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

MARK D. MARSHALL, HELEN O. LEUNG, TASHA L. DRAKE, TADEUSZ PUDLIK, NAZIR SAVJI, and DANIEL W. McCUNE, *Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000*.

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 CH_2CF_2–HF and the deuterium nuclear quadrupole coupling interaction in CH_2CF_2–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, CH_2CF_2–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.

[a] H. O. Leung and M. D. Marshall, J. Chem. Phys. 125, 154301 (2006).