

Large vibrational contributions to the nonlinear optical properties of an isolated buckminsterfullerene molecule.

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Abstract

The vibrational contributions to the nonlinear optical properties of an isolated buckminsterfullerene molecule have been computed within the double harmonic oscillator and infinite optical frequency approximations. In our treatment, normal coordinates from density functional theory are combined with Hartree-Fock electrical properties. Values obtained for the ratio of vibrational to static electronic contributions vary from 0.01 for second harmonic generation to 0.64 for electro optic Kerr effect to 1.26 for degenerate four wave mixing.

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