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Low- and high-temperature single crystal X-ray diffraction study of CaGeO$_3$ perovskite synthesized at 12 GPa and 1253 K AKIHIKO NAKATSUKA, NORIAKI NAKAYAMA, Graduate School of Science and Engineering, Yamaguchi University, HIROSHI ARIMA, Institute for Materials Research, Tohoku University, AKIRA YOSHIASA, Graduate School of Science and Technology, Kumamoto University — The perovskite (pv) phase of CaGeO$_3$ has the $Pbnm$ structure (orthorhombic) at ambient condition and is the best analogue of MgSiO$_3$ pv, a major constituent of the earth’s lower mantle. The CaGeO$_3$ pv was previously reported to undergo the phase transition to the $Cmcm$ structure (orthorhombic) at 520 K. However, there is some doubt as for the existence of this high-$T$ phase, and the structural behavior of the $Pbnm$ phase at high-$T$ is also unclear. Clarifying these is important to help the crystal chemical understanding of MgSiO$_3$ pv in the lower mantle. For this purpose, we have conducted the single crystal X-ray diffraction study of CaGeO$_3$ pv in the range from 98 to 873 K. The crystal structures were successfully refined in the $Pbnm$ structure up to 873 K, and the $R$-factors reached $R = 0.0142-0.0229$ and $wR = 0.0117-0.0184$ for each temperature. The structural parameters, such as lattice constants and volume, varied monotonously with temperature. No phase transition was thus observed in the investigated temperature range. The further detailed structural properties of CaGeO$_3$ pv at high-$T$ will be discussed.

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