Poster Presentation

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Crystal structure analysis of LiN(DxH1-x)4SO4 by neutron diffraction

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The crystal structure of Li(ND4)SO4 was analysed by neutron diffraction method. The crystal is a partially deuterated Li(NH4)SO4 and one of the ferroelectric materials with hydrogen atoms. The crystal is orthorhombic at room temperature with lattice parameters of a=5.2773(5) Å, b=9.124(2) Å, c=8.772(1) Å and Z=4. Neutron intensity data were collected on the Four-Circle Diffractometer (FCD) at HANARO in Korea Atomic Energy Research Institute. The structure was refined by full-matrix least-square to final R value of 0.049 for 745 observed reflections by neutron diffraction. All atomic positions of four hydrogen atoms at NH4 and the occupation factors of D and H were refined. From these results we obtained the average chemical structure of this sample, LiND3.05H0.95SO4. Five years later, neutron intensity data were collected and analysed once more with same crystal. The crystal is orthorhombic but with different lattice parameters, or hexagonal. We will report and discuss these results in this presentation.

Keywords: hydrogen bond, neutron diffraction, FCD at HANARO