HIGH-PRECISION CAVITY-ENHANCED SPECTROSCOPY FOR STUDYING THE H_2-AR COLLISIONS AND INTERACTIONS

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information about molecular collisions is encoded in the shapes of collision-perturbed molecular resonances. This connection between molecular interactions and line shapes is most clearly seen in simple systems such as the molecular hydrogen perturbed by a noble gas atom. We study the H_2-Ar system by means of highly accurate absorption spectroscopy and *ab initio* calculations. On the one hand, we use the cavity-ring-down-spectroscopy technique to record the shapes of the S(1) 3-0 line of molecular hydrogen perturbed by argon. On the other hand, we simulate the shapes of this line using *ab initio* quantum-scattering calculations performed on our accurate H_2-Ar potential energy surface (PES). In order to validate the PES and the methodology of quantum-scattering calculations separately from the model of velocity-changing collisions, we measured the spectra in experimental conditions in which the influence of the latter is relatively minor. In these conditions, our theoretical collision-perturbed line shapes reproduce the raw experimental spectra at the percent level. However, the collisional shift, δ_0, differs from the experimental value by 20%. Compared to other line-shape parameters, collisional shift displays much higher sensitivity to various technical aspects of the computational methodology. We identify the contributors to this large error and find the inaccuracies of the PES to be the dominant factor. With regard to the quantum scattering methodology, we demonstrate that treating the centrifugal distortion in a simple, approximate manner is sufficient to obtain the percent-level accuracy of collisional spectra.

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