Study of Structural Phase Transitions in $[Mg(H_2O)_6][SiF_6]$ by Means of Single Crystal ^2H NMR

Takahiro Iijima, Motohiro Mizuno, Masahiko Suhara, and Kazunaka Endo

Department of Chemistry, Faculty of Science, Kanazawa University, Kanazawa 920-1192, Japan

Reprint requests to Dr. M. M.; E-mail: mizuno@wriron1.s.kanazawa-u.ac.jp

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The temperature and angular dependences of ^{2}H NMR spectra were measured for single crystal of $[Mg(H_2O)_6][SiF_6]$. At 283 K, $(e^2Qq/h, \eta)$ of ^{2}H, averaged by fast 180° flip of water molecules, were obtained as (128 kHz, 0.72), (123 kHz, 0.82) and (106 kHz, 0.80), corresponding to three unequal water molecules in $[Mg(H_2O)_6]^{2+}$. At 338 K, $(e^2Qq/h, \eta)$ averaged further by the fast reorientation of $[Mg(H_2O)_6]^{2+}$ around the C_3 axis was obtained as (57 kHz, 0.01). In phase II, the jumping rate for the reorientation (k) and the amplitude of the rotational modulation ($\Delta\alpha$) of $[Mg(H_2O)_6]^{2+}$ about the C_3 axis were obtained from the simulation of ^{2}H NMR spectra. The jumping rate at infinite temperature and the activation energy were estimated from the temperature dependence of k as $k_0 = 9 \times 10^{17}$ s^{-1} and $E_a = 78$ kJmol^{-1}, respectively. The II-III phase transition was found to be related with the freeze of this motion.

Key words: Nuclear Quadrupole Interaction; ^{2}H NMR; Incommensurate Phase; Rotational Modulation; Molecular Dynamics.