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The infrared spectrum of gibbsite: Theory vs. Experiment

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The theoretical infrared (IR) spectrum of gibbsite (alpha-Al(OH)3) was computed using ab-initio quantum mechanical calculations. Calculations were performed by using the Density Functional Theory, with the generalized gradient approximation. The low-frequency dielectric tensor of gibbsite was determined as a function of the light frequency using the linear response theory. The influence of the particle shape on the IR spectrum was then investigated. In the region of OH stretching bands, an excellent agreement between theory and experiment was obtained by considering spherical particles. This agreement provides an unambiguous interpretation of the OH bands in terms of vibrational modes.