MICROWAVE INVESTIGATION OF $CIS, TRANS$-1,4-DIFLUOROBUTADIENE AND A PARTIAL STRUCTURE FOR THIS MOLECULE

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The cis,trans isomer of 1,4-difluorobutadiene has been investigated with a pulsed-beam, Fourier transform microwave spectrometer in the spectral range of 5-17 GHz. This molecule is a near-symmetric top with κ = -0.9744. Sufficient *b*-type and *a*-type transitions for the parent species have been observed to fit a Watson-type Hamiltonian with A = 12,982.1, B = 1467.82, and C = 1318.64 MHz. From a Stark-effect study of three transitions of the parent, the two components of the dipole moment have been determined as μ_b = 2.213 (5) D and μ_a = 0.660 (4) D. Fewer transitions have been observed for each of the four different ^{13}C isotopomers in natural abundance. Fitting Hamiltonians for the ^{13}C isotopomers has required the transfer of some centrifugal distortion constants from the parent. Cartesian coordinates and geometric parameters for the carbon-atom backbone have been found by the substitution method. All the bond angles and bond lengths differ in this planar molecule. Thus, its complete structure is an eighteen-parameter problem. Partially deuterated material has been prepared by isotopic exchange in basic D_2O. From a study of this mixture a full structure should be determinable.