NMR Relaxation Time Simulation for Different Models of Motion in $(CH_3)_3NBH_3$

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Monte Carlo simulations of complex rotation of single $-CH_3$ groups, $-(CH_3)_3$ groups and $-BH_3$ groups were performed for trimethylamine borane $(CH_3)_3NBH_3$. In the course of these simulations the correlation functions for different models of rotation were determined. Knowledge of these functions and of some data extracted from NMR experiments allowed for the calculation of the longitudinal magnetic relaxation time T_1 as a function of temperature. The values of relaxation times obtained from Monte Carlo simulations are compared to experimental results published by other authors. There is a clear relation between the assumed model of rotation and the shape of the T_1 curve versus temperature.

Key words: Correlation Function; Monte Carlo; NMR, Relaxation.