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Assignment of the structural OH stretching bands of gibbsite

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ABSTRACT

Single-crystal Raman and FTIR methods have been combined to study the structural OH groups of gibbsite, $Al(OH)_3$. According to factor group analysis, six unique OH stretching bands [ν(OH)] bands are expected to occur in both IR and Raman spectra. In this study, six ν(OH) bands were observed in both the Raman and IR spectra. Analysis of the gibbsite crystal structure reveals two distinct types of structural OH groups: interlayer and intralayer hydrogen-bonded OH groups. The ν(OH) bands corresponding to these two types of OH groups were clearly resolved using polarized single-crystal Raman spectroscopy. The interlayer hydrogen-bonded OH groups are oriented along the *c* axis of the crystal and are represented by three ν(OH) bands at 3433, 3370, and 3363 cm^{-1}. In contrast, the intralayer hydrogen-bonded OH groups are oriented nearly parallel to the (001) face and are represented by the ν(OH) bands at 3623, 3526, and 3519 cm^{-1}. Assignment of the ν(OH) bands was based, in part, upon the Lippincott and Schroeder one-dimensional (LS-1D) model of the hydrogen bond. Based upon the known geometry of each OH group, the LS-1D model was used to predict the ν(OH) frequencies corresponding to each OH group. Additional support for the band assignments was obtained by correlation between the single-crystal Raman band intensities and the OH bond orientations obtained from the crystal structure.