



COMPARATIVE STUDY OF TEN DIFFERENT LEVEL THEORY USING THE GIAO METHOD

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Abstract

Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful experimental techniques for obtaining three-dimensional structures of complex molecules, mainly for the analysis of the relative and absolute configurations of organic compounds¹⁻². We present a new GIAO-HDFT universal scaling factor each one level of theory and a comparative study in which investigate its ability to predict NMR ¹³C chemical shifts with high cost-effectiveness ratio. Considering a set of 22 molecules with different behaviors (27 different chemical shifts), we got to generate a universal GIAO-HDFT with a basis set consistent with 6-31G(d) basis set and linear scaling factors using a “chemical shift – chemical shift” correlation approach. NMR chemical shifts were computed with ten different level theory using the GIAO method and are given relative to that of TMS calculated at the same level of theory³. Thus the best a scale factor equation generated for 6-31G basis set was applying PBE1PBE level that was the $\delta_{\text{scal}} = 1.01 \delta_{\text{calc}} + 0.20$, where δ_{calc} and δ_{scal} are the calculated and the linearly scaled values of the ¹³C chemical shifts, respectively). In order to achieve widespread application of a scaling factor to GIAO-HDFT ¹³C chemical shifts, it is desirable to combine excellent accuracy of MAD (mean absolute deviation) and RMS (root mean square). The data comparison demonstrated a great agreement between experimental and calculated NMR chemical shifts. For these set of 22 molecule MAD and RMS are: 3.79 and 4.99 respectively. The prediction of ¹³C chemical shifts by calculation using DFT mPBE1PBE/6-31G* is a very powerful tool for screening proposed structures and be used more widely.

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