THE SHAPES OF CHLOROPENTAFLUOROACETONE AND 1,3-DICHLOROTETRAFLUOROACETONE IN THE GAS PHASE

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The pure rotational spectra of the two title molecules have been recorded using a chirped pulse Fourier transform microwave (CP-FTMW) spectrometer and also using a Balle-Flygare FTMW spectrometer. In both cases sufficient resolution was available to determine the full chlorine nuclear electric quadrupole coupling tensor(s). Supporting quantum chemical calculations, coupled with the data available, show that for both molecules the ClCCO dihedral angle is approximately 90^o. The 1,3-dichlorotetrafluoroacetone species possesses a C_2 symmetry axis with the Cl centers on opposite sides of the CCC plane. Spectroscopic parameters and structural parameters will be presented.