NITROGEN BROADENING AND SHIFT COEFFICIENTS IN THE ν_5 AND ν_6 FUNDAMENTAL BANDS OF $^{12}CH_3D$

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A multispectrum nonlinear least-squares fitting technique[a] has been used to determine Lorentz N_2-broadening and pressure-induced shift coefficients for a large number of transitions in the ν_5 and ν_6 fundamental bands of $^{12}CH_3D$ in the region from 1060 to 1640 cm^{-1}. We analyzed a total of 17 high-resolution (0.002 to 0.006 cm^{-1}) room temperature absorption spectra recorded with the Bruker IFS 120 HR at PNNL and the 1-m Fourier transform spectrometer (FTS) at the McMath-Pierce facility of the National Solar Observatory at Kitt Peak. Our multispectrum analysis technique allowed us to simultaneously analyze both self-broadened and N_2-broadened spectra. The data set included 13 spectra of 98% pure CH_3D at pressures of 0.1 to 303 torr in cells with path lengths of 10 to 2486 cm and 4 spectra of lean mixtures ($\approx 1\%$) of CH_3D in research grade nitrogen at total pressures between 100 and 400 torr in a 25 cm cell.

N_2-broadening coefficients for over 800 transitions and shift coefficients for more than 600 transitions in the ν_5 and ν_6 bands were determined. Transitions with rotational quantum numbers up to $J'' = 15$ and $K'' = 14$ were analyzed. N_2-broadening coefficients were measured in all six ν_6 sub-bands (^PP, ^PQ, ^PR, ^RP, ^RQ and ^RR). The measured broadening coefficients vary from about 0.02 to 0.09 cm^{-1} atm^{-1} at 296K. Most of the measured pressure-shift coefficients are negative with values extending from about -0.014 to +0.005 cm^{-1} atm^{-1}. Very few of the measured shift coefficients are positive, and the positive shifts are mostly associated with the $J'' = K''$ transitions in the ^PQ sub-bands. $J'' = K''$ transitions are also associated with the smallest broadening coefficients in both the ν_5 and ν_6 bands.

[a] D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Atkins, *JQSRT* **53**, 705-721 (1995).