

LETTER

**Crystal structure of single-crystal CaGeO<sub>3</sub> tetragonal garnet synthesized at 3 GPa and 1000 °C**

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ABSTRACT

Single crystals of CaGeO<sub>3</sub> garnet were synthesized at 3 GPa and 1000 °C using a cubic anvil type of high pressure apparatus and the crystal structure was refined from single crystal X-ray diffraction data. This garnet is tetragonal with lattice parameters of  $a = 12.535(2)$  Å,  $c = 12.370(2)$  Å,  $V = 1943.5(5)$  Å<sup>3</sup> and belongs to space group  $I4_1/a$ . Two dodecahedral sites are occupied only by Ca with mean Ca-O bond lengths of 2.480(4) and 2.467(4) Å. The Ca and Ge cations are completely ordered at two octahedral sites with mean Ca-O = 2.301(3) Å and mean Ge-O = 1.910(3) Å. Three tetrahedral sites are occupied only by Ge, and their mean Ge-O bond lengths are 1.753(3), 1.787(4), and 1.764(4) Å. Furthermore, the present tetragonal garnet has an unusual feature in that the mean value [2.704(5) Å] of the shared edge lengths of GeO<sub>6</sub> octahedron is larger than that [2.699(5) Å] of the unshared ones, as has also been observed for other tetragonal garnets with  $I4_1/a$ .