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Applicability of DFT functionals for evaluating the first hyperpolarizability of phenol blue in solution

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ABSTRACT

The first electronic hyperpolarizability (β) of phenol blue (PB) in several solvents in a wide range of dielectric constants is investigated using the density functional theory (DFT). The reliability of various exchange-correlation functionals is assessed by a comparison to reference Møller-Plesset second-order perturbation theory (MP2) calculations. The equilibrium geometry of PB in each solvent is obtained by using the average solvent electrostatic configuration/free energy gradient method, which performs optimizations on the free energy hyper-surface by employing iteratively the sequential quantum mechanics/molecular mechanics methodology. The dependence of β on the bond length alternation (BLA) coordinate is rationalized by means of the two-level model. Within the employed exchange-correlation functionals, the LC-BLYP functional shows the best performance for describing the static and dynamic MP2 results of β , which increases as the BLA diminishes, reaching a maximum in an intermediate value of BLA. The results also illustrate the role played by the difference between the ground- and excited-state dipole moments ($\Delta\mu$) in determining the hyperpolarizability behavior in solution. Particularly, in the aqueous solution case, $\Delta\mu$ goes to around zero when BLA is near zero, leading to an abrupt decline in the β value. The DFT results of this study, therefore, indicate a clear relationship between the first hyperpolarizability and the BLA coordinate for the PB in solution, in agreement with experiment.

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