DENSITY FUNCTIONAL THEORY PREDICTIONS OF ONE-BOND CARBON-CARBON NMR COUPLING CONSTANTS

Reynier Suardíaz, José M. García de la Vega, Jesús San Fabián, R. Crepo-Otero, C. Pérez

a Dpto. de Química Física, Facultad de Química, Universidad de la Habana. La Habana 10400, Cuba.
reynier@fq.uh.cu
b Dpto. de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, España.

The reliability of density functional theory (DFT) in the determination of one-bond carbon-carbon spin-spin coupling constants ($^{1}J_{CC}$) is examined. Predictions using four functionals PBE, PW91, B3LYP, B3P86 and four basis set functions 6-311G**, TZVP, EPR-III and aug-cc-pVTZ-J are made and compared to experimental values. The set of 51 organic molecular systems with 71 $^{1}J_{CC}$ include different types of hybridized carbon atoms. The geometries of the studied systems were obtained by theoretical optimization at B3LYP/6-31G** level of theory. Regression analysis is used as a basic and appropriate methodology for this kind of comparative study. We conclude that DFT prediction of $^{1}J_{CC}$ of Csp3-Csp3 and Csp3-Csp2 are reliable for B3LYP/aug-cc-pVTZ-J and B3LYP/TZVP combinations. For Csp2-Csp2 couplings, B3P86/augcc-pVTZ-J seems to be the best choice but further studies are required. Additional experimental data is needed for the rest of the $^{1}J_{CC}$. 