American Mineralogist, Volume 87, pages 1286–1290, 2002

First-principles calculation of the infrared spectrum of lizardite

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ABSTRACT

The theoretical infrared spectrum of lizardite [$Mg_3Si_2O_5(OH)_4$] was computed using first-principles quantum mechanical calculations. Density functional perturbation theory allowed us to derive the low-frequency dielectric tensor of lizardite as a function of the light frequency. The infrared spectrum was then calculated using a model that takes into account the platy shape of particles. A very good agreement was obtained between theory and experiment. This agreement allows us to make an unambiguous assignment of the major absorption bands observed in the IR spectrum of lizardite, including the stretching bands of OH groups.