

## FTIR JET SPECTROSCOPY OF THE FUNDAMENTAL PARALLEL BANDS OF PERFLUOROCYCLOBUTANE IN THE MID-INFRARED

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Rotationally resolved spectra have been obtained for five fundamental bands and associated hot bands for perfluorocyclobutane using a Bruker IFS 120HR Fourier transform infrared spectrometer interrogating a continuous slit jet expansion of a 10%  $c\text{-C}_4\text{F}_8$ -in-helium mixture. The rotational temperature of the expansion is approximately 10 K. The ring of perfluorocyclobutane is slightly puckered and the molecule has  $D_{2d}$  symmetry. The  $B_2$  parallel bands at 1240.3 and 1292.6  $\text{cm}^{-1}$  correspond to  $\text{CF}_2$  stretches and have been assigned and fit with a rigid rotor, symmetric top Hamiltonian. The fundamental band at 1292.6  $\text{cm}^{-1}$  has the following fit constants:  $\nu_0 = 1292.56039(3) \text{ cm}^{-1}$ ,  $B' = 0.0354142(4) \text{ cm}^{-1}$ , and  $B'' = 0.0354367(4) \text{ cm}^{-1}$ . The band at 1240.3  $\text{cm}^{-1}$  correlates with an  $B_{1g}$  symmetry mode in planar  $c\text{-C}_4\text{F}_8$  and consequently has IR allowed transitions from the excited ring puckering states. Indeed, we observe that the transitions in this band are split into strong and weak components corresponding to transitions from the ground and first excited ring puckering states, respectively. The stronger component has the following fit constants:  $\nu_0 = 1240.34858(4) \text{ cm}^{-1}$ ,  $B' = 0.0354192(7) \text{ cm}^{-1}$ , and  $B'' = 0.0354356(7) \text{ cm}^{-1}$ ; and for the weaker component  $\nu_0 = 1240.34674(5) \text{ cm}^{-1}$ ,  $B' = 0.0354188(9) \text{ cm}^{-1}$ , and  $B'' = 0.0354360(9) \text{ cm}^{-1}$ . No  $K$  structure was observed in any of the parallel bands and attempts to fit distortion constants to these bands were unsuccessful. Rotationally resolved bands were also observed at 964.3  $\text{cm}^{-1}$  ( $E$ ), 1223.5  $\text{cm}^{-1}$  ( $B_2$ ), and 1343.2  $\text{cm}^{-1}$  ( $E$ ).