

ACCURATE EXPERIMENTAL VALIDATION OF AB INITIO QUANTUM SCATTERING CALCULATIONS USING THE SPECTRA OF He-PERTURBED H₂

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Due to its simplicity, molecular hydrogen perturbed by helium atom constitutes a great benchmark system for tests of *ab initio* quantum scattering calculations as a method of precise description of collisional effects in ultra-accurate experimental spectra. Here we present our recent cavity-enhanced measurements of H₂ lines perturbed by He. Our results exhibit an unprecedented subpercent agreement with fully quantum *ab initio* calculations. We investigate collisional line-shape effects that are present in highly accurate experimental spectra of the 3-0 S(1) and 2-0 Q(1) lines. We clearly distinguish the influence of six different collisional effects (i.e.: collisional broadening and shift, their speed dependences and the complex Dicke effect) on the shapes of H₂ lines. We demonstrate that if any of the six contributions is neglected, then the experiment-theory comparison deteriorates at least several times. We also analyze the influence of the centrifugal distortion on our *ab initio* calculations and we demonstrate that the inclusion of this effect slightly improves the agreement with the experimental spectra.

In addition, we describe the theoretical calculations that were performed to obtain the subpercent agreement with experiment. In the analysis described here, we employed the state-of-the-art statistical model of the collision-perturbed shape of molecular lines. We obtained all the parameters of this model from quantum scattering calculations, and the dynamical calculations were performed on the most accurate potential energy surface (PES) to date.