Simulation of the NMR Second Moment as a Function of Temperature in the Presence of Molecular Motion. Application to $(CH_3)_3NBH_3$

Roman Goc

Institute of Physics, A. Mickiewicz University, Umultowska 85, 61-615 Poznań

Reprint requests to Dr. R. G.; E-mail: goc@amu.edu.pl

Z. Naturforsch. **57 a,** 29–35 (2002); received November 20, 2001

The method for simulating the second moment of the NMR absorption spectrum as a function of temperature is presented. The second moment is first calculated as a function of the number of jumps of rotating molecules or their parts (like methyl groups). This number of jumps is rescaled into the frequency of internal rotation and these frequencies are recalculated into equivalent temperatures. The relation between frequency of rotation, and temperature is established on the basis of the Arrhenius relation $\nu_c = \nu_0 \exp(-E_a/RT)$. The described method is then applied to the analysis of molecular motion in trimethylamine borane $(CH_3)_3NBH_3$. The proposed method is especially useful in the case of complex structures, where combined motions are possible, because the NMR second moment is much more sensitive to the geometry of motion than the magnetic relaxation times T_1 or $T_{1\rho}$ usualy used in studies of the internal dynamics of solids.

Key words: NMR; Second Moment; Internal Rotation; Simulation.