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

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A high-resolution (0.0018 cm^{-1}) infrared spectrum has been recorded for the C-type band (a_u) for CH out-of-plane flapping at 934 cm^{-1} of *trans,trans*-1,4-difluorobutadiene (ttDFBD). Considerable progress has been made in analyzing the rotational structure of this band despite hot band structure and numerous perturbations. Assigned series extend from K_a" of 4 to 28 in the R branch and K_a" = 6 to 30 in the P branch. Pertubations due to Coriolis coupling occur for K_a' = 4, 11, 16, 24, and 28, for which perturbing states are suggested. More than 1150 ground state combination differences have been fitted to a Watson-type Hamiltonian to give A = 1.0507503(7), B = 0.0389679(5), and C = 0.0375835(4) cm^{-1} for the ground state of this near-prolate top, which has κ = -0.9973. The goal is to obtain a structure for ttDFBD as part of a study of the three isomers of DFBD, in which the cis effect is observed.