Studies of Successive Phase Transitions and Molecular Motions in $[Mg(H_2O)_6][SiF_6]$ by $^{1,2}H$ and ^{19}F NMR*

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The successive phase transitions of $[Mg(H_2O)_6][SiF_6]$ were studied by measuring ^2H NMR spectra. The quadrupole coupling constant e^2Qq/h and asymmetry parameter η changed drastically at each transition temperature. $^{1,2}H$ and ^{19}F NMR T_1 were measured for this compound to study the relation between the molecular motions and the successive phase transitions. The activation energy E_a and the pre-exponential factor τ_0 for the reorientation of $[SiF_6]^{2-}$ were estimated as 28 kJmol^{-1} and 6.0×10^{-14} s, and those of the 180° flip of H_2O as 33 kJmol^{-1} and 4.0×10^{-14} s. These two motions occur rapidly even in phase V. For the reorientation of $[Mg(H_2O)_6]^{2+}$, E_a = 62 kJmol^{-1} and $\tau_0 = 1.1\times10^{-16}$ s were obtained from the simulation of ^2H NMR spectra. The jump rate of this motion is of the order of 10^4 - 10^6 s^{-1} in phase II. These results suggest that the successive phase transitions are closely related to the motion of $[Mg(H_2O)_6]^{2+}$.

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