

Compressibility of stottite, $\text{FeGe}(\text{OH})_6$: An octahedral framework with protonated O atoms

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ABSTRACT

The evolution of the unit-cell parameters of stottite [$\text{FeGe}(\text{OH})_6$], a compound with a tetragonal octahedral framework related to the perovskite structure, has been determined to a maximum pressure of 7.8 GPa by single-crystal X-ray diffraction at room temperature. Stottite does not exhibit any phase transitions in this pressure range. A fit of a third-order Birch-Murnaghan equation of state to the pressure-volume data yields values of $V_0 = 425.67(2) \text{ \AA}^3$, $K_{T0} = 78.4(3) \text{ GPa}$ and $K'_0 = 6.18(10)$. Analysis of the unit-cell parameter data shows that **c** is approximately 10% more compressible than **a**. Compressional moduli for the axes are $K_{a0} = 81.3(3) \text{ GPa}$ and $K'_{a0} = 6.4(1)$, $K_{c0} = 73.3(6) \text{ GPa}$ and $K'_{c0} = 5.7(2)$. We relate these axial compressibilities to the structure of stottite, which, unlike related cubic protonated octahedral frameworks such as burtite [$\text{CaSn}(\text{OH})_6$], is expected to have a highly anisotropic hydrogen-bonding topology: a high degree of hydrogen-bonded connectivity parallel to (001) and very little parallel to [001]. Enhanced hydrogen bonding within the (001) plane may stiffen the structure along $\langle 100 \rangle$. We also make some provisional comparisons with structural and elasticity data for perovskites and show that the absence of a central, non-framework cation in the stottite structure allows octahedral tilts in excess of 40° . The stottite structure is much softer than any known oxide perovskite. The relative importance of an empty cavity site vs. the role of hydrogen bonding is likely to be a major issue in understanding the compressional behavior of protonated octahedral frameworks.