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Compression of $CaTiO_3$ and $CaGeO_3$ perovskites

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ABSTRACT

High-pressure single-crystal X-ray diffraction measurements of $CaTiO_3$ and $CaGeO_3$ perovskite have been carried out to 9.7 and 8.6 GPa, respectively, at room temperature. Fitting a third-order Birch-Murnaghan equation-of-state to the *P-V* data yields values of V_0 = 223.764 ± 0.017 Å^3, $K_{T,0}$ = 170.9 ± 1.4 GPa, and $K' = \partial K/\partial P$ = 6.6 ± 0.3 for $CaTiO_3$ and V_0 = 206.490 ± 0.017 Å^3, $K_{T,0}$ = 194.0 ± 2.1 GPa, and K' = 6.1 ± 0.5 for $CaGeO_3$. A similar analysis of the axial compressibilities shows that the degree of anisotropic compression in both perovskites is less than 10%. In $CaTiO_3$ the *a* and *b* axes have similar compressibilities (K_a = 168.7 ± 2.1 GPa, K_b = 168.3 ± 1.9 GPa) whereas the *c* axis is the least compressible (K_c = 175.3 ± 1.5 GPa). In $CaGeO_3$, the *b* axis (K_b = 188 ± 4 GPa) and the *a* axis (K_a = 195 ± 5 GPa) are more compressible than the *c* axis (K_c = 204 ± 3 GPa). The variations with pressure of all axes show significant curvature with increasing pressure and have K' values ranging from 5.7 ± 0.5 to 7.0 ± 0.4 in $CaTiO_3$ and 5.0 ± 0.9 to 6.9 ± 1.2 in $CaGeO_3$. No phase transition was detected. There is evidence, however, that in $CaGeO_3$ the tetragonal to orthorhombic spontaneous strain decreases slightly with pressure which may indicate that a phase transition occurs at a pressure above 10 GPa. Elasticity trends of Ca-perovskites relating bulk modulus and molar volume are independent of both the degree of distortion from cubic symmetry and the symmetry of the structure.