BROADENING AND SHIFT COEFFICIENTS IN THE 3-μm BANDS OF HCN

M. A. H. SMITH, C. P. RINSLAND, *Atmospheric Sciences, NASA Langley Research Center, Mail Stop 401A, Hampton, VA 23681-2199*; V. MALATHY DEVI, D. CHRIS BENNER, *Department of Physics, The College of William and Mary, Box 8795, Williamsburg, VA 23187-8795*; and M. DULICK, *National Solar Observatory, P. O. Box 26732, Tucson, AZ 85726-6732*.

While there have been a number of recent studies of room-temperature N_2-broadening of spectral lines in various molecular bands of HCN, the corresponding pressure-induced line shifts have not been measured. Only three limited studies of the temperature-dependence of N_2-broadening in HCN have been reported, and air- and O_2-broadening have been examined only at room temperature for single $HC^{15}N$ rotational line.[a] We have recorded over 80 new infrared spectra of HCN broadened by N_2, O_2, or air at room temperature and low temperatures using a 50-cm coolable cell with the McMath-Pierce Fourier transform spectrometer (FTS) of the National Solar Observatory on Kitt Peak, Arizona. Most of these spectra cover bandpasses of either 2750-3950 cm^{-1} at 0.008 cm^{-1} resolution or 600-3000 cm^{-1} at 0.005 cm^{-1} resolution. Volume mixing ratios of HCN in the broadening gases were 0.1% or less, and total sample pressures ranged from 12 Torr to over 500 Torr. Most spectra were recorded at temperatures from room temperature down to near the freezing point of HCN (-13°C), and some spectra were successfully recorded at temperatures down to about -60°C. Several spectra of low pressures (about 0.1 Torr) of purified HCN were also recorded to provide line positions unaffected by pressure-induced shifts. An initial group of 19 of these absorption spectra have been analyzed simultaneously using our multispectrum nonlinear least-squares technique[b] to determine N_2-broadening and shift coefficients and their temperature dependences for transitions up to $J'' = 30$ in the ν_1 fundamental band of $H^{12}C^{14}N$. The results for N_2-broadening compare well with available values reported in the literature. In particular, the N_2-broadening temperature-dependence exponent n shows a quantum-number dependence similar to that observed in the ν_2 band by Schmidt et al.[c] Analysis of air-broadening and shifts in the ν_1 band is in progress, as well as work on the ν_2 and $2\nu_2$ band systems.

[a] J.-M. Colmont, *J. Mol. Spectrosc.* **114**, 298-304 (1985).
[b] D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith and D. Atkins, *JQSRT* **53**, 705-721 (1995).
[c] C. Schmidt, J.-C. Populaire, J. Walrand, G. Blanquet and J.-P. Bouanich, *J. Mol. Spectrosc.* **158**, 423-432 (1993).