

INFRARED AND RAMAN SPECTRA OF *ZE*-1,4-DIFLUOROBUTADIENE

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Gas-phase infrared and liquid-phase Raman spectra have been recorded for the *ZE* (*cis*, *trans*) isomer of 1,4-difluorobutadiene. Based on these spectra and unscaled calculations made by the hybrid Hartree-Fock/density-functional theory adiabatic connection method, a complete assignment of vibrational fundamentals is proposed. For this molecule of C_8 symmetry, the fundamentals are (in cm^{-1}): (a' : R, pol; IR, A/B-type bands) 3114, 3082, 3062, 3036, 1690, 1629, 1391, 1313, 1253, 1224, 1138, 1129, 1008, 706, 504, 308, 138; (a'' : R, dpol; IR, C-type bands) 929, 887, 824, 758, 526 (calc.), 230, 155. The interplay between calculated frequencies and infrared intensities and experiment is emphasized in making this assignment and the previously reported assignments for the *trans,trans* and *cis,cis* isomers. These three isomers illustrate the *cis* effect in which the most electronically crowded *cis,cis* isomer has the lowest electronic energy. For all three isomers the *s-trans* rotamer is dominant.