AN INVESTIGATION OF THE NUCLEAR QUADRUPOLE COUPLING TENSORS OF 2-BROMOPYRIDINE USING THE EXTENDED TOWNES-DAILEY ANALYSIS

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The rotational spectrum of 2-bromopyridine was measured with a cavity FTMW spectrometer, and the complete nuclear quadrupole coupling tensors of ^{79}Br, ^{81}Br, and ^{14}N were determined. These tensors are interpreted using the Extended Townes-Dailey (ETD) analysis[a]. which allows us to predict orbital electron populations. These results are compared to *ab initio* Intrinsic Atomic Orbital (IAO) populations. The ETD analysis for the ^{14}N nucleus requires expressing the orbitals as sp^2 hybrids and performing rotations on the measured quadrupole tensors and the calculated IAO populations.

[a]S. E. Novick *J. Mol. Spectrosc.* **267** 13-18, 2011.