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LETTERS

$MnSi_2O_5$ with the titanite structure: A new high-pressure phase in the MnO-SiO_2 binary

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ABSTRACT

Single crystals of $MnSiO(SiO_4)$ with the titanite structure together with $MnSiO_3$ clinopyroxene were synthesized from a MnO-SiO_2 oxide mixture at 1000 °C and 9.2 GPa in a multi-anvil press. The crystal structure of $MnSi_2O_5$ [space group $C2/c$, a = 6.332(1) Å, b = 8.161(1) Å, c = 6.583(1) Å, β = 114.459(3)°, and V = 309.66 Å^3] was refined at room temperature from single-crystal X-ray data to R1 = 2.23%. The monoclinic $MnSi_2O_5$ phase has the titanite aristotype structure and is similar to the monoclinic Ca-analogue $CaSi_2O_5$. Si occurs in compressed octahedral coordination, replacing Ti in titanite, and in tetrahedral coordination as an orthosilicate group. Mn has a distorted sevenfold coordination with Mn-O distances between 2.086 and 2.365 Å.