American Mineralogist, Volume 104, pages 897–904, 2019

High-pressure phase transitions of clinoenstatite

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Abstract

Clinoenstatite ($Mg_2Si_2O_6$) undergoes a well-known phase transition from a low-pressure form (LPCEN, space group $P2_1/c$) to a high-pressure form (HPCEN, space group $C2/c$) at ~6 GPa. High-pressure structure refinements of HPCEN were carried out based on single-crystal X-ray diffraction experiments between 9.5 and 35.5 GPa to determine its *P-V* equation of state and structural evolution over an expanded pressure range relevant to pyroxene metastability. The best-fit isothermal equation of state to our data combined with the five data points between 5.34 and 7.93 GPa from Angel and Hugh-Jones (1994) yields a second-order Birch-Murnaghan equation with K_{T0} = 121(2) GPa and V_0 = 403.9(5) Å^3 (with K'_{T0} = 4 implied). Further reduction of misfit upon fitting a third-order Birch-Murnaghan equation is not significant at the 90% confidence level. At ~45 GPa, a transition from HPCEN to a $P2_1/c$-structured polymorph (HPCEN2) was observed, which is isostructural to the $P2_1/c$ phase recently observed in diopside ($CaMgSi_2O_6$) at 50 GPa (Plonka et al. 2012) and in clinoferrosilite ($Fe_2Si_2O_6$) at 30–36 GPa (Pakhomova et al. 2017). Observation of HPCEN2 in $Mg_2Si_2O_6$ completes the third apex of the pyroxene quadrilateral wherein HPCEN2 is found, facilitating a broader view of clinopyroxene crystal chemistry at conditions relevant to metastability in the Earth's mantle along cold subduction geotherms.

Keywords: $MgSiO_3$, clinoenstatite, enstatite, pyroxene, single-crystal X-ray diffraction