VIBRATIONAL ACTIVITY IN THE S_1-S_0 SPECTROSCOPY OF PARA, META, AND ORTHOFLUOROTOLUENES

TODD STONE, QUAN JU, CHARLES S. PARMENTER, *Department of Chemistry, Indiana University, Bloomington, IN 47405*; AND ZHONG-QUAN ZHAO, *ThermoTrex Corp, 9550 Distribution Ave., San Diego, CA 92121-2306.*

In support of IVR studies involving internal rotation in these fluorotoluenes, we have extended the cold jet S_1-S_0 fluorescence excitation (FE) and single vibronic level fluorescence (SVLF) spectroscopy from the benchmark work of Okuyama, Mikami and Ito[a]. The goal is to characterize the dominant vibrational activity. P-difluorobenzene (pDFB) has been used for comparison. A close correspondence occurs between pDFB and pFT. The main structure in both the zero point level SVLF spectrum and the FE spectrum is assigned with activity in the same three modes. If one does not look too closely, the molecules are twins. Two of these modes also contribute to the dominant vibrational structure in mFT and oFT. Additional dominant activity is also apparent in these molecules, but it comes from only two other modes even though the reduced symmetry allows about two-thirds of the modes to be totally symmetric. Thus the principal S_1-S_0 vibrational activity in these fluorotoluenes have more similarities than differences. On the other hand, an abundance of low intensity vibrational structure makes mFT and oFT spectra appear qualitatively different from those of pFT and pDFB.

[a]K. Okuyama, N. Mikami and M. Ito, *J. Phys. Chem.* **89**, 5617 (1985).