HIGH RESOLUTION INFRARED SPECTRA OF SPIROPENTANE, (C_5H_8)

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Infrared spectra of spiropentane have been recorded at a resolution (0.002 cm^{-1}) sufficient to resolve for the first time individual rovibrational lines. This initial report presents the ground state constants for this molecule determined from the detailed analysis of the ν_{16} (b_2) parallel band at 993 cm^{-1}. In addition, the determination included more than 2000 ground state combination-differences deduced from partial analyses of four other infrared-allowed bands, the $\nu_{24}(e)$ perpendicular band at 780 cm^{-1}, and three (b_2) parallel bands at 1540 cm^{-1}(ν_{14}), 1568 cm^{-1}(ν_5+ν_{16}), and 2098 cm^{-1}(ν_5+ν_{14}). In each of the latter four cases, the spectra show complications; in the case of ν_{24} due to rotational l-type doublings and in the case of the parallel bands, perturbations due to Fermi resonance and Coriolis interactions of the upper states with nearby levels. The unraveling of these is underway but the assignment of many of these transitions permits the confident use of ground state combination-differences in determining the following constants for the ground state (in units of cm^{-1}) B_0 = 0.13947360(2), $D_J = 2.458(1) \times 10^{-8}$, and $D_{JK} = 8.30(3) \times 10^{-8}$. For the unperturbed ν_{16} fundamental, more than 3000 transitions were fit and the band origin was found to be at 992.53792(3) cm^{-1}. The numbers in parentheses are the uncertainties (two standard deviations) in the values of the constants. The results are compared with those computed at the ab initio anharmonic level using the B3LYP density functional method with a cc-pTVZ basis set.