

## **Equation of state of brucite: Single-crystal Brillouin spectroscopy study and polycrystalline pressure-volume-temperature measurement**

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### **ABSTRACT**

Acoustic velocities of brucite were measured at room pressure in over 48 directions from Brillouin spectroscopy using a natural sample. These data are supplemented with volume measurements as a function of pressure and temperature that range from ambient conditions to 11 GPa and 873 K using synchrotron X-ray radiation at the National Synchrotron Light Source (NSLS) in a cubic-anvil apparatus (SAM-85) with a synthetic polycrystalline sample. The diffraction patterns are collected during cooling cycles to minimize the effect of deviatoric stress on the measurements. These data yield internally consistent thermoelastic parameters defining the equation of state of brucite along with the single-crystal elastic moduli. The Brillouin spectroscopy measurements are best fit with the following elastic model:  $C_{11} = 156.7(8)$ ,  $C_{33} = 46.3(8)$ ,  $C_{44} = 21.7(5)$ ,  $C_{12} = 44.4(10)$ ,  $C_{13} = 12.0(15)$ , and  $C_{14} = 0.2(8)$  GPa. The resultant linear compressibilities of the  $a$  and  $c$  axes are  $3.8(1) \times 10^{-3}$  and  $19.6(6) \times 10^{-3}$  (GPa $^{-1}$ ), respectively, with the Reuss bound for the bulk modulus,  $K_R = 36.7(10)$  GPa and the Hill average,  $K_H = 46(1)$  GPa. The unit-cell parameters ( $a$ ,  $c$ , and volume) determined from the diffraction measurements were fit with a Birch-Murnaghan equation of state, yielding  $K_0 = 39.6(14)$  GPa,  $K' = 6.7(7)$ ,  $(\partial K_T / \partial T)_P = -0.0114(16)$  GPa/K, and  $\alpha = 5.0(7) \times 10^{-5}$ /K. The bulk modulus and linear compressibilities from X-ray diffraction are in agreement with those from Brillouin spectroscopy. The ratio of linear compressibility of the  $a$  to  $c$  axes is about five times at ambient conditions and reduces to almost unity by 10 GPa. The axial thermal expansions reflect a similar pressure dependence. The ambient shear anisotropy ( $C_{44}/C_{66}$ ) is about 2.5.