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On the crystal structure of delta-Al(OH)3

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A high pressure phase of Al(OD)3, called delta phase, was synthesized at 18 GPa and 973 K using a Kawai-type multi-anvil apparatus (Komatsu et al., 2007a). Based on powder X-ray diffraction at ambient conditions, Komatsu et al.(2007a) confirmed that delta-Al(OD)3 is isostructural with delta -Al(OH)3 with space group Pnam, as previously reported by Dachille and Gigl(1983). However, successive neutron diffraction measurements at ambient conditions (Komatsu et al., 2007b) revealed that the real space group of delta-Al(OD)3 is P212121, but not Pnam as obtained by X-ray diffraction experiments. Komatsu et al.(2007b) suggested that the positions of D atoms may be in ordered in hydrogen bonds in the P212121 structure, while they were proposed to be in disordered in the Pnam structure. Here we use the Vienna ab initio simulation package VASP (Kresse and Furthmuller, 1996) to study the structural and enegetic properties of delta-Al(OH)3 in more detail. The structures of the three known Al(OH)3 polymorphs, gibbsite, bayerite, and eta -Al(OH)3, were also calculated using VASP to check the reliability and applicability of the computations.

Keywords: Al(OH)3, high pressure, phase transition, first-principles calculation