Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Using Monte Carlo Simulations to Develop an Understanding of the Hyperpolarizability Near the Fundamental Limit SHORESH SHAFEI, Washington State University, MARK C. KUZYK, University of Oregon, MARK G. KUZYK, Washington State University — The hyperpolarizability governs all light-matter interactions. In recent years, quantum mechanical calculations have shown that there is a fundamental limit of the hyperpolarizability of all materials. The fundamental limits are calculated only under the assumption that the Thomas Kuhn sum rules and the three-level ansatz hold. (The three-level ansatz states that for optimized hyperpolarizability, only two excited states contribute to the hyperpolarizability.) All molecules ever characterized have hyperpolarizabilities that fall well below the limits. However, Monte Carlo simulations of the nonlinear polarizability have shown that attaining values close to the fundamental limit is theoretically possible; but, the calculations do not provide guidance with regards to what potentials are optimized. The focus of our work is to use Monte Carlo techniques to determine sets of energies and transition moments that are consistent with the sum rules, and study the constraints on their signs. This analysis will be used to implement a numerical proof of three-level ansatz.

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Date submitted: 16 Nov 2009 Electronic form version 1.4