AN INVESTIGATION OF THE DIPOLE FORBIDDEN TRANSITION EFFECTS IN BROMOFLUOROCARBONS AS IT PERTAINS TO 3-BROMO-1,1,1,2,2-PENTAFLUOROPROPANE USING CP-FTMW SPECTROSCOPY

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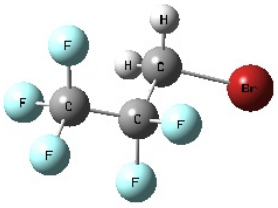

As part of a series of bromofluorocarbon species and analogues, the microwave spectrum of the molecule 3-bromo-1,1,1,2,2-pentafluoropropane has been measured on a CP-FTMW spectrometer located at Missouri S&T. The resultant spectrum is dense with transitions occurring at a rate of ≈1 transition/MHz! Within the spectrum, ^{79}Br and ^{81}Br isotopologues of multiple conformers of 3-bromo-1,1,1,2,2-pentafluoropropane have been identified. Rotational constants, centrifugal distortion parameters, nuclear quadrupole coupling constants and how each compare with theory for each conformer will be discussed.

Due to the large quadrupolar moment of bromine, heavy, brominated molecules are good candidates for dipole-forbidden transitions. Previous studies with bromoperfluoroacetone[a] provided a rich spectrum full of dipole forbidden transitions that 3-bromo-1,1,1,2,2-pentafluoropropane does not share. This difference will be explained using structural considerations along with the matrix elements needed to enact these transitions.

[a]F. E. Marshall, D. J. Gillcrist, T. D. Persinger, S. Jaeger, C. C. Hurley, N. E. Shreve, N. Moon, and G. S. Grubbs II, *J. Mol. Spectrosc.* **328** (2016) 59.