A COMPLETE STRUCTURE OF *TRANS*-3,4-DIFLUOROCYCLOBUTENE FROM MICROWAVE SPECTROSCOPY

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Microwave spectra have been observed in the 6-17-GHz region for $trans$-3,4-difluorocyclobutene, two $^{13}C_1$ modifications, two d_1 modifications, and the perdeutero species. Watson-type Hamiltonians have been fit with a full set of quartic centrifugal distortion constants for all species except for the d_4 species. Rotational constants for the normal species in MHz are A = 5664.02410(29), B = 3366.07000(19), and C = 2345.58058(16). Complete structures fit with an r_s/r_0 treatment and an r_0 treatment are in satisfactory agreement. Preferred r_s/r_0 results with Costain uncertainties in parentheses are 1.349(4) $\AA$ for the C=C bond, 1.503(9) $\AA$ for the contiguous C-C bonds, 1.534(4) $\AA$ for the unique C-C bond, 1.398(6) $\AA$ for the C-F bond, 1.081(3) $\AA$ for the =C-H bond, and 1.102(5) $\AA$ for the -C-H bond. Consistent with C_2 symmetry, the ring is slightly puckered. Compared with cyclobutene, the C=C bond is slightly longer and the C-C bonds are shorter, adjustments which are familiar consequences of fluorine substitution on small rings.