Quantum Mechanical Prediction of ^{1}H and ^{13}C NMR Chemical Shifts in Large Protein Systems

Duane Williams[1], Bing Wang[1] and Kenneth M. Merz, Jr.[1]

[1]University of Florida, Department of Chemistry & Quantum Theory Project, Gainesville, FL 32611

Abstract

We have implemented a methodology for qualitative description Nuclear Magnetic Resonance (NMR) chemical shift tensors at the semi-empirical AM1 level and have generated the associated ^{1}H and ^{13}C protein NMR-specific AM1 parameters. Using our linear-scaling divide-and-conquer algorithm to perform the quantum mechanical calculations, we carried out this parameterization using a series of globular protein systems with a variety of secondary structure as the training set. Our approach can be employed using semi-empirical (AM1/PM3) geometries and can be executed at a fraction of the cost of *ab initio* methods, thus providing an attractive option for the quantum mechanical studies of NMR on large protein systems.