^{2}H NMR Study of Molecular and Electron Spin Dynamics in Paramagnetic $[Co(H_2O)_6][SiF_6]$

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The temperature dependences of ^{2}H NMR spectra and the spin-lattice relaxation time T_1 were measured for $[Co(H_2O)_6][SiF_6]$. The variation of the spectrum above room temperature can be explained by the reorientation of $[Co(H_2O)_6]^{2+}$ about the C_3 axis. The activation energy E_a and the jumping rate at infinite temperature k_0 for the three site jump of $[Co(H_2O)_6]^{2+}$ were obtained as 82 kJmol^{-1} and 2×10^{17}s^{-1} from the spectral simulation. Below room temperature, the spectral line shape was dominated by the 180° flip of the water molecule. The minimum of T_1 caused by the 180° flip of the water molecule was observed at ca. 260 K. The jumping rate of the 180° flip of the water molecule was estimated from the ^{2}H NMR T_1 and the spectral simulation. E_a = 38 kJmol^{-1} and $k_0 = 6\times10^{15}$s^{-1} for the 180° flip of the water molecule were obtained from T_1.

Key words: Phase Transition; ^{2}H NMR; Nuclear Quadrupole Interaction; Paramagnetic Shift; Molecular Dynamics.