## Nuclear quadrupole coupling and electric dipole forbidden transitions in the spectrum of cyclopropylchloromethyldifluorosilane

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Chemistry Seminar on rotational spectroscopy



## Monday Feb. 19 at 4 pm in 303 Schrenk

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**Abstract**: Rotational spectroscopy is a powerful tool to understand the geometric and electronic nature of molecules as the induced rotations tell us about how the mass is distributed about the so-called principal inertial axes. Like electronic and vibrational spectroscopy, the rotations of molecules are also subject to a set of selection rules that are derived from quantum mechanics. However, as I have discussed before, these selection rules are based upon a number of approximations and assumptions, such as the rigid rotor and Born-Oppenheimer approximation, and, in certain cases, these selection rules do not necessarily apply to the system and, as such, we observe "forbidden" transitions.

In particular, we discuss the observation of *x*-type transitions (no change in parity of the  $K_a$  and  $K_c$  quantum numbers), and the more traditional  $\Delta J = 2$  transitions, and how these are facilitated by the (small) quadrupole moment associated with the chlorine nucleus. To our knowledge, we are the first to report the appearance of *x*-type transitions arising from the quadrupolar moment of <sup>35</sup>Cl and <sup>37</sup>Cl. We shall also use our analysis and understanding of the rotational spectrum to propose various eigenstate coupling mechanisms that lead to the breakdown of these selection rules and how *J*,  $K_a$  and  $K_c$ , three important quantum numbers in rotational spectroscopy, are "bad" quantum numbers to describe the system.

**About the speaker:** Alex joined the Grubbs group at the department of chemistry at Missouri S&T in August 2022, as a post-doctoral research fellow, to construct and test a novel, state-of-the-art chirped-pulse Fourier transform microwave spectrometer.

He competed his PhD in physical and theoretical chemistry at the University of Nottingham in the United Kingdom focusing largely on the vibrational and electronic spectroscopy of small, aromatic molecules, notably *meta*fluorotoluene and *N*-methylpyrrole, as well as van der Waals complexes of the latter with the rare gases. Theoretical projects have included predicting the spectroscopy of small vdW complexes using both high-level single- and multi-reference *ab initio* methods.

He completed his master's degree in 2019 at the same institution, with time spent at the University of Canterbury in New Zealand, working on understanding the fluxional Cope rearrangement in bullvalene and how various substituents can affect the energy barrier and the timescale of this fluxionality.