MICROWAVE SPECTRA AND MOLECULAR STRUCTURES OF THE GAS-PHASE HOMOCHIRAL HOMODIMERS OF 3,3-DIFLUORO-1,2-EPOXYPROPANE AND 3-FLUORO-1,2-EPOXYPROPANE

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Density functional theory is used to examine the possible conformations of both homochiral (RR or SS) and heterochiral (RS or SR) homodimers of 3,3-difluoro-1,2-epoxypropane and 3-fluoro-1,2-epoxypropane as a guide in the search for their microwave spectra. Similar to the analogous homodimers of 3,3,3-trifluoro-1,2-epoxypropane, the lowest energy heterochiral dimers of these species contain an inversion center and are microwave silent. However, spectra are obtained for the lowest energy conformers of the homochiral dimers. Analysis of the spectra confirms the theoretically predicted geometries.