¹H NMR Study of Molecular Motions in Thiourea Pyridinium Halide Inclusion Compounds

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The proton NMR second moment and spin-lattice relaxation time have been studied for polycrystalline inclusion compounds of thiourea pyridinium chloride, bromide, iodide and their perdeuterated analogues in a wide temperature range. The pyridinium cation reorientation around the pseudohexagonal C₆' symmetry axis over inequivalent barriers and hindered rotation of the thiourea molecule around its C=S bond have been revealed. The activation parameters of the both motions have been found.

Key words: NMR; Molecular Motion; Inclusion Compounds.