

# Performance of QTP functionals for NMR and static polarizability properties

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There is no doubt that Kohn-Sham Density functional theory (KS-DFT) holds the position as the most widely employed method in quantum chemical modeling nowadays since it offers an optimal equilibrium between cost and accuracy. However, from its foundation, KS-DFT suffers from some ubiquitous issues, i.e., incorrect one-particle spectrum, lack of an integer discontinuity, and self-interaction error (Devil's Triangle of KS-DFT) [1]. The Quantum Theory Project (QTP) exchange-correlation (XC) functionals, developed following the rigorous Correlated Orbital Theory (COT) arguments [2], were able to mitigate the errors previously mentioned. These functionals also delivered superior results for several chemical properties, e.g., ionization potential, electron affinity, reaction barriers, excitation energies to charge and Rydberg states, among others [3-5]. This way, the natural path regarding the knowledge about the quality of QTP functionals lies on the investigation of second-order response properties such as those obtained from Nuclear Magnetic Resonance (NMR) and the non-linear static polarizabilities. In this context, we tested 33 XC functionals from the different Jacob's ladder rungs (i.e., LDA, GGA, global hybrids, RSH, and double hybrids) for NMR spin-spin coupling constants, NMR chemical shift, and static polarizability. The reference method for such an investigation was the EOM-CCSD. Initial results show the great performance of the QTP XCs. For example, for NMR spin-spin coupling constants, the smallest value for the total percentage error was presented by QTP-01 (11.84 %), followed by QTP-02 (12.36 %), then mPW1LYP (12.54 %), and  $\omega$ B97X (12.60 %). Finally, for static polarizability, the smallest mean absolute deviations come from the following, QTP-01 (0.22 a.u.), LC-QTP (0.24 a.u.), PBE0 (0.24 a.u.).

## REFERENCES:

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