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Helium-perturbed H_2 spectra: a benchmark system for *ab initio* line-shape calculations

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Synopsis We report the results of the investigation of the line-shape parameters of the S and O branches of the helium-perturbed hydrogen, based on *ab initio* quantum-scattering calculations. We provide the pressure broadening and shift coefficients and the complex Dicke parameters for 60 lines and 17 temperatures, ranging from 5 to 2000 K. The results are in a good agreement with available experimental works. The investigation is important for astrophysical studies, for example as a reference data for studying the gas giants' atmospheres.

Hydrogen molecule is the most abundant molecule in the Universe. It is investigated in various physical fields, ranging from astrophysics and the analysis of gas giants atmospheres [1, 2]or collisions in the interstellar medium [3], to ultra-accurate measurements in molecular spectroscopy [4, 5, 6], and even in the search for physics beyond the Standard Model [7]. Recently [8] it was pointed out, that the available data regarding the line-shape parameters of hydrogen is rather sparse. The development of experimental techniques in molecular spectroscopy requires a sub-percent accuracy of the theoretical calculations. Such requirements could be fulfilled with the *ab initio* quantum-scattering calculations, based on the close-coupling scheme.

The collisional system of hydrogen molecule and helium atom is a perfect benchmark system for performing *ab initio* investigation of the line-shape parameters. It involves only four electrons, allowing researchers to calculate the potential energy surface of such system by means of the state-of-the-art methods of quantum chemistry. Moreover, because of the small mass of the system and large rotational constant of the hydrogen molecule, the dynamical calculations can be performed in reasonable computational time.

Using the recently reported ultra-accurate potential energy surface for the H_2 -He system [9], we performed close-coupling calculations of generalized cross sections for lines of the S and

O branches [10]. We investigated 60 lines in total, for vibrational bands from 0-0 to 0-5 and rotational levels up to j=5. Generalized spectroscopic cross sections were obtained from Smatrix elements for a wide range of kinetic energies (from 0.1 to 9000 cm⁻¹). The cross sections were later averaged over the relative speed distribution of the colliding pair, leading to the final line-shape parameters: pressure broadening and shifting coefficients and real and imaginary part of the Dicke contribution to the Hess profile. The parameters are obtained for 17 temperatures, ranging from 5 to 2000 K. This is the first complex investigation of the S and O branches in the H₂-He system using *ab initio* methods.

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