HIGH-RESOLUTION INFRARED SPECTRA OF BICYCLO[1.1.1]PENTANE: ANALYSES OF THE ν_{14}(e') AND $\nu_{18}(a_2")$ BANDS

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Infrared spectra of the ν_{14}(e') 540 cm^{-1} and $\nu_{18}(a_2")$ 835 cm^{-1} bands of bicyclo[1.1.1]pentane have been recorded at a resolution sufficient (0.0015 cm^{-1}) to resolve for the first time individual rovibrational lines. This report presents the ground state constants for this molecule determined from two of the ten infrared-active fundamental bands. The fitted transitions were judged to be free of perturbations of their upper state levels. A combined total of more than 6000 lines with J and K quantum numbers of the two bands ranging up to about 60 were fit with an obs-calc RMS deviation of 0.00021 cm^{-1}. The following principal constants (in units of cm^{-1}) of the rovibrational ground state were obtained: B_0 = 0.23994136(30), D_J = 5.9959(96)x10^{-8}, and D_{JK} = -1.5052(98)x10^{-8}. The band centers were found to be ν_{14} = 540.326397(19) cm^{-1} and ν_{18} = 832.92902(3) cm^{-1}. The values in parentheses represent the uncertainties (2 standard deviations) in the last digits of the value of the constants. The results are compared with those obtained for [1.1.1]propellane and with those computed at the ab initio anharmonic level using the B3LYP density functional method with a cc-pVTZ basis set.