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Rietveld refinement of $\text{Ca}_2\text{TiSiO}_6$ perovskite

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ABSTRACT

The structure of the high-pressure cubic double perovskite $\text{Ca}_2\text{TiSiO}_6$ was refined using synchrotron X-ray powder data [S.G. $Fm\bar{3}m$, $a = 7.4105(1)$ Å, $Z = 4$]. Ti and Si are fully ordered into alternating octahedra in the perovskite framework, with Ca occupying a tetrahedrally distorted cuboctahedron. The cation-anion bond lengths are Ti-O = 1.947(3) Å, Si-O = 1.758(3) Å, and Ca-O = 2.622(1) Å.