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Self-perturbed rovibrational lines in the region of the first overtone of HBr. What I have learned from my mistakes

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The sequence of the spectra of pure HBr at different sub-atmospheric pressure was recorded in the region of the first overtone with a Bruker IFS 120 HR Fourier spectrometer at resolution of 0.003 cm⁻¹. The rovibrational lines of H⁷⁹Br and H⁸¹Br with the same line index *m* were fitted with Voigt profiles simultaneously. This profile was found to describe adequately the experimental lines. The self-broadening and self-shifting coefficients as well as the intensities of the lines were obtained [1]. It was not found the statistically significant difference between both broadening and shifting coefficients for different isotopologues.

The obtained broadening coefficients are in good agreement with literature data, however they have a smaller error, about 1%. It should be noticed that the HITRAN values in P-branch, which are mirroring from R-branch, differ essentially from the experimental ones. To the best of our knowledge, the shifting coefficients [1] were reported for the first time. The intensities of the line are in the reasonable agreement with literature and HITRAN values.

Unfortunately, some methodical errors were made during the experiment. Particular two aperture sizes were used during recording of the different spectra. This led to unexpected results. The influence the aperture size on the spectra and the ways to remedy the described situation are discussed.

Reference:

1. R.E. Asfin, A. Domanskaya, C. Maul, Opt. Spectr. 130, 1 (2022).