THE ν_3 BAND OF NO_2: ANALYSIS TECHNIQUE

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In the next paper results will be presented for an analysis of the ν_3 band of $^{14}N^{16}O_2$. The rovibrational spectrum of NO_2 contains numerous doublets, most of them very closely spaced. Most of the doublets were unresolved at the resolution of the FTS spectra used for their measurement, and an even greater number were unresolved in broadened spectra. Many of the doublets are separated by amounts comparable to the Doppler width at room temperature and at atmospheric temperatures, so the unresolved area of the absorption of the doublet is highly dependent upon the separation of the lines.

The positions of the closely spaced lines of a doublet are very unstable in the multispectrum least squares solution[a] due to the strongly nonlinear derivatives of the calculated spectrum with respect to the line positions. By means of constraints[b] the problem was reformulated to one of solving for the mean of the two positions and the separation of the lines. While the mean position is generally very well determined, the separation is highly correlated with the intensities of the lines. Thus, in most cases it is necessary to constrain the ratio of the intensities of the two lines to be the ratio of their HITRAN intensities. The air-broadened Lorentz halfwidths of the two lines are constrained to be equal since they cannot usually be determined separately. Likewise, the air pressure-induced line shift and the temperature dependences of the halfwidths and shifts were also constrained to be the same for the two lines. In some cases the two lines were separated well enough to test these assumptions. The assumptions in these cases were generally quite good, but there are cases in which they are not.[c]

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

[b] D. Chris Benner, this symposium

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