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Subject: Assessment doctoral dissertation Hubert Jozwiak

It is my great pleasure to give an assessment of the PhD Thesis by candidate Hubert Jozwiak. The theoretical work, dealing with collisions of simple molecules and atoms in fundamental studies in atomic and molecular physics, is performed in the world-leading environment on this subject built by the thesis advisor. The thesis involves detailed studies of the effects of collisions on line-shape parameters and rate constants for simple molecules of astrophysical, environmental, and fundamental importance - most importantly the simplest molecule in our universe, molecular hydrogen. In addition to providing key reference data for the whole scientific community, the PhD candidate developed a software package for state-of-the-art scattering calculations, benchmarked ab initio potential energy curves and studied fundamental aspects of the theoretical description of collisions processes, involving the hyperfine structure and the indistinguishability of the involved particles. As such, the work involves the analysis and derivation of fundamental equations and computations at a very high level of sophistication, improving existing data in the literature and significantly extending the understanding of the matter at a point where physics and chemistry merge.

The major achievement of the thesis resides in (i.) developing and implementing a quantum scattering approach for the calculation of collision effects in the spectroscopy of simple molecules; (ii.) providing state-of-the-art reference rate coefficients and line-shape parameters under various conditions for H_2-He, H_2-H_2 (and isotopologues), and N_2-CO. This data is not only important for astrophysical and atmoshperic studies, but also for fundamental physics tests using precision measurements of molecular hydrogen; (iii.) providing reference data for the hyperfine structure of spectroscopic lines for various molecular hydrogen species and (iv.) providing crucial calculations/simulations for the next generation of precision measurements of the hydrogen molecules based on optical and magnetic traps.

These achievements require a wide variety of skills and are of high importance for the planning and analysis of various measurements carried out around the world. Let me highlight two examples, that I think exemplify the scientific approach of Hubert Jozwiak: when reaching some limitations with widely used existing legacy code for the quantum scattering calculations, he developed his own scattering code, overcoming these limitations. Secondly, while existing studies on collisional effects treat the collision partners as indistinguishable, the candidate studied the effect of the spin-statistics theorem and showed that for example the pressure broadening shows different behavior in the low-temperature regime.

In part I of the thesis, revised rate coefficients were obtained for the H_2-He system using new ab initio data, revealing an improved treatment of vibrational excitations. In addition, beyond Voigt-line-shape effects and a pure ab initio approach were studied to describe collisional widths and shifts of molecular lines, aiming for a description of the system at low and high pressure conditions. The results were made available also via databases such as HITRAN, after benchmarking them by comparing to experimental data.

While part I focused on astrophysical applications, part II aims at terrestrial applications and provides data, for example, for N_2-CO. Various approximations were tested and a new scattering code was developed to handle the resulting complexity of the scattering calculations.

In part III of the thesis, the focus lies on precise measurements of molecular hydrogen and its isotopologues for fundamental tests of physics, including QED. Here, Raman transitions, as well as the hyperfine structure for electric-dipole and quadrupole transitions were calculated. The resulting dataset is of immense value for ongoing experimental studies and fills existing gaps in the scientific literature. Very relevant and impressive were two studies for future experiments with molecular hydrogen in dipole and magnetic traps, identifying magic wavelength conditions using the quadrupole polarizability and showing the H_2 molecules could be sympathetically cooled using Li atoms.

In conclusion, this doctoral dissertation shows par excellence the theoretical knowledge of the candidate at the merger point of physics and chemistry. For the problems tackled in the dissertation, it provides original solutions as discussed above. I should also highlight the broad scope and the level of independence that the candidate shows, which is exemplified by his exceptional publication track record, with ten first author publications contained in this thesis, for many of which he also took over the role as corresponding author. In addition, the candidate is involved in several collaborations/joint publications with other theoretical and experimental groups, indicating his ability to foster scientific collaborations and bringing his theoretical predictions into action.

I confirm, without hesitation, that the candidate deserves the doctoral degree for this excellent work, fulfilling all the conditions specified in Art. 187 of the Law on Higher Education and Science. I am not familiar with the Polish system, but I would fully support awarding a high degree of distinction associated with the PhD degree bestowed upon him.

Maximilian Beyer