ASSIGNMENTS FOR THE VIBRATIONAL FUNDAMENTALS OF THE ROTAMERS OF 1,1,2,2-TETRAFLUOROETHANE-D_2 AND -$^{13}C_2$

NORMAN C. CRAIG, JESSICA I. CHUANG, CHRISTIANA C. NWOFOR, and CATHERINE M. OERTEL,
Department of Chemistry, Oberlin College, Oberlin, OH 44074.

The d_2 and $^{13}C_2$ isotopomers of 1,1,2,2-tetrafluoroethane have been synthesized, and their infrared and Raman spectra have been investigated. An assignment for the normal species has already been proposed.[a] Infrared spectra of the d_2 and $^{13}C_2$ species were recorded in the gas phase and crystal phase; Raman spectra were recorded in the liquid phase and crystal phase. Because only the anti rotamer is present in the crystal phase, complete assignments of vibrational fundamentals for this rotamer of the d_2 and $^{13}C_2$ species are made with confidence from experimental data. At room temperature only about 25% of the gas is the gauche rotamer. Thus, assigning the fundamentals of the gauche rotamers is challenging even with the aid of calculated frequencies and infrared intensities for the normal species.[b]

[a] V. F. Kalasinky, H. V. Anjaria, and T. S. Little, *J. Phys. Chem.* **86**, 1351, (1982).
[b] S. Papasavva, K. H. Illinger, and J. .E. Kenny, *J. Phys. Chem.* **100**, 10100, (1996).