The Crystal Structure of Boehmite

Gary G. Christoph[1], Charles E. Corbató[2], Douglas A. Hofmann[2] and Rodney T. Tettenhorst[2]

The Ohio State University, Columbus, Ohio 43210

[1] Department of Chemistry.
[2] Department of Geology and Mineralogy.

Abstract: The crystal structure of a synthetic boehmite sample has been refined to an R of 0.047 in the space group Amam from X-ray powder diffraction data. Inclusion of hydrogen atoms and/or refinement in the space group $A2_1am$ gave poorer results. Cell dimensions were determined as a = 3.6936 (± 0.0003), b = 12.214 (± 0.001), c = 2.8679 (± 0.0003) Å. All Al-O(OH) distances lie between 1.88 and 1.91 Å. Shared octahedral edges are 2.51 – 2.52 Å, and unshared octahedral edges are 2.86 – 2.87 Å, in excellent agreement with those for layered silicates. The O-H … O distance between contiguous octahedral sheets is 2.71 Å. The computed X-ray pattern matches closely with the experimental pattern, indicating the degree to which the crystal structure has been determined.

Key Words: Boehmite • Crystal Structure • O-OH Distances • Powder X-ray Diffraction • Synthesis

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