

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

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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 C₁, C₂ and C₃ 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 (≈ 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).