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LETTER

A new high-pressure $CaGe_2O_5$ polymorph with 5- and 6-coordinated germanium

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ABSTRACT

We discovered a new $CaGe_2O_5$ polymorph in high-pressure experiments (above 8 GPa). The phase is orthorhombic, space group *Pbam*, with $a = 7.306(2)$, $b = 8.268(2)$, $c = 5.714(1)$ Å, $V = 345.2(1)$ Å^3, and $Z = 4$. The new phase, which we call post-titanite $CaGe_2O_5$, is the high-pressure polymorph of titanite $CaGe_2O_5$. The structure of this new polymorph is based on a network of 5- and 6-coordinated Ge polyhedra and 8-coordinated Ca atoms. Following the germanate analog to silicate, post-titanite $CaSi_2O_5$ could be expected to form at high-pressure conditions and thus might exist in Earth's mantle.

Keywords: $CaGe_2O_5$ polymorph, post-titanite, 5- and 6-coordinated Ge, Earth's mantle