

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE 1,1-DIFLUOROETHYLENE–HF COMPLEX

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The rotational spectra of six isotopomers of 1,1-difluoroethylene–HF have been collected in the 7 - 22 GHz region with a Fourier transform microwave spectrometer. These include the most abundant isotopomer, its DF counterpart, and four singly substituted ^{13}C species in natural abundance. Both *a*- and *b*-type transitions have been observed for all species. In addition, the hydrogen-fluorine spin-spin coupling interaction in the HF subunit for $\text{CH}_2\text{CF}_2\text{--HF}$ and the deuterium nuclear quadrupole coupling interaction in $\text{CH}_2\text{CF}_2\text{--DF}$ have been observed and analyzed. The rotational constants are consistent with a planar complex, with the two subunits interacting through a hydrogen bond formed between the H atom of HF and an F atom in 1,1-difluoroethylene and via a secondary interaction between the F atom in HF and the H atom located *cis* to the hydrogen-bonded F atom in 1,1-difluoroethylene. The rotational constants, hyperfine coupling constants, and results from the analogous complex, $\text{CH}_2\text{CF}_2\text{--HCCH}$,^a are combined to determine the structural parameters of 1,1-difluoroethylene–HF and 1,1-difluoroethylene–DF, which are found to be slightly different.

^aH. O. Leung and M. D. Marshall, *J. Chem. Phys.* 125, 154301 (2006).