EXTENDED TOWNES-DAILEY ANALYSIS OF THE NUCLEAR QUADRUPOLE COUPLING TENSOR

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One simple way to understand nuclear quadrupole coupling constants is by invoking the model of Townes and Dailey.[a] This model, involving the field gradients generated by *p* electrons, has usually been used to estimate the fractional ionic character of diatomic molecules from a single nuclear quadrupole coupling constant. We will extend the model to three dimensions for polyatomic molecules and use it to rationalize the perhaps unexpected nuclear quadrupole coupling tensor for molecules such as monobromogermylene (HGeBr) and compare this simple calculation with *ab initio* results.

[a] C. H. Townes, B. P. Dailey, *J. Chem. Phys.* **17**, 782 (1949)