CALCULATION OF NUCLEAR ISOTROPIC SHIELDINGS AND INDIRECT NUCLEAR SPIN-SPIN COUPLING CONSTANTS IN THE COMPLETE BASIS SET LIMIT (CBS)

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Computational chemistry has been widely used to support analysis of NMR data including chemical shifts, related to nuclear isotropic shieldings, and indirect nuclear spin-spin coupling constants. Besides, prediction of NMR parameters is invaluable in studying new molecular systems. The accuracy of theoretical predictions depend on the quality of method on calculations (e. g. RHF, MP2, DFT or CCSD(T)) and the completeness of basis set describing molecular system.

The presented paper discusses the importance of basis set selection and simple mathematical fitting toward complete basis set limit (CBS). The CBS approach in the current work is based on fitting the results of NMR calculations with regularly converging basis set families using three-parameter and two-parameter functions:

$$Y(x) = Y(\infty) + A\exp(-x/B) \quad \text{and} \quad Y(x) = Y(\infty) + A/x3$$

The CBS approach provides a reliable test for calculation methods and is mainly designed for small molecules. In case of larger systems, for example, enzyme active site, the "locally dense basis set" method is suitable.

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