THE CHEMISTRY AND PHYSICS OF NONLINEAR OPTICAL MATERIALS:
A NEW LOOK AT AN OLD FIELD

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Recent efforts to "engineer" new nonlinear optical materials with specific desired characteristics has engendered a need for a theoretical description of optical properties which is readily accessible to chemists, yet correctly treats the essential physics of dielectric response. This paper describes a simple empirical molecular orbital model which gives useful insights into the relationship between chemical composition, crystalline structure, and optical susceptibilities. We compare the probabilities of finding new harmonic generators in various chemical classes. Rigorous bounds on the magnitudes of linear and nonlinear optical coefficients and their anisotropies are also discussed.

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