

ELECTRIC DIPOLE FORBIDDEN, QUADRUPOLE ALLOWED TRANSITIONS IN THE PURE ROTATIONAL SPECTRUM OF CYCLOPROPYLCHLOROMETHYLDIFLUOROSILANE

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Last year¹, we presented the rotational spectrum of cyclopropylchloromethyldifluorosilane (synthesised by the Guirgis group at the College of Charleston, SC) in the 5.0–19.0 GHz region of the electromagnetic spectrum. We noted that the quadrupole coupling tensor for the most populous conformation in the free-jet expansion was unusual, in that the value of χ_{aa} was very close to zero. Upon further analysis, and the subject of this talk, we have observed electric dipole forbidden, quadrupole allowed transitions (including the somewhat enigmatic x -type transition) in the rotational spectra of the ³⁷Cl isotopologue of the most populous conformation in the free-jet expansion, and the parent species of a higher-energy conformation also present in the free-jet expansion. These transitions are highly unusual in chlorine containing species owing to the relatively small quadrupolar moment of chlorine and the (generally) higher rotational constants in chlorine-containing species when compared to brominated or iodated species. We present and discuss pathways through which the zero-order rotational state wavefunctions can be viewed to mix together in order to give rise to these transitions.

¹ A. R. Davies, A. G. Hanna, A. Lutas, G. A. Guirgis and G. S. Grubbs II, TK05 — “*Rotational spectroscopy and structure of cyclopropylchloromethyldifluorosilane*”, International Symposium on Molecular Spectroscopy (ISMS), 2023.