STRUCTURAL DETERMINATION OF THE CHIRAL MOLECULE 2-BROMO-1,1,1,3-TETRAFLUOROETHANE BY CP-FTMW SPECTROSCOPY

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Dipole forbidden, nuclear electric quadrupole allowed transitions in microwave spectroscopy are manifested through a linkage in off-diagonal components of the quadrupole coupling tensor. It is hypothesized that these transitions, due to their transition pathways, could possibly be used to differentiate chirality in a microwave three-wave mixing (3WM)-type experiment. In order to test this hypothesis, 2-bromo-1,1,1,3-tetrafluoroethane was chosen, as it is chiral, possesses a large quadrupolar nucleus and is heavy enough to generate the needed mixing to bring about these forbidden transitions. Because this the first known rotational study of the molecule, traditional rotational spectroscopy utilizing CP-FTMW techniques was performed first. This presentation will describe the collection of spectra, structural analysis, and observed dipole forbidden transitions of the title molecule.