

Abstract Submitted
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Evaluating Molecular Hyperpolarizabilities with MOPAC SEAN SMITH, STEVEN ALEXANDER, Southwestern University — Molecules with high second-order nonlinearities have a number of industrial applications including high-speed low-power electronics. Accurate calculations can help identify molecules that have these properties. We have used the MOPAC semiempirical molecular orbital program to calculate the first order hyperpolarizabilities for several molecules and we compare these results to the experimental values reported in the literature. There is good correlation between these two data sets for most of the molecules though some have hyperpolarizabilities that differ by several orders of magnitude.

Steven Alexander
Southwestern University

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