


Received: 23 March 2018 | Revised: 22 May 2018 | Accepted: 7 June 2018

DOI: 10.1002/qua.25708

WILEY International Journal of
QUANTUM CHEMISTRY

FULL PAPER

Density functional electric response properties of molecules in Cartesian grid

Abhisek Ghosal | Tanmay Mandal | Amlan K. Roy 

Abstract

Within the finite-field Kohn–Sham framework, static electric response properties of diatomic molecules are presented. The electronic energy, dipole moment (μ), static dipole polarizability (α), and first-hyperpolarizability (β) are calculated through a pseudopotential-DFT implementation in Cartesian coordinate grid, developed in our laboratory earlier. We engage the Labello–Ferreira–Kurtz (LFK) basis set; while four local and nonlocal exchange–correlation (LDA, BLYP, PBE, and LBVWN) functionals have been adopted. A detailed analysis of *grid convergence* and its impact on obtained results is presented. In each case the *electric field optimization* was carefully monitored through a recently prescribed technique. For all three molecules (HCl, HBr, HI) considered, the agreement of all these quantities with widely successful and popular atom-centered-grid procedure, is excellent. To assess the efficacy and feasibility, companion calculations are performed for these on a representative molecule (HCl) at distorted geometries, far from equilibrium. Wherever possible, relevant comparison is made with available *all-electron* data and experimental results. This demonstrates that Cartesian grid provides accurate, reliable results for such properties of many-electron systems within pseudopotential representation.