EVIDENCE FOR A NON-PLANAR C=(CCC) STRUCTURE IN HEXAFLUOROISOBUTENE AND HEXAFLUOROACETONE IMINE: A PURE ROTATIONAL SPECTROSCOPIC STUDY

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The pure rotational spectra of the parent and all ^{13}C isotopologues of hexafluoroisobutene, $(CF_3)_2C{=}CH_2$, have been recorded using chirped pulse Fourier transform microwave spectroscopy. The spectra observed consist of only b-type transitions all of which are doubled by between $\approx$ 1 MHz to 60 MHz. This doubling phenomena may be rationalized by the assumption that the methylene carbon is slightly out of the plane formed by the remaining carbons, similiar to that observed in methylene cyclobutane[a]. For the parent species 235 transitions have been fitted simultaneously using rotational constants, centrifugal distortion constants, the Coriolis coupling constant F_{ac}, and the vibrational energy spacing ΔE_{01}. The results are compared to those recently obtained for the related species hexafluoroacetone imine, $(CF_3)_2C{=}NH$.

[a] W. Lin, J. A. Gayle, W. C. Pringle, and S. E. Novick *J. Mol. Spectrosc.* **251**, 210-216, 2008.