AIR-BROADENING AND SHIFT COEFFICIENTS AND LINE MIXING IN THE ν_3 BAND OF $^{12}CH_3D$

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A multispectrum nonlinear least squares fitting technique[a] has been used to determine Lorentz air-broadening coefficients and air-induced shift coefficients for transitions in the ν_3 fundamental band of $^{12}CH_3D$ in the spectral region between 1154 and 1430 cm^{-1}. Eleven high-resolution (0.005 cm^{-1}) room-temperature absorption spectra, recorded using the 1-m Fourier transform spectrometer (FTS) at the McMath-Pierce facility of the National Solar Observatory at Kitt Peak, were simultaneously analyzed. The data set included both low-pressure (1 to 3 Torr) spectra of 98% pure CH_3D and spectra of lean mixtures ($\approx 1\%$) of CH_3D in dry air at total pressures from about 100 Torr to 400 Torr. Cell path lengths of 25 and 150 cm were used.
Air-broadening coefficients were determined for for more than 360 ν_3 transitions with rotational quantum numbers as high as $J'' = 17$ and $K'' = 17$. Air-induced shift coefficients were also determined for most of these transitions. The measured broadening coefficients range from 0.016 to 0.073 cm^{-1} atm^{-1} at 296K, and the shift coefficients range vary from about -0.0086 to +0.0058 cm^{-1} atm^{-1}. The majority of the shifts are negative, and the positive shifts often involve transitions with $J'' = K''$. The ^{Q}Q sub-band $J'' = K''$ transitions are also associated with the smallest broadening coefficients. Weak line mixing effects have been observed in a few high-J transitions with $K'' = 3$, and we have determined off-diagonal relaxation matrix element coefficients for several $A^+A^-(A1A2)$ split components. At low to medium values of J'', the A^+A^- splittings are very small, and the two components are practically unresolved. Variations of the measured parameters with rotational quantum numbers and differences between the A and E symmetry species will be discussed. We will also compare our measurements with the values on the current HITRAN compilation[b] and with other available measurements.

[a] D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Atkins, *JQSRT* **53**, 705-721 (1995).
[b] L. S. Rothman *et al.*, *JQSRT* **53**, 665-710 (1998).