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Pressure-temperature stability studies of FeOOH using X-ray diffraction

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Abstract

The Mie-Grüneisen formalism is used to fit a Birch-Murnaghan equation of state to high-temperature (T), high-pressure (P) X-ray diffraction unit-cell volume (V) measurements on synthetic goethite (α-FeOOH) to combined conditions of T = 23–250 °C and P = 0–29.4 GPa. We find the zero-pressure thermal expansion coefficient of goethite to be $\alpha_0 = 2.3\ (\pm 0.6) \times 10^{-5}\ K^{-1}$ over this temperature range. Our data yield zero-pressure compressional parameters: $V_0 = 138.75\ (\pm 0.02)$ Å^3, bulk modulus $K_0 = 140.3\ (\pm 3.7)$ GPa, pressure derivative $K_0' = 4.6\ (\pm 0.4)$, Grüneisen parameter $\gamma_0 = 0.91\ (\pm 0.07)$, and Debye temperature $\Theta_0 = 740\ (\pm 5)$ K. We identify decomposition conditions for 2α-FeOOH $\rightarrow$ α-Fe_2O_3 + H_2O at 1–8 GPa and 100–400 °C, and the polymorphic transition from α-FeOOH (*Pbnm*) to ε-FeOOH ($P2_1mn$). The non-quenchable, high-pressure ε-FeOOH phase P-V data are fitted to a second-order (Birch) equation of state yielding, $K_0 = 158\ (\pm 5)$ GPa and $V_0 = 66.3\ (\pm 0.5)$ Å^3.

Keywords: Goethite, XRD data, diamond-anvil cell, compressibility measuresments