EXTENDED TOWNES-DAILEY ANALYSIS II

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Last year at this conference, I presented the Extended (to three dimensions) Townes-Dailey analysis for calculating p-orbital populations from measured nuclear quadrupole coupling tensors.[a] That analysis was limited to molecules containing atoms from the third row and higher. That is, the analysis was limited to unhybridized p-orbitals. Here I will generalize the method to include hybridized orbitals.

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[a] S. E. Novick, *OSU International Symposium on Molecular Spectroscopy*, RH04 (2009)