Nuclear Magnetic Resonance Shielding Tensors: A Quasi-Relativistic Approach Including Electroweak Interaction Effects

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We present a two-component zeroth-order regular approximation (ZORA) approach to the calculation of nuclear magnetic resonance (NMR) shielding tensors at the density functional theory level. Our method is similar to that of [1], but in addition to the standard electromagnetic contributions we also incorporate effects of the parity-violating (PV) weak interaction of the standard model of physics. These effects are especially fascinating in chiral molecules, where the weak interaction is predicted to cause NMR frequency splittings $\Delta\nu_{\mathrm{pv}}$ between enantiomers [2, 3, 4, 5]. Due to the smallness of the effect, these have not yet been observed experimentally. However, a measurement with sufficient resolution would not only reveal an intriguing aspect of molecular chirality but could potentially also offer an appealing low energy gateway to the investigation of fundamental forces in nature, thus complementing current high energy particle physics experiments. Here, we report conventional NMR shielding constants and PV contributions to them for experimentally suitable compound classes. The impact of nuclear charge dependence and conformational effects is investigated.

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