

PRELIMINARY ANALYSIS OF A C-TYPE BAND IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF *EE*-1,4-DIFLUOROBUTADIENE

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As part of a study of nonpolar molecules that exhibit surprising energy relationships among isomers, a C-type band in the infrared spectrum of the *EE* (*trans-trans*) isomer of 1,4-difluorobutadiene is being investigated. This band, centered at 934 cm^{-1} , is due to CH out-of-plane flapping. Although the band structure contains evidence of substantial perturbations, the rotational structure at 0.002 cm^{-1} resolution appears to be fully assignable. Preliminary rotational constants for the ground state are $A = 1.0507499$ (14), $B = 0.0389603$ (47), and $C = 0.0375881$ (40) cm^{-1} for this near-prolate symmetric top with $\kappa = -0.99729$. A synthetic method has been found to make the deuterated isotopomers needed for the complete structural analysis of the isomers of 1,4-difluorobutadiene.