Structure Refinement of Deuterated Boehmite

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Abstract: The crystal structure of a deuterated synthetic boehmite powder, γ-AlOOD, has been determined by time-of-flight neutron diffraction and Rietveld profile refinement in space group *Cmcm* to a weighted profile R of 3.71%. Cell dimensions are a = 2.868(1), b = 12.2336(4), and c = 3.6923(1) Å. Alternate space groups for the boehmite structure suggested in the recent literature were found to be unacceptable. Atom positions, bond distances, and angles, with the exception of those involving hydrogen, were nearly identical to those determined by R. J. Hill in 1981 who studied a single crystal of boehmite by X-ray diffraction. All atoms were refined with anisotropic thermal parameters. The b value is 0.013 Å larger, and the thermal ellipsoids of oxygen are slightly more anisotropic than those reported by Hill and may reflect the different samples studied.

Key Words: Boehmite • Crystal structure • Deuterium • Hydrogen position • Neutron diffraction • Rietveld refinement

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