PWPB95-D3: AN EFFICIENT AND ACCURATE DOUBLE-HYBRID-META-GGA DENSITY FUNCTIONAL

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A new double-hybrid-meta-GGA density functional called PWPB95 is presented.\cite{1} It contains reparameterized Perdew-Wang exchange, Becke95 correlation and 50\% of Fock-exchange. Furthermore, it includes 26.9\% of spin-opposite scaled perturbative correlation and, consequently, has a better formal scaling behavior than other double-hybrids. This can be achieved with the help of the Laplace transformation algorithm $[O(N^4)]$. Additionally, PWPB95 is combined with our latest atom-pair-wise London-dispersion correction (DFT-D3).\cite{2}

The functional’s applicability is investigated with an extended and improved version of our recently published database for general main group thermochemistry, kinetics and noncovalent interactions (GMTKN30).\cite{3} PWPB95-D3 is in detail compared with various other double-hybrid approaches for GMTKN30 and dissociation reactions of transition metal carbonyls.

PWPB95-D3 turns out to be the least basis set dependent double-hybrid and it is in general more accurate and robust. An overall statistical analysis of about 47 density functionals shows that it belongs to the best functionals for GMTKN30.\cite{4} It is, thus, recommended for future usage in general chemistry applications.

The analysis of 47 functionals with GMTKN30, furthermore, allows a thorough evaluation of these. Recommendations for different rungs on Jacob’s Ladder are given. This analysis also sheds some light on ’modern’ approaches like range-separated hybrids and Truhlar’s M0X classes of functionals.