A COMPLETE STRUCTURE FOR *CIS,TRANS*-1,4-DIFLUOROBUTADIENE FROM MICROWAVE SPECTROSCOPY

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Microwave spectra have been observed for cis, $trans$-1,4-difluorobutadiene, for the four ^{13}C isotopomers in natural abundance, and for five deuterium isotopomers in a mixture prepared by partial exchange in NaOD/D_2O. Watson-type Hamiltonians have been fitted to the a-type and b-type transitions observed for each species. For the normal species, which is a near prolate top, A = 12988.3327(11), B = 1467.8791(3), and C = 1318.5845(3) MHz. From Stark effect measurements, the dipole moment components are μ_a = 0.660(4) D and μ_b = 2.213(5) D. A Kraitchman substitution analysis succeeds for the carbon atom backbone and for the hydrogen atoms on the end carbon atoms but does not for the interior hydrogen atoms. Most notably, I_b' for the 2-d_1 species is smaller than I_b for the normal species. To obtain a complete structure, results of DFT calculations with the adiabatic connection method were used for the bond lengths and bond angles of the interior C-H bonds. Otherwise the agreement of experiment and theory is good.