The Vibrational Properties of Katoite $Ca_3Al_2[(OH)_4]_3$: A Periodic *ab-initio* Study

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The vibrational spectrum of katoite was simulated by using the periodic *ab initio* CRYSTAL program [1].

In spite of the structural similarities with garnets [2], katoite presents a quite different spectrum, due to the presence of hydrogen atoms and lack of connectivity among the $Al(OH)_6$ octahedra. A deep analysis of the dynamical-matrix eigenvectors, including isotopic substitutions and modes visualization, was performed in order to assign the 345 modes. Hydrogen related modes, namely OH strectching, AlOH bending and H rotation with respect to the Al-O axis can be identified as nearly pure modes, although only the former form a separated band.

For the OH strectching, anharmonicity effects, that are as large as 150 cm^{-1}, have been taken into account. The calculated values are in very good agreement with available experimental data. [3]

[1] Saunders V.R., Dovesi R., Roetti C., Orlando R., Zicovich-Wilson C., Harison N.H., Doll K., Civalleri B., Bush I.J., D'Arco Ph., Llunell M., *CRYSTAL2003 user's manual,* University of Torino, Torino, 2003. [2] Pascale F., Zicovich-Wilson C., Orlando R., Dovesi R., 2005, *in press*. [3] Rossman G.R., Aines R.D., *Am. Mineral.*, 1991, **76**, 1153.

Keywords: ab-initio calculations, hydrogernet, vibration