# INVESTIGATION OF COLLISIONAL EFFECTS IN MOLECULAR SPECTRA - COMPREHENSIVE DATASET OF LINE-SHAPE PARAMETERS FROM AB INITIO CALCULATIONS FOR He-PERTURBED HD

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The abundance of molecular hydrogen and atomic helium in the universe makes them an important system to study in various fields. A mixture of molecular hydrogen and helium is the main component of the atmospheres of gas giants in the Solar System and is predicted to be a dominant constituent of the atmospheres of some types of exoplanets. The hydrogen molecule is also the simplest molecule, the structure of which can be calculated from first principles, which makes it well suited for accurate tests of *ab initio* calculations. In particular HD molecule, despite its lower abundance than $H_2$ isotopologue is noticeable in spectroscopic studies due to the presence of its dipole moment. Studies show that in some cases the uncertainty of astronomical observations (f.e. measuring the D/H ratios) of hydrogen molecule spectra is dominated by the uncertainties of collisional parameters, including pressure broadening and pressure shift coefficients.

We utilize the methodology of populating line-by-line spectroscopic databases with beyond-Voigt line-shape parameters [a] , which is based on *ab initio* quantum scattering calculations and was first applied to the He-perturbed $H_2$. We report a comprehensive dataset of beyond-Voigt line-shape parameters (pressure broadening and shift coefficients, their speed-dependences, and the complex Dicke parameters) for all electric dipole and quadrupole transitions within the ground electronic state in He-perturbed HD that are present in HITRAN (11 575 lines) at temperatures spanning from 20 to 1000 K. We parametrize the temperature dependence of the line-shape parameters with double-power-law representation (DPL), recommended for the HITRAN database. In addition to the presentation of the calculations, we will discuss our latest experimental determination of collisional line-shape parameters for He-perturbed $H_2$ and its comparison with theoretical results.

[a] P. Wcisło et al., J Quant Spectrosc Radiat Transf 2021;260:107477. doi: 10.1016/j.jqsrt.2020.107477