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

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The crystal structure of aluminium trideuteroxide, delta-Al(OH)3, 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)3 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. 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)3 has the lower symmetry space group from Pnam due to the ordering of D atoms. The framework of the derived structure model is isostructural with the distorted ReO3-type structure, which is considered as an A-site deficient hydroxy-perovskite.