

COMPLETE ASSIGNMENT OF THE VIBRATIONAL FUNDAMENTALS OF ZZ-1,4-DIFLUOROBUTADIENE.

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From infrared and Raman spectra a complete assignment was proposed for the 24 vibrational fundamentals of the ZZ (*cis-cis*) isomer of 1,4-difluorobutadiene, which is a centrosymmetric molecule of C_{2h} symmetry. A few adjustments in this initial assignment were made on the basis of ab initio predictions of all the frequencies and the intensities in the infrared spectrum. The experimental assignments in cm^{-1} are: (a_g : R, pol; IR, -) 3088, 3047, 1676, 1410, 1247, 1133, 946, 750, 232; (a_u : R, -; IR, C-type bands) 914, 762, 330, 78; (b_g : R, dpol; IR, -) 897, 789, 559; (b_u : R, -; IR, A/B-type bands) 3109, 3042, 1624, 1340, 1215, 1044, 649, 165. These experimental values will be compared with the ab initio predictions, which were based on the hybrid density-functional theory/Hartree-Fock Adiabatic Connection Method (ACM) with use of a TZ2P basis set.