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_s 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.