolupráce; účastnil se např. čtyř European research networks on Theoretical Chemistry a po pět let působil v této společnosti jako koordinátor. Uznávaná míra přínosu Pavla Rosmuse do světové vědecké literatury je přesvědčivě doložitelná citační analýzou jeho publikací (viz ICI Web of Knowledge): 238 stávajících vědeckých publikací dosud získalo 5149 citací a autorův *h*-index činí **38**.

Jiří Čížek, Rudolf Polák, Lubomír Skála a Vladimír Špirko



Professor Pavel Rosmus

Pavel Rosmus

In September 2006, Pavel Rosmus retired from his Professorship at the Université de Marne-la-Vallée and he became a Professor emeritus. This event was celebrated in an international symposium on the *Interplay of Theory and Experiment in Molecular Spectroscopy and Dynamics*, which took place in the Heyrovsky Institute of Physical Chemistry in Prague on 15 September 2006. About 60 of his colleagues and friends attended this meeting. To honour the scientific achievements of Pavel Rosmus his friends agreed to contribute to this special issue of *Molecular Physics*.

Pavel was born in Prerov, province of Moravia of the Czech Republic, on 11 August 1938. He began his studies of Chemistry in 1957 at the Technical University of Prague. In 1960, after a stay of four months at the Institute of Chemical Technology in Moscow, he changed to the Technical University Dresden, East Germany. There he gained a Diploma degree at the Institut für Organische Chemie for work on 'Spectroscopy and Chromatography of Sulfur Heterocycles' in 1964. He continued as a research associate under the supervision of Professor R. Mayer and obtained his PhD in 1968 with a thesis on 'The Effects of Substituents on the Reactivities of Tiocarbonyles'.

Shortly thereafter, during the events of the Prague Spring, Pavel denied the demands of East German authorities to cooperate in a radio campaign in the Czech language, and he and his young family were immediately expelled from East Germany. Back in Prague he found support by Professor Zahradnik at the Heyrovsky Institute of Physical Chemistry of the Czech Academy of Science. He studied the role of orbital localization in transition metals by means of semi-empirical calculations – his first step into theoretical chemistry.

In spring 1971, Pavel was fortunate to take advantage of the non-citizenship of his family to leave the Czech republic for West Germany where his family finally settled in Frankfurt. Supported by Professor H. Hartmann he continued his research work at the Institute of Physical Chemistry of the Johann Wolfgang Goethe-Universität Frankfurt, investigating the possibility of an analytical description of electron correlation by means of Methieu functions. During 1973 he was as a post-doc with Professor R. McWeeny at the

University of Sheffield, UK, and participated in the development of a new pseudo-potential method for heavy atoms.

In the beginning of 1974, Pavel joined the group of Professor W. Meyer at the Institute of Physical Chemistry of the Johannes Gutenberg-Universität Mainz as a research associate. During the following years Pavel found his final field of research: the application of advanced quantum chemical methods to problems of molecular spectroscopy. He was the main author of a series of papers on diatomic hydrides, providing highly accurate molecular constants, dissociation energies, ionization potentials and electron affinities. They were essential to establish the potential of a new method, the coupled electron pairs approximation using pseudo natural orbitals (PNO-CEPA). One of us (WM) is happy to acknowledge that this work would never have been possible without Pavel's energetic efforts to overcome the poor computational situation in Mainz by exhausting travels to the computing center of the Max-Planck Institute for Plasma Physics in Munich.

Also in 1974, Pavel began computational investigations and simulations of PE spectra in a cooperation with Professor Bock of the Institute of Inorganic Chemistry of the Johann Wolfgang Goethe-Universität Frankfurt who offered him a tenure position. Thus, in 1978 Pavel moved to Frankfurt. He habilitated for Theoretical Chemistry in 1982 and became tenure Professor. During his 15 years at the Frankfurt Department of Chemistry Pavel greatly extended his research interests to virtually all fields of molecular properties and related spectroscopies, excelling in particular in the calculation of high-quality potential energy surfaces, dipole and transition moment surfaces and the simulation of high-resolution IR and UV spectra. This work was done in close cooperation with Professor E.A. Reinsch and one of us (HJW) who at that time had just developed the first version of the internally-contracted multi-reference configuration interaction (MRCI) as part of the MOLPRO program. This program became the main working horse of Pavel's research. He was the driving force behind many impressive applications. One of us (HJW) is very grateful for a wonderful and very fruitful collaboration

with Pavel, which continued until now. It has resulted in 61 common publications.

In 1993, Pavel was appointed Professor de Première Classe at the Université de Marne la Vallée in France. Since then he has been leading a very productive Theoretical Chemistry research group. His research, carried on in close collaboration with his colleague Professor G. Chambaud, embraced the study of rovibronic spectra of a large variety of ionic molecules and ion–molecule complexes, the investigation of Renner–Teller systems and processes of unimolecular or photo dissociation. In recognition of his scientific achievements, he received in 2000 the very prestigious nomination for Membre Senior Institut Universitaire de France. In 2007 he was nominated Gauss-Professor by the Academy of Sciences in Göttingen, Germany.

Given Pavel's affinity to unsolved problems in spectroscopy and his ability to design an appropriate theoretical treatment, he could establish very successful cooperations all over the world: 1984 he was Visiting Professor at the Institute of Physics Manne Siegbahn, Stockholm, Sweden, where he worked with Professor Larsson on radiative transition probabilities; 1985 he was elected Visiting Fellow of JILA, Colorado, USA, which marked the beginning of a long-time cooperation with Dr S. V. O'Neil on radiative transition probabilities, negative ion states and charge transfer processes; 1987 he was elected an Overseas Fellow of Churchill College, Cambridge, UK, resulting in an extensive research cooperation with one of us (NH) with the focus on dipole moment surfaces as prerequisites for ro-vibrational transition probabilities and simulation of IR spectra; 1997 and 2000 he was invited to the Center of Intensive Calculations – CINECA in Bologna, Italy, where he worked with Professor Palmieri on spin–orbit interactions and molecular ion lifetimes. In a long-time cooperation with Professor J. P. Maier, University of Basel, Switzerland, Pavel has made crucial contributions to the understanding of spectra of matrix-trapped ionic molecules. We should finally note that for more than a decade he participated in four European research networks on Theoretical Chemistry. This community is particularly indebted to him for acting as Coordinator for about five years.

The research interests of Pavel Rosmus have centred on the quest to predict and interpret the properties of molecular matter through the computational exploitation of theory and modelling of electronic structure. His entire effort is guided by what is computationally feasible, and therefore embrace detailed consideration of the advanced topics in computational chemistry. He has always put a strong emphasis on computations of measurable data directly comparable with experiments. Pavel has truly set new standards in Theoretical

Spectroscopy. His work and his personality have deeply influenced all of us who work in Theoretical Chemistry. We are very grateful to him.

Wilfried Meyer
Kaiserslautern
Hans-Joachim Werner
Stuttgart
Nicholas Handy
Cambridge

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