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Identifying molecular features that maximize the second hyperpolarizability CHRISTOPHER BURKE, TIMOTHY ATHERTON, Department of Physics and Astronomy, Tufts University, JOSEPH LESNEFSKY, Department of Physics, University of Illinois at Chicago, ROLFE PETSCHKEK, Department of Physics, Case Western Reserve University — Designing materials with high non-linear optical properties is of importance for a variety of applications ranging from optical switching to chemical sensing. A key figure of merit is the intrinsic molecular second hyperpolarizability γ_{int} , a dimensionless quantity which measures how close a molecule's second hyperpolarizability is to the theoretical maximum. By modeling a molecule as a one dimensional linear piecewise potential, γ_{int} was optimized with respect to the shape of the potential. The number of parameters needed to describe the potential was varied. Searches were carried out for extrema in both the positive and negative directions, finding optimum potentials with γ_{int} of 0.60 and -0.15. The optimum potentials possess parity symmetry and are specified by a very small number of parameters due to our simple and well chosen representation. Based on the shape of the optimized potentials, we use these results to suggest possible routes for synthesizing molecules with high γ_{int} .

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