

ANALYSIS OF A/C-TYPE AND B-TYPE BANDS IN THE HIGH-RESOLUTION INFRARED SPECTRA OF 1,1,2,2-TETRAFLUOROETHANE RECORDED AT -100°C .

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The high-resolution (0.002 cm^{-1}) infrared spectrum of 1,1,2,2-tetrafluoroethane was recorded on the Bruker IFS120HR spectrometer at Giessen in a 3-m cell cooled to -100°C . At this temperature only the anti rotamer makes a significant contribution to the spectrum. The two antisymmetric CF stretching modes in the 1135-cm^{-1} region have sufficient intensity to be observable. Our analysis of the A-type and C-type bands centered at 1127.434 cm^{-1} built on the jet-cooled, diode-laser experiments of the NIST/BNL groups.^a The analysis of the B-type band centered at 1144.339 cm^{-1} is completely new. Ground state (GS) rotational constants have been fit to more than 811 ground state combination differences derived from the analysis of both bands. The GS rotational constants for this very asymmetric top ($\kappa = -0.2958$) are (in cm^{-1}) $A = 0.171328(6)$, $B = 0.105003(1)$, and $C = 0.0689585(4)$. Upper state constants were also fit for both bands. This rotational analysis is the first step toward obtaining the complete structure of the anti rotamer from infrared spectra of the d_2 and $^{13}\text{C}_2$ species as well as from the spectrum of the normal species.

^aS. C. Stone, L. A. Philips, G. T. Fraser, F. J. Lovas, L. -H. Xu, and S. W. Sharpe, *J. Mol. Spectrosc.* **192**, 72, (1998).