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An ab initio study of hydrogarnets

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ABSTRACT

The structural properties of katoite, $Ca_3Al_2(O_4H_4)_3$, are investigated as a function of applied pressure. The calculated structure at ambient pressure, the bulk modulus and its pressure derivative are in good agreement with the available experimental data. The strength of the hydrogen bond increases under pressure, accompanied by a lengthening of the O-H bonds. This conclusion agrees with experimental spectroscopic data and casts serious doubts on the reliability of neutron diffraction results that predict strong compression of the O-H bonds. Calculations for $Mg_3Al_2(O_4H_4)_3$ have been used to predict the structure and relative stability of the hypothetical hydropyrope.