

## DETERMINING THE GROUND STATE GEOMETRY OF THE (*E*)-1-CHLORO-1,2-DIFLUOROETHYLENE–HYDROGEN FLUORIDE COMPLEX USING MICROWAVE SPECTROSCOPY

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To better understand the effects of chlorine substitution on the intermolecular interactions between fluorinated ethylenes and linear, protic acids, the structure of the (*E*)-1-chloro-1,2-difluoroethylene–hydrogen fluoride complex has been investigated via *ab initio* calculations and microwave spectroscopy. It was necessary first to determine an improved experimental structure of (*E*)-1-chloro-1,2-difluoroethylene itself, and the rotational spectra of four isotopologues of this monomer have been obtained in the 6-21 GHz range using Fourier transform microwave spectroscopy for this purpose. *Ab initio* calculations for the van der Waals complex with hydrogen fluoride, performed at the MP2 level of theory, predict that the lowest energy conformation is similar to that observed for the trifluoroethylene–HF dimer.<sup>a</sup> Based on these predictions, rotational spectra of three isotopologues of the (*E*)-1-chloro-1,2-difluoroethylene–hydrogen fluoride complex spanning 7-19 GHz are collected. Rotational constants, centrifugal distortion constants, and chlorine quadrupole coupling constants are determined using a least-squares fitting program. The data obtained so far are consistent with a planar ground-state structure in which the HF molecule binds to the side of the substituted ethylene by forming a hydrogen bond to fluorine and a secondary interaction with the geminal hydrogen.

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<sup>a</sup>H.O. Leung and M.D. Marshall, *J. Chem. Phys.* 126, 114310 (2007).