EXTENDED TOWNES-DAILEY ANALYSIS II

STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*.

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.

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