Evaluation of DFT Methods for the Evaluation of NMR Chemical Shifts of Transition Metal Complexes

Mark A. Iron

Computational Chemistry Unit, Department of Chemical Research Support,
Weizmann Institute of Science, Rehovot 7610001, Israel

At one of my first Sanibel symposia, I presented an in-depth evaluation of the factors influencing the calculation of ^{13}C and ^{1}H NMR chemical shifts of organic compounds.[1] In this presentation, I will present my findings in expanding this study to transition metal complexes, including ^{51}V, ^{103}Rh and ^{195}Pt chemical shifts as well as ^{1}H, ^{13}C and ^{31}P directly bound to the metal centre. To this end, a large collection of complexes with experimentally measured NMR spectra has been collated. Since relativistic effects can be significant with platinum, the reliability of using an RECP is also considered.

1.   Iron, M. A. Evaluation of the Factors Impacting the Accuracy of ^{13}C NMR Chemical Shift Predictions using Density Functional Theory – The Advantage of Long-Range Corrected Functionals. *J. Chem. Theory Comput.* **2017,** *13*, 5798-5819.