Hydrogen Isotope Effect on the Temperature Dependence of the ^{35}Cl-NQR Frequency in $(NH_4)_2IrCl_6$

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The ^{35}Cl-NQR frequencies and spin-lattice relaxation times of $(NH_4)_2IrCl_6$ and $(ND_4)_2IrCl_6$ were measured in the temperature range 4.2 - 300 K. It was confirmed that no phase transition takes place down to 4.2 K. The observed frequency at 4.2 K in $(ND_4)_2IrCl_6$ was higher by 18 kHz than that in the non-deuterated analogue. This discrepancy was attributed to a difference between the lowest rotational states of the ammonium ions in these compounds. The energy separation between the ground state and excited state of rotational motion, in which N-H of the ammonium ion rotates among the three directions slightly apart from the triad axis, was estimated by fitting analysis to be 31 cm^{-1} and 93 cm^{-1} for $(ND_4)_2IrCl_6$ and $(NH_4)_2IrCl_6$, respectively. The activation energy of the reorientation of the ammonium ion among the four directions of the triad axis was estimated to be 6.9 and 7.6 kJ mol^{-1}, respectively.

Key words: Isotope Effect; Tunneling Motion; Chlorine NQR; Ammonium Hexachloroiridate.