

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

NORMAN C. CRAIG, LEWIS V. MCCARTY, PETER T. LINGENFELTER, A. SONAN OSMANI, and OSMAN RATHORE, *Department of Chemistry, Oberlin College, Oberlin, OH 44074*; MICHAEL J. TUBERGEN, *Department of Chemistry, Kent State University, Kent, OH 44242.*; ROBERT L. KUCZKOWSKI, *Department of Chemistry, University of Michigan, Ann Arbor, MI 48109.*

Microwave spectra have been observed in the 6-17-GHz region for *trans*-3,4-difluorocyclobutene, two $^{13}\text{C}_1$ 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) Å for the C=C bond, 1.503(9) Å for the contiguous C-C bonds, 1.534(4) Å for the unique C-C bond, 1.398(6) Å for the C-F bond, 1.081(3) Å for the =C-H bond, and 1.102(5) Å 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.