Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra

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Abstract

We present a composite procedure for the quantum-chemical computation of spin-spin-coupled ^{1}H NMR spectra for general, flexible molecules in solution. The procedure is based on four main steps, namely an initial conformer/rotamer ensemble (CRE) generation by the fast tight-binding method GFN-xTB and a newly developed search algorithm, computation of the relative free energies and NMR parameters, and solving the spin Hamiltonian. In this way the NMR-specific nuclear permutation problem is solved, and the correct spin symmetries are obtained. Energies, shielding constants, and spin-spin couplings are computed at state-of-the-art DFT levels with continuum solvation.