FORBIDDEN TRANSITIONS IN THE VERY RICH PURE ROTATIONAL SPECTRUM OF TRANS-1-IODOPERFLUOROPROPANE

CHRISTOPHER T. DEWBERRY, GARRY S. GRUBBS II, and STEPHEN A. COOKE, *The Department of Chemistry, University of North Texas, P.O. Box 305070, Denton, TX, 76203-5070*.

Using both chirped pulse-, and low frequency cavity-based Fourier transform spectroscopy over 700 transitions have been recorded for the title molecule for the first time. The C_1, C_2 and C_3 carbon-13 species have been observed in natural abundance allowing a substitution structure for the CCC backbone to be determined. Nearly all the transitions observed were either a-type R branches or b-type Q branches. No c-type transitions were observed. The χ_{aa}, χ_{bb}, χ_{cc} and χ_{ab} components of the iodine nuclear quadrupole coupling tensor have been determined. Of note, several forbidden transitions were also observed, such as $J_{k_{-1},k_{+1}}$ F = $14_{4,10}$ 23/2 $\leftarrow$ $12_{5,7}$ 21/2. In this particular case it seems that the upper energy level is nearly degenerate with a level connected to the lower energy level by a μ_a dipole component term, but the lower energy level is also nearly degenerate with a second level connected to the upper energy level, again by a μ_a dipole component term. The two intermediate energy levels are themselves connected by a μ_b dipole component term. Near degeneracies such as these, together with a large χ_{ab} value ($\approx$ 1 GHz) mean that certain $\Delta J = 2$ transitions become allowed. This phenomena has been previously observed for 1-iodopropane by Fujitake and Hayashi (J. Mol. Spect, 127, (1988), 112-124).