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Report on the habilitation thesis of Dr. Karel Houfek

entitled

Resonant collisions of electrons and anions with molecules: from diatomics to polyatomics

The research described in the habilitation thesis of Dr. Houfek is concerned with the broad field of electron-driven chemistry and physics. This field is much less widely known than photochemistry to which it may be compared, but affects many areas of science (e.g., astronomy, plasma science and technology), industry and even medicine (radiotherapy, sterilization). With respect to applications of electron-driven chemistry a colleague working in the industry referred to the electron-beam (EB) technologies as a "sleeping giant" – vast but unseen by the public because many companies using it do not publicize that they do. The uses encompass polymer crosslinking during fabrication of tires, crosslinking of the polymer on a sticky tape and many others.

The Habilitation Thesis consists of a very readable and compact introduction in chapter 1 – the "Overview of studied problems" – and a collection of original papers in chapter 2. This format is entirely appropriate.

The papers are exceptionally well written, not only scientifically, but also from a didactic point of view. Some of the theoretical papers of Karel Houfek refer to experimental work of my group in Fribourg. The experimental results were often puzzling to us when they were recorded and the understanding was provided by the work of Karel Houfek. Important is that Houfek provided not only the rigid understanding in the sense of theoretically reproducing the experimental data, but also, even primarily, provided physical insight, showing which physics caused the puzzling shapes of the spectra. I also experienced the exceptional didactic capacity of Houfek at numerous discussions at conferences where he succeeded to explain to me – an experimentalist – the theoretical intricacies and the underlying insight. This didactic talent makes him even more suitable for a position at a university.

Houfek's work includes several ground-breaking studies. My favorite work is described in chapter 1.1 of the Habilitation Thesis. It is to my knowledge the only

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work on temporary negative ions going beyond Born-Oppenheimer approximation. The point is that quantum mechanics demands that, in an electron-molecule collision, the motion of the electron and the motion of the nuclei are treated simultaneously, requiring one equation combining both nuclear and electronic motion and resulting in only one wave function describing the motion of both the electron and the nuclei. Solving this task is extremely demanding, however, and researchers therefore use the Born-Oppenheimer approximation, splitting the calculation into two parts, calculating the electronic motion for fixed nuclei and then calculating the motion of the nuclei on a potential surface obtained in the first step. The use of the approximation results in an error, however, and little was known about the nature and magnitude of this error. Houfek shed light into this problem by solving the full equation, without the Born-Oppenheimer approximation, for three cases which modeled the three important molecules NO, F_2 and N_2, and subsequently comparing the exact results to those obtained by various methods using the Born-Oppenheimer approximation.

Another favorite publication of mine is paper 2.3, which provides detailed interpretation of the shapes of the vibrational excitation cross sections in NO, which were very puzzling to us when we recorded them in Fribourg. The puzzling point is that two kinds of vibrational structure appear in the cross sections even though a diatomic molecule has only one vibrational coordinate.

A strong experimental group working on the theme of the electron-molecule processes has recently emerged at the Heyrovský institute of the Academy, around Juraj Fedor, in the domain led by Michal Fárník. This makes it even more meaningful to have Karel Houfek as professor at the Charles University, making Prague a competence center for electron-driven physics and chemistry both theoretically and experimentally.

To conclude, Karel Houfek is a leading scientist in the field of theory of physics of extremely short-lived states such as resonances in electron-molecule (or ion) collisions. He has a very impressive list of innovative papers. He has an exceptional didactic talent. I recommend that his Habilitation Thesis is accepted by the Faculty and that he is appointed as an associate professor at the Charles University.

Fribourg, 24. June 2018

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