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Confrontation of the molecular hydrogen spectra in the presence of noble gases with *ab initio* calculation

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Hydrogen molecule in its ground electronic state perturbed by the helium atom constitutes the simplest system of molecule perturbed by atom. This gives possibility to make a link between the experiment and the theory from the first principles. allowing to use *ab initio* calculations to make the physical interpretation of the experimental spectra.¹ This also gives an opportunity to thoroughly study collisional line-shape effects on both experimental and theoretical ground.²

We utilize highly accurate cavity ring-down spectroscopy^{1,2} to study the H₂-He collisions and interactions.³ In contrast to most of the previous studies, we do not fit spectra with phenomenological line shapes, but directly superimpose theoretical profiles on the raw experimental spectra without fitting any of the line-shape parameters. Within this approach not only the shapes of experimental lines are reliably reproduced, but also the underlying physics of molecular collisions can be traced. Besides the analysis of the basic line-shape effects (such as relaxation or phase changes of the internal states of the molecule), we also analyse the more sophisticated ones such as speed-dependent effects or velocity-changing collisions (complex Dicke parameter)^{4,5}, which are particularly pronounced for the H_2 -He system.^{3,6,7,8}

According to our knowledge, this is the first comparison of highly accurate experimental spectra with advanced *ab initio* models which includes the speed-dependent effects and velocity-changing collisions. It allows us to study quantum scattering for molecules as well as to validate *ab initio* quantum potentials in ranges very challenging for quantum chemistry methods.

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