

A high-temperature neutron diffraction study on $\text{Mg}(\text{OD})_2$

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The structure of deuterated brucite, $\text{Mg}(\text{OD})_2$, was investigated by measuring neutron diffraction at high temperature and at atmospheric pressure to see the dynamic behavior of D atoms with increasing temperature. The neutron diffraction experiments from 202K to 600K were carried out at the beamline of Wide-Angle Neutron Diffractometer (WAND) in the High Flux Isotope Reactor (HRIR), Oak Ridge National Laboratory, USA. Rietveld analysis was performed with both the single D site model and the three-site D model. D atom sits at a crystallographic $2d$ site on the 3-fold rotation axis in the single D site model and at a $6i$ site with occupation factor of 1/3 in the three-site D model. Analysis for 600 K data was not successful using the single D site model but was successfully converged using the three-site D model. This is possibly due to the strongly anisotropic D motion.

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