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Gauge-including atomic orbital could not be the best choice for carbon-13 nuclear magnetic resonance calculations for terpenes

Terpenes are natural products that have several biological and pharmacological properties that are directly related to their chemical structures. In the structural determination of organic molecules, nuclear magnetic resonance is used on a large scale. The present study aims to develop and test chemical shift scaling factors from carbon-13 to terpenes, based on linear regressions. The geometries were optimized at the B3LYP/6-311+G(d,p) level, in the gaseous phase, and the chemical shift will be obtained at the PBE0/aug-cc-pvdz level with three different approaches gauge-including atomic orbital, continuous set of gage transformations, and individual gages for atoms in molecules, in phase gaseous and liquid, where the polarized continuum model was used. The tetramethylsilane was used as a reference and the experimental data of carbon-13 were obtained in chloroform. The results indicate that the gauge-including atomic orbital method presented a lower performance than the other 2 used. Thus, for studies with terpenes, with this level of theory, the use of the gauge-including atomic orbital method is not indicated.

Keywords: Terpenes; scaling factors; linear regressions; chemical shift.