

## Crystal structure of high pressure Al(OH)<sub>3</sub> polymorphs: II. Powder X-ray diffraction study of delta-Al(OH)<sub>3</sub>

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The crystal structure of aluminium trideuterioxide, delta-Al(OH)<sub>3</sub>, synthesized at 18 GPa and 700 C using a Kawai-type multi-anvil apparatus was investigated by powder X-ray diffraction method at ambient condition. The space group assuming the delta-Al(OH)<sub>3</sub> has a centrosymmetric space group is to Pnam (#62) with lattice constants of a=5.14036(9)Å, b=5.06489(9)Å, c=7.25745(13)Å, and V=188.950(6)Å<sup>3</sup>. The crystal structure was solved by a direct method, and the MEM/Rietveld method revealed the positions of D atoms. It is possible that the structure of delta-Al(OH)<sub>3</sub> has the lower symmetry space group from Pnam deu to the ordering of D atoms. The framework of the derived structure model is isostructural with the distorted ReO<sub>3</sub>-type structure, which is considered as an A-site deficient hydroxy-perovskite.