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First-principles study of the OH-stretching modes of gibbsite

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Abstract

The theoretical infrared (IR) and Raman spectra of gibbsite [α-$Al(OH)_3$] were computed using ab initio quantum mechanical calculations. The low-frequency dielectric tensor and the Raman tensors of gibbsite were determined using linear response theory. The transmission powder IR spectrum was found to strongly depend on the shape of the gibbsite particles. In the region of the OH-stretching bands, an excellent agreement between theory and experiment was obtained, providing an unambiguous interpretation of the OH bands in terms of vibrational modes. In contrast, the assignment of the bands observed at lower frequency is complicated by the significant overlap between neighboring bands together with their sensitivity to particle shape.

Keywords: IR spectroscopy, Raman spectroscopy, quantum mechanical calculation, gibbsite