ACCURATE CAVITY RING-DOWN SPECTROSCOPY OF D₂ AND COMPARISON WITH AB INITIO CALCULATIONS

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Nowadays highly refined theoretical determinations of rovibrational transition energies of molecular hydrogen can reach the remarkable level of $2 \times 10^{-5}$ cm$^{-1}$.\(^1\) This opens a promising way to test quantum electrodynamics for molecules as well as to study new physics beyond the Standard Model.\(^2\) Nonetheless, these advances are hindered by the difficulty of modeling line shapes of molecular hydrogen due to very pronounced collisional effects.\(^3\)

We present and discuss highly accurate measurements of the quadrupole transitions of the D$_2$ 2 − 0 band. Self-perturbed spectra were collected with a cavity ring-down spectrometer linked to an optical frequency comb referenced to a GPS-disciplined Rb clock.\(^4\) The line-shape analysis was performed using the Hartmann-Tran profile as well as the speed-dependent billiard ball profile. To describe the collisional line-shape effects and mitigate the collisional systematics we performed ab initio quantum scattering calculations obtaining the differences between theoretical and experimental values of the line positions of about 1.5 MHz. The uncertainty of the measured line positions is about 700 kHz, which in the case of the S(3) and S(4) transitions represents a 50-fold improvement compared to the previously available data.\(^5\)

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