Nuclear magnetic dipole moments from NMR experiments

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We discuss new values of nuclear magnetic dipole moments, obtained from accurate absolute shielding constants and experimental NMR data, for a series of nuclei. The generally accepted literature values of magnetic moments were for many isotopes derived from NMR spectra. However, in the procedure applied to determine the moments of bare nuclei the effects of the molecular electronic structure have been often described in a very approximate manner. Accurate absolute shielding scales can be presently established analysing NMR spectra and shielding constants determined by ab initio methods of quantum chemistry.

We focus on the ^{209}Bi magnetic moment, which is of importance for the interpretation of Bi^{82+} ion hyperfine splitting experiments. Our values derived from NMR experiment and calculated shielding constants of Bi^{3+} ions in aqueous solutions of $Bi(NO_3)_3$ and $Bi(ClO_4)_3$ salts differ from old literature data and represent an independent confirmation of ^{209}Bi magnetic moment recently determined. The accuracy limit of the ^{209}Bi magnetic moment set by the present computational chemistry methods is discussed.

References

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