MAGNETIC-FIELD-INDUCED QUADRUPOLE SPLITTING IN GASEOUS AND LIQUID ^{131}Xe NMR: QUADRATIC AND QUARTIC FIELD DEPENDENCE

J. Vaara and P. Pyykkö

Department of Chemistry, P.O.B. 55 (A. I. Virtasen aukio 1)
FIN-00014 University of Helsinki, Finland
email: jvaara@chem.helsinki.fi

A theory for the magnetic-field-dependent quadrupole splitting in the ^{131}Xe NMR spectra in isotropic media is presented and tested by *ab initio* electronic structure calculations. [1] Evidence only exists for even-power magnetic field dependence. The dominant mechanism is verified to be the electric field gradient caused by the diamagnetic distortion of the atomic electron cloud, quadratic in the magnetic field. The computed results are in excellent agreement with the recent experiment by Meersmann and Haake. [2]

1. J. Vaara and P. Pyykkö, Phys. Rev. Lett. 86 (2001) 3268.
2. T. Meersmann and M. Haake, Phys. Rev. Lett. 81 (1998) 1211.