

## ROTATIONAL SPECTROSCOPY AND STRUCTURE OF CYCLOPROPYLCHLOROMETHYLDIFLUOROSILANE

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The rotational spectrum of cyclopropylchloromethyldifluorosilane has been investigated in the 5 — 19 GHz region of the electromagnetic spectrum using a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer. The molecule was synthesised by collaborators in the Guirgis group at the College of Charleston. Owing to sample limitations, it was only possible to acquire ~80,000 free induction decays (FIDs), although this was sufficient to yield a spectrum with appreciable signal to noise. As a result, both  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$  isotopologues have been observed, primarily arising from the high relative natural abundances of the Cl isotopes, and their spectra have been assigned. The presence of the Cl nuclei, both with  $I = 3/2$ , leads to transitions splitting into multiple hyperfine components, and thus a good estimation of the nuclear electric quadrupole coupling constants is essential for an accurate assignment. The observation of the Cl isotopologues allows some conclusions to be made pertaining to the electronic and geometric structure of the molecule, and shall be compared to the equilibrium structures obtained from both DFT and *ab initio* methods. Additionally, a conformer arising from a rotation of the chloromethyl group has also been observed.