AB INITIO CALCULATIONS OF COLLISIONAL EFFECTS IN MOLECULAR SPECTRA OF SIMPLE MOLECULES

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The simple structure of molecular hydrogen isotopologues provides a great opportunity for testing the *ab initio* quantum scattering theory on the ultra-accurate experimental spectra and analysis of their spectral lines plays a crucial role in studies of atmospheres of gas giants. We present the results of *ab initio* calculations of collisional cross sections and line-shape parameters for the simple benchmark systems of D_2 perturbed by He and H_2. In our analysis, we use the state-of-the-art statistical model of the collision-perturbed molecular lineshapes and we obtain all the parameters for this model from quantum scattering calculations with use of the highly accurate *ab initio* potential energy surface.