

# Temperature Dependence of $^2\text{H}$ Quadrupole Coupling Constants in $^2\text{H}_2\text{O}$ and Ionic Motions in Crystalline $[\text{M}(^2\text{H}_2\text{O})_6][\text{SnCl}_6]$ (M: Mg, Ca), Studied by $^2\text{H}$ NMR and Neutron Powder Diffraction \*

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The temperature dependence of  $^2\text{H}$  NMR spectra was measured at 130–430 K on  $[\text{M}(\text{D}_2\text{O})_6][\text{SnCl}_6]$  (M: Mg, Ca) (rhombohedral, space group:  $R\bar{3}$ ), and neutron powder diffraction on the Mg salt was performed at room temperature. Based on the accurate orientation of  $\text{D}_2\text{O}$  molecules in an octahedral cation, spectra with a large asymmetry parameter  $\eta$ , observed around 200 K, were explained by a model of  $180^\circ$  flip of water molecules. Another motional narrowing observed above room temperature was assigned to a cationic overall reorientation about the  $C_3$ -axis.

*Key words:*  $^2\text{H}$  NMR; Neutron Diffraction; Molecular Motion; Quadrupole Coupling Constant; Spectrum Lineshape.

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