

ANALYSIS OF THE ROTATIONAL STRUCTURE IN SEVERAL BANDS IN THE HIGH-RESOLUTION INFRARED SPECTRA OF BUTADIENE-*TRANS,TRANS*-1,4-*d*₂ AND -*CIS,CIS*-1,4-*d*₂.

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Butadiene-*trans,trans*-1,4-*d*₂ and -*cis,cis*-1,4-*d*₂ were prepared from *trans,trans*-1,4-dichlorobutadiene. Gas-phase spectra were recorded at 0.002 cm⁻¹ resolution in the mid-infrared region on a Bruker IFS 120HR FT spectrometer at PNNL. For the *trans,trans* isotopomer the C-type band at 1002.553 cm⁻¹, which was not perturbed near the band center, was more fully analyzed than another C-type band at 825.5 cm⁻¹, which was extensively perturbed. Ground state rotational constants for this near-symmetric top ($\kappa = -0.9810$) were fit to 1828 ground state combination differences (GSCDs) derived from the two bands. *A*, *B* and *C* rotational constants for the ground state are 1.3397796(7), 0.1306985(2), and 0.1191086(3) cm⁻¹, respectively. For the *cis,cis* isotopomer the C-type band at 808.367 cm⁻¹ was analyzed. Fitting 1559 GSCDs gave $\kappa = -0.9707$ and 1.1398737(6), 0.1380156(3), and 0.1231302(3) cm⁻¹ for *A*, *B* and *C*, respectively. These rotational constants along with those of other deuterium and ¹³C isotopomers will be used to determine a complete equilibrium rotational structure of butadiene.