THE MICROWAVE SPECTRUM AND MOLECULAR STRUCTURE OF 2-CHLORO-1,1-DIFLUOROETHYLENE AND PROGRESS TOWARDS ITS COMPLEXES WITH ARGON AND HYDROGEN FLUORIDE

MARK D. MARSHALL, HELEN O. LEUNG, and JASMINA C. CHEUNG-LAU, *Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000*.

Substitution of fluorine for hydrogen in 1,1-difluoroethylene leads to the observation of unexpected, but ultimately understandable, structures for the complexes of 1,1,2-trifluoroethylene with both hydrogen fluoride[a] and acetylene.[b] As a first step towards investigating the effect of chlorine substitution on the same carbon atom, it is necessary to refine the molecular structure of 2-chloro-1,1-difluoroethylene available in the literature.[c] Fourier transform microwave spectra of six isotopomers of 2-chloro-1,1-difluoroethylene are obtained in the 7–21 GHz region. Strong b-type and weaker a-type transitions, which are split by the chlorine nuclear quadrupole hyperfine interaction, are observed. Kraitchman substitution coordinates, fits to the molecular moments of inertia, and *ab initio* results are used to determine bond lengths and angles for the molecule of sufficient quality to be used in determining the structures of its complexes. *Ab initio* calculations on the complexes of 2-chloro-1,1-difluoroethylene with argon and with hydrogen fluoride are used to assist in the analysis of spectra obtained in pulsed jet expansions of mixtures of 2-chloro-1,1-difluoroethylene with hydrogen fluoride in both argon and first run neon.

[a] H. O. Leung and M. D. Marshall, *J. Chem. Phys.* **126,** *in press* (2006).
[b] H. O. Leung, M. D. Marshall, and W. T. Cashion, *61st Ohio State University International Symposium on Molecular Spectroscopy*, RE12 (2006).
[c] D. R. Jenkins, and T. M. Sugden, *Trans. Faraday Soc.* **55,** 1473 (1959); S. Chandra, *J. Phys. Chem.* **71,** 1927 (1967).