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 \(A = 1.0507499 \pm 0.0000014\), \(B = 0.0389603 \pm 0.0000047\), and \(C = 0.0375881 \pm 0.0000040\) 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.