

Sodium heptasilicate: A high-pressure silicate with six-membered rings of tetrahedra interconnected by SiO₆ octahedra: (Na₈Si[Si₆O₁₈])

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ABSTRACT

Crystals of sodium heptasilicate (Na₈Si₇O₁₈) have been grown at 9 GPa, 1000 °C using the MA6/8 superpress at Edmonton. The X-ray structure was determined at room pressure ($R = 5.8\%$). Sodium heptasilicate is trigonal with $a = 7.180(1)$ Å, $\alpha = 87.26(1)^\circ$, space group $R\bar{3}m$, $Z = 1$, and $D_x = 3.009$ g/cm³. The structure contains isolated six-membered UDUDUD rings of SiO₄ tetrahedra interconnected by SiO₆ octahedra with ⁶Si:⁴Si = 1:6, giving a structural formula of Na₈Si[Si₆O₁₈]. The mixed ⁴Si,⁶Si framework is undersaturated because only one of the non-bridging O atoms in the SiO₄ tetrahedron is shared with the SiO₆ octahedron. Six Na cations per formula unit (pfu) are in eightfold coordination with O, and two are in a distorted and compressed octahedral coordination. Sodium heptasilicate belongs to the homologous series Na_{2k}Na_{2(m-k)}}Si_{m-k}[Si_{n-m+k}O_{2n+m}], with $k < m < n$ and $(n - m + k) \geq (3/2)(m - k)$. The X-ray structure is consistent with microprobe analysis data and revises the earlier characterization of this phase as ζ -Na₂Si₂O₅. The sodium heptasilicate structure does not fully relax with decompression and undergoes incipient displacive transformation ($R\bar{3}m \rightarrow R\bar{3}$) with minor positional disorder of Na cations.