

Research Article

GIAO/DFT evaluation of ^{13}C NMR chemical shifts of selected acetals based on DFT optimized geometries

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NMR • ^{13}C NMR • chemical shifts • GIAO/DFT • acetals • Rychnovsky's acetonide method

ABSTRACT

DFT/B3LYP calculations of the ground-state conformation of eight cyclic and acyclic acetals are presented and compared with experimental data. Results of single-point GIAO/DFT calculations at five different levels of theory show that isotropic shieldings need to be empirically scaled to achieve agreement with experimental chemical shifts. Statistical evaluation of data indicates that the most accurate prediction of ^{13}C chemical shifts is achieved at the MPW1PW91/6-311G** level of theory. An empirical equation describing the relationship between δ values and shielding constants is postulated. This equation has been applied to the non-chair ground-state conformation of the six-membered acetonide and to the conformationally flexible benzodioxonine derivative. The agreement observed between the experimental and predicted chemical shifts shows that calculations at the MPW1PW91/6-311G** level of theory are adequate for addressing questions of conformation. Copyright © 2004 John Wiley & Sons, Ltd.

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