

Crystal chemistry of high-pressure BaSi₄O₉ in the trigonal (*P3*) barium tetragermanate structure

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ABSTRACT

Crystals of BaSi₄O₉ synthesized at 4 GPa and 1000 °C were determined to be isostructural with barium tetragermanate [trigonal, space group *P3*, $a = 11.2469(11)$ and $c = 4.4851(6)$ Å, $V = 491.3(1)$ Å³]. The structure ($R = 2.4\%$) features a corner-linked framework of three-member silicate tetrahedral rings, which are cross-linked by isolated silicate octahedra. Ba cations occupy tenfold-coordinated sites in channels defined by the silicate framework. This structure is 4.2% denser than the topologically similar benitoite form of high-pressure BaSi₄O₉, which was produced by grinding the barium tetragermanate-type crystals described in this report.