

ROTATIONAL ANALYSIS OF BANDS IN THE HIGH-RESOLUTION INFRARED SPECTRA OF *trans,trans*- AND *cis,cis*-1,4-DIFLUOROBUTADIENE-2-*d*<sub>1</sub>

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Ground state rotational constants for a series of isotopomers are being sought for use in determining the semi-experimental equilibrium structures of the isomers of 1,4-difluorobutadiene. Because fluorine substitution has a large influence on CC bond lengths in C<sub>3</sub> and C<sub>4</sub> rings, we asked how fluorine substitution affects butadiene. *trans,trans*- and *cis,cis*-1,4-Difluorobutadiene-2-*d*<sub>1</sub> have been synthesized, and high-resolution (0.0013 cm<sup>-1</sup>) infrared spectra have been recorded for these nonpolar species. Analysis of the rotational structure in several bands is reported. For the *trans,trans* isomer, the C-type band at 709.0 cm<sup>-1</sup> for  $\nu_{21}(a'')$  has been fully analyzed, and the C-type band at 914.3 cm<sup>-1</sup> for  $\nu_{18}(a'')$  has been partially analyzed. Interfering with the analysis of the second band is overlap of its R branch with the P branch of the A/B-type band for  $\nu_{13}(a')$  at 933 cm<sup>-1</sup>. For the *cis,cis* isomer, as much as possible of the C-type band ( $K'_a = 10$  to 34) for  $\nu_{20}(a'')$  at 775.4 cm<sup>-1</sup> has been analyzed. An A-type band for  $\nu_{13}(a')$  at 865.8 cm<sup>-1</sup> has also been analyzed into the band center. Small inertial defects confirm that these molecules are planar. Ground state rotational constants are reported for both isomers in comparison with those for the normal species.<sup>a</sup>

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<sup>a</sup>N. C. Craig, M. C. Moore, C. F. Neese, D. C. Oertel, L. Pedraza, and T. Masiello, *J. Mol. Spectrosc.* 254, 39-46 (2009).