Second Moment Simulations for Different Models of Rotations and Oscillations in Polycrystalline Thiourea Pyridinium Nitrate Inclusion Compound and its Two Perdeuterated Analogues

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The second moment of ^{1}H NMR absorption spectra was calculated for three samples of $[(NH_2)_2CS]_2(C_5H_5NH)^+NO_3^-$, two of which were deuterated at different positions. The calculations were performed for different rotations and oscillations, and for a wide range of frequencies of these motions. These frequencies were then transformed into temperatures resulting in the temperature dependence of the second moment. The calculations were undertaken in order to analyze the experimental results obtained in our laboratory. Special attention was paid to molecular reorientations through unequal potential barriers. Comparison of the second moment values calculated for different models of rotation with the experimental ones enabled a deeper insight into the internal motion in this material as a function of temperature.

Key words: NMR; Second Moment; Simulation; Internal Reorientation; Inclusion Compounds.