MEASUREMENTS OF AIR-BROADENING AND PRESSURE-SHIFT COEFFICIENTS AND LINE MIXING IN THE ν_6 FUNDAMENTAL BAND OF $^{12}CH_3D$

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A multispectrum nonlinear least-squares spectral fitting technique[a] has been used to measure air-broadening and air induced pressure-shift coefficients for more than 670 transitions in the ν_6 fundamental band of $^{12}CH_3D$ in the 1040 and 1410 cm^{-1} spectral region. Additionally, line mixing effects were observed and values for off diagonal relaxation matrix coefficients were determined for the first time in several of the $K'' = 3$, A^+A^- split components in the ^PP, ^PQ, ^PR, ^RP, ^RQ, and ^RR sub-band transitions. These results were obtained from simultaneous analysis of 11 room temperature laboratory absorption spectra recorded with the McMath-Pierce Fourier transform spectrometer at the National Solar Observatory on Kitt Peak, Arizona. Low-pressure (1 to 3 torr) spectra of 98% pure CH_3D and lean mixtures ($\approx 1\%$) of CH_3D in dry air (100 to 400 torr) in 25 and 150 cm pathlength absorption cells were used in the analysis. Measurements involved transitions with quantum numbers as high as $J'' = 17$ and $K'' = 15$ and also included 34 transitions with $2 \leq \Delta K \leq 4$. The air-broadening coefficients range between 0.016 and 0.076 cm^{-1} atm^{-1} at 296K and the pressure-shift coefficients vary from about -0.012 to +0.008 cm^{-1} atm^{-1}. For each J series in the ^PP and ^RR sub-bands, the $J'' = K''$ (or the $J' = K'$) transition exhibited the smallest broadening coefficient. In the ^PQ sub-band, $J'' = K''$ transition in each J series had the largest negative pressure-shift coefficient while the $J' = K'$ transition lines in the ^RQ sub-band showed the largest positive pressure-shift coefficients. These and several other interesting patterns observed during the analysis will be discussed. The results will be compared to previous measurements and to other values reported in the literature.

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