Studies of Successive Phase Transitions and Molecular Motions in $[\text{Mg(H}_2\text{O)}_6][\text{SiF}_6]$ by $^{1,2}$H and $^{19}$F NMR

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The successive phase transitions of $[\text{Mg(H}_2\text{O)}_6][\text{SiF}_6]$ were studied by measuring $^2$H NMR spectra. The quadrupole coupling constant $\hat{Q}/h$ and asymmetry parameter $\eta$ 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 $\tau_0$ for the reorientation of $[\text{SiF}_6]^{2-}$ were estimated as $28 \text{ kJmol}^{-1}$ and $6.0 \times 10^{-14} \text{ s}$, and those of the $180^\circ$ flip of $\text{H}_2\text{O}$ as $33 \text{ kJmol}^{-1}$ and $4.0 \times 10^{-14} \text{ s}$. These two motions occur rapidly even in phase V. For the reorientation of $[\text{Mg(H}_2\text{O)}_6]^{2+}$, $E_a = 62 \text{ kJmol}^{-1}$ and $\tau_0 = 1.1 \times 10^{-16} \text{ s}$ were obtained from the simulation of $^2$H NMR spectra. The jump rate of this motion is of the order of $10^4 - 10^6 \text{ s}^{-1}$ in phase II. These results suggest that the successive phase transitions are closely related to the motion of $[\text{Mg(H}_2\text{O)}_6]^{2+}$.

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