MULTISPECTRUM ANALYSIS OF THE ν_1 BAND OF HCN: INTENSITIES, BROADENING AND SHIFT COEFFICIENTS

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Infrared spectra of HCN in the 3200−3400 cm^{-1} region have been recorded at 0.008 and 0.005 cm^{-1} resolution using two different Fourier transform spectrometers (FTS), the McMath-Pierce FTS at the National Solar Observatory on Kitt Peak and the Bruker IFS 120 HR FTS at the Pacific Northwest National Laboratory. Spectra were recorded with pure HCN at room temperature as well as mixtures of HCN in N_2 or HCN in air at temperatures from $+26°$C to $-60°$C.

Using our multispectrum technique,[a] we fit up to 27 spectra simultaneously to determine positions, absolute intensities, self-broadening and self-shift coefficients at room temperature for lines belonging to the $H^{12}C^{14}N$ ν_1 band centered near 3311 cm^{-1}. In addition, we were able to determine intensities, self-broadening and self-shift coefficients for some lines of the $\nu_1 + \nu_2^1 - \nu_2^1$ hot band and several line intensities for $H^{13}C^{14}N$ and $H^{12}C^{15}N$. The measured line intensities in the ν_1 band of the main isotope were further analyzed to derive the vibrational band intensity and Herman-Wallis coefficients.[b]

Parameters for broadening and shifts by N_2, along with their temperature-dependences, were determined from simultaneous fits to 27 spectra, and we fit 22 spectra simultaneously to obtain the air-broadening and shift parameters. We were able to determine these parameters for both broadening gases for transitions of the ν_1 band of $H^{12}C^{14}N$ with assignments between P(29) and R(28).[c] Differences between our results, previous measurements, and the parameters in the current HITRAN database[d] will be quantified and discussed.

[a] D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith and D. Atkins, *JQSRT* **53**, 705-721 (1995).
[b] V. Malathy Devi et al., *JQSRT*, in press (2003).
[c] C. P. Rinsland et al., *JQSRT*, in press (2003).
[d] L. S. Rothman et al., *JQSRT*, in press (2003).