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Direct magnetic field dependence of NMR shielding

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Nuclear shielding is considered independent of the magnetic field strength when analysing NMR experiments. However, already in 1970, Ramsey proposed on theoretical grounds that this may not be valid for heavy nuclei. Here we present experimental evidence for the direct field dependence of shielding, using 59Co shielding in Co(acac)3 dissolved into chloroform as an example. This low-spin diamagnetic Co(III) complex features a very large and negative nuclear shielding constant of the central Co nucleus. We carry out variable temperature NMR experiments in four different field strengths ranging from 7.05 to 18.79 T. As there is a well-known sensitivity of the 59Co NMR frequency to temperature, we introduce Xenon gas into the sample and use the known temperature dependence of the 129Xe signal to calibrate the temperature. Signal from a Xenon gas sample is used as a frequency reference. The experiments result in temperature dependent magnetic field dependence in the order of -10-3 ppm T-2 for the 59Co shielding constant, arising from the direct modification of the electron cloud of the complex by the field. First-principles non-linear response theory results in values ranging from -10-5 to -10-3, in reasonable agreement with the experiment. Upon increasing field strengths available in contemporary NMR setups, the direct magnetic field dependence of NMR parameters becomes a factor to take into account in studies of materials and molecular structures. Furthermore, direct field-induced effects may in the future provide entirely new tools for materials characterisation.

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