

# Water Molecular Motion and Hydrogen Bond in Paramagnetic [Cu(H<sub>2</sub>O)<sub>6</sub>][PtCl<sub>6</sub>] as Studied by Single Crystal <sup>2</sup>H NMR

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The temperature and angular dependences of the <sup>2</sup>H NMR spectrum were measured for single crystal [Cu(H<sub>2</sub>O)<sub>6</sub>][PtCl<sub>6</sub>]. ( $e^2Qq/h, \eta$ ) = (132 kHz, 0.72) were obtained for the D nucleus averaged by the fast 180° flip of the water molecule at 297 K. D<sub>1</sub>(236 kHz, 0.10) and D<sub>2</sub>(246 kHz, 0.09) were obtained for two unequal D nuclei of the water molecule at 133 K. Below  $T_c$ , at least three nonequivalent waters were found to exist. The jumping rate for the 180° flip of the water molecule ( $k$ ) was obtained from the simulation of <sup>2</sup>H NMR spectra at  $H_0 \parallel [111]$  direction. The activation energy  $E_a$  and the jumping rate at infinite temperature were estimated from the temperature dependence of  $k$  to be 24 kJ mol<sup>-1</sup> and  $1 \times 10^{13} \text{ s}^{-1}$ .

*Key words:* Phase Transition; <sup>2</sup>H NMR; Nuclear Quadrupole Interaction; Paramagnetic Shift; Molecular Dynamics.