P. Wcisło¹, F. Thibault², H. Cybulski¹, I.E. Gordon³, L.S. Rothman³, R. Ciuryło¹

1. Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland

2. Institut de Physique de Rennes, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, Bât.11B, F-35042 Rennes, France

3. Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics, Cambridge MA 02138, USA

* piotr.wcislo@fizyka.umk.pl

A proper treatment of non-Voigt line-shape effects is crucial to reliably interpret and reconstruct accurate molecular spectra as well as to reduce the systematic errors in atmospheric measurements of the Earth and other planets. This fact has stimulated development of a new structure of modern spectroscopic databases [1-3] and incorporation of an extensive set of new line-shape parameters [4]. It turned out, however, that the most challenging issue is to determine the values of these parameters for a wide range of pressures and temperatures covering all the bands and branches. Currently a set of available experimental data is relatively sparse and even if the experimental data can be reliably fitted and reproduced with the non-Voigt line-shape model then their extrapolations to other transitions and other thermodynamic conditions would result in very large errors [4]. Following [5, 6] we present our proposal for overcoming this difficulty by performing a set of *ab initio* lineshape calculations. We calculate from first principles the phase-/state-changing contribution by full quantumscattering calculations [7-9] and velocity-changing one from the Boltzmann collisional operator based on the billiard-ball approximation [10, 11]. After validation with experimental spectra for several particular lines we will be able to generate a complete dataset of *ab initio* line-shape parameters for a given molecular system. Finally, they will be projected [4] on a simple structure of the quadratic correlated speed-dependent hard collision profile [12, 13] also called the Hartmann-Tran profile [14], hence making them ready to be included into the new structure [1, 2] of the HITRAN database [15].

To validate our concept, we chose H_2 perturbed by helium which, on one hand, is the simplest possible system for such studies while, on the other hand, it is relevant for the studies of the atmospheres of gas giants and hence required to be stored in the spectral line databases. Our preliminary results for pure rotational and fundamental bands demonstrate that our *ab initio* approach not only well reproduces experimental spectra, but can also be used to validate the potential energy surfaces available in the literature [8]. In the next step we will repeat these calculations for higher H_2 vibrations with an extended version of the recent highly accurate PES [16]. A positive validation of our calculations will open a way for generating the first complete *ab initio* dataset of the line-shape parameters for a particular molecular system. In a long-term perspective we would like to focus on the CO-N₂ system, which is not only relevant for the investigations of Earth's atmosphere but can also be a feasible objective of *ab initio* studies.

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