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Report on the doctoral thesis of Mr Hubert Jóźwiak

The doctoral thesis of Mr Hubert Jóźwiak, entitled "Collisions of simple molecules and atoms in fundamental studies", was prepared under the supervision of prof. Piotr Wcisło at the Institute of Physics of the Nicolaus Copernicus University, in the group which has extensive experience in both theoretical and experimental studies of various aspects of spectral line broadening. This particular thesis has predominantly theoretical character, although the candidate does not avoid comparing his results with the experiments. The first impression after a cursory examination of the thesis is the impressive range of content, its volume and its form, more typical of a habilitation dissertation. The core of the work consists of 12 publications in prestigious scientific journals. Although these publications have between 2 and 18 authors, in 10 of them Mr Jóźwiak is listed in the first place, and his dominant contribution to most papers is confirmed by statements of (altogether 29) co-authors, again written in a form more typical of habilitation procedures. The collection of publications is preceded by a comprehensive, almost 50-page Introduction, which is a useful guide to the published works, and their main results are summarised in 4 pages at the end of the thesis. The dissertation is completed by 4 Appendices which give details of some technical aspects of the publications and an exhaustive bibliography of 283 items. It should not be assumed that Mr Jóźwiak has included all of his work in the presented thesis, as it counts a total of 28 papers published between 2017 and 2024, which is also an achievement worthy of the highest praise.

Understandably, such extensive work addresses a number of issues, which can be divided into two main groups. The first concerns collisions of diatomic molecules with perturbers - atoms and other molecules - and their effect on the shape of the spectral lines. Using the best available theoretical potential energy surfaces, systems such as H_2-He, HD-H_2 or CO-N_2 were studied, assuming various conditions characteristic of both interstellar space and the atmospheres of planets, including the Earth. Mr Jóźwiak calculated the rate coefficients for rovibrational transitions in the studied molecules, for the first time taking into account higher vibrational levels, and determined precise parameters describing the shapes and shifts of the corresponding spectral lines. The results obtained may have immediate applications in testing models of interstellar clouds, models of the atmospheres of Solar System planets or, in the Earth's environment, in climate modelling or pollution monitoring.

The second group of papers concerns the field of high precision spectroscopy of the hydrogen molecule, which at the highest level of accuracy can shed light on fundamental problems in physics, such as the validation of the Standard Model of particle physics. In particular, the author investigated the influence of the hyperfine structure of rovibrational transitions on the observed line shapes. The isotopologues of diatomic hydrogen H_2, HD, HT and DT were considered, as well as the dipole and quadrupole transitions between the corresponding levels. To illustrate the scale of the work, one of the papers provides frequencies and intensities of more than 300,000 hyperfine lines for more than 18,000 rovibrational transitions. The ultimate goal for high-precision spectroscopy of H_2 is to cool the molecules to temperatures in the mK range and trap them in an optical dipole trap. However, the trap is formed by a strong laser field which, in contrast to the spectroscopic requirements, can significantly shift the molecular energy levels. In the following work, Mr Jóźwiak identified a few so-called 'magic wavelengths' of the trapping laser at which the AC Stark shift would be eliminated for the selected rovibrational molecular transition. The two groups of topics are linked by the last paper, in which the influence of hyperfine and magnetic interactions on collisions between hydrogen molecules and ultracold ^{6}Li atoms was investigated in the context of the feasibility of sympathetic cooling of H_2.

The twelve articles that make up the thesis have been published in the following prestigious journals: Physical Review A (3), Journal of Quantitative Spectroscopy and Radiative Transfer (3), Journal of Chemical Physics (2), Astronomy & Astrophysics (2), Communication Physics and Scientific Reports. This means that Mr Jóźwiak's work has undergone detailed peer review by experts probably better than me and possible revision. I believe that this relieves me of the obligation to evaluate each paper in detail. However, I can state with confidence that these publications represent original and lasting contributions to the field of high resolution molecular spectroscopy.

Before moving on to the final conclusions of the report, I would like to make a few comments on the style of presentation. The thesis is well organised. In particular, I find the Introduction to be clearly written and of great help in understanding the ideas underlying the calculations presented in the following publications. The Appendices provide insight into the details of the calculations and I found the one discussing the role of quantum indistinguishability in spectral line shape theory particularly interesting. Numerous references illustrate the author's scholarship. A small criticism is that in the section containing reprints of publications, the consecutive page numbering is not displayed, which makes it difficult to navigate through them. For example, in order to find paper H, which according to the Table of Contents begins on page 117, the reader must either count 65 pages from the last numbered page 52 of the Introduction or count back 53 pages from page 170, where the numbering resumes. However, this is a minor point and in no way affects my assessment of the thesis.

In conclusion, the thesis is of a very high scientific quality and provides results that are very valuable for the field. I therefore recommend that Mr Hubert Jóźwiak be admitted to the next stages of the procedure for awarding a doctoral degree. In my opinion, the quality and scope of the results go far beyond what can be expected from a doctoral dissertation, and I propose the thesis for distinction. When applying for a distinction, it is advisable to indicate the most valuable result. In this case it is difficult because the candidate has achieved an outstanding level in every aspect of the research undertaken, but I suggest that the description of the influence of hyperfine interactions and external magnetic fields on precise spectroscopic measurements of the hydrogen molecule be cited as justification for the distinction.

P. Kowalczyk