

EQUILIBRIUM STRUCTURES FOR THE *CIS* and *TRANS* ISOMERS OF 1,2-DIFLUOROETHYLENE AND THE *CIS,TRANS* ISOMER OF 1,4-DIFLUOROBUTADIENE

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Microwave spectra for seven isotopomers of *cis*-1,2-difluoroethylene have been reinvestigated and extended with the pulsed-molecular-beam Fourier-transform method. Rotational Hamiltonians that include a full set of quartic centrifugal distortion constants have been fit for each isotopomer. Ground state rotational constants for the *trans* isomer were available from an investigation of the high-resolution infrared spectra of several isotopomers. Equilibrium rotational constants have been extracted for the *cis* and *trans* isomers from the experimental ground state constants and the vibration-rotation constants computed at the MP2/6-31G(d) level. Equilibrium structures have been fit to the equilibrium principal moments of inertia for both isotopomers, and isomeric differences in the bond lengths and bond angles are interpreted in terms of the strong influence of fluorine substitution. For *cis,trans*-1,4-difluorobutadiene a similar derivation of the equilibrium structure has been achieved through the combination of published microwave data and quantum chemical calculations. This substance provides an opportunity to examine the influence of *cis* and *trans* fluorine substitution within a single molecule.