# ANALYSIS OF THE ROTATIONAL STRUCTURE IN TWO BANDS OF THE ANTI ROTAMERS OF 1,1,2,2-TETRAFLUOROETHANE AND ITS $d_2$ ISOTOPOMER IN HIGH-RESOLUTION INFRARED SPECTRA

NORMAN C. CRAIG, CATHERINE M. OERTEL and DAVID C. OERTEL, *Department of Chemistry, Oberlin College, Oberlin, OH 44074*; MICHAEL LOCK, *Physikalisch-Chemisches Institut, Justus Liebig Universität, D-35392 Giessen, Germany*.

Structures of the rotamers of 1,1,2,2-tetrafluoroethane are of interest as part of the study of the gauche effect, in which rotamers of fluorocarbons exhibit surprising energy relationships. The structure of the polar gauche rotamer has been determined in cooperation with the microwave group at NIST. The structure of the nonpolar anti rotamer can be found by analysis of the rotational structure in high-resolution (0.0018 $cm^{-1}$) infrared spectra of the gas phase at $-100°C$. Analyzing this structure is challenging for this rather heavy molecule which is also a very asymmetric top ($\kappa$ = -0.30). For the parent molecule, a good start had been made at NIST and PNL on the analysis of the spectrum of an A/C-type band observed by a jet-cooled-beam, diode-laser technique.[a] We have greatly extended the analysis of this band with the new spectrum and have also analyzed the rotational structure of a B-type band. In the spectrum of the $d_2$ species, we have completed the analysis of the rotational structure of the B-type band and the A-type component of the A/C-type band. The analysis of the B-type bands for both isotopomers includes assignments of oblate series for small $K_c$ values. Rotational constants for the anti rotamer of both isotopomers will be reported.

[a]Stone, S. C.; Philips, L. A.; Fraser, G. T.; Lovas, F. J.; Xu, L. -H.; Sharpe, S. W. *J. Mol. Spectrosc.* **1998**, *192*, 75.