

Ba₃Nb₆Si₄O₂₆ [1]; Ba₃(Ti_{1.2}Nb_{4.8})Si₄O_{25.4} [4], belkovite

Structural features: Triple infinite chains of vertex-linked NbO₆ octahedra share vertices with units of two vertex-linked SiO₄ tetrahedra to form a 3D-framework; Ba in channels parallel to [001]. See Fig. IV.8.

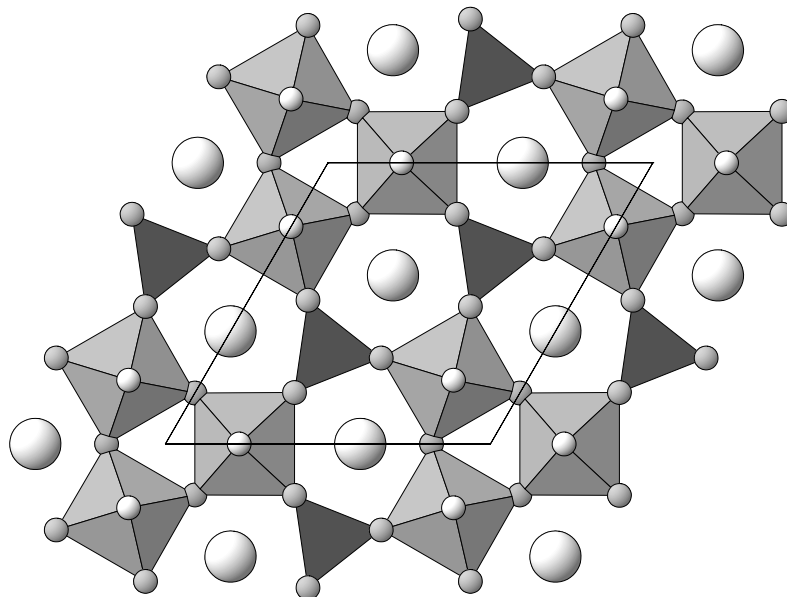


Fig. IV.8. **Ba₃Nb₆Si₄O₂₆**

Arrangement of SiO₄ tetrahedra (dark), NbO₆ octahedra (light) (O atoms small) and Ba atoms (large) viewed along [001].

Shannon J., Katz L. (1970) [1]

Ba₃Nb₆O₂₆Si₄

a = 0.9, *c* = 0.789 nm, *c/a* = 0.877, *V* = 0.5535 nm³, *Z* = 1

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|---------------------|-----------------------------|-----------------------------|-----------------------------|------|--------------------------------------|
| O1 | 12 <i>l</i> | 1 | 0.183 | 0.4888 | 0.2159 | | non-colinear SiNb |
| Nb2 | 6 <i>i</i> | .. <i>m</i> | 0.23809 | 0 | 0.26061 | | octahedron O ₆ |
| O3 | 6 <i>i</i> | .. <i>m</i> | 0.8188 | 0 | 0.2642 | | non-colinear Nb ₂ |
| Si4 | 4 <i>h</i> | 3.. | ¹ / ₃ | ² / ₃ | 0.29691 | | tetrahedron O ₄ |
| O5 | 3 <i>g</i> | <i>m</i> 2 <i>m</i> | 0.2734 | 0 | ¹ / ₂ | | non-colinear Nb ₂ |
| O6 | 3 <i>f</i> | <i>m</i> 2 <i>m</i> | 0.2269 | 0 | 0 | | non-colinear Nb ₂ |
| Ba7 | 3 <i>f</i> | <i>m</i> 2 <i>m</i> | 0.59952 | 0 | 0 | | 12-vertex polyhedron O ₁₂ |
| O8 | 2 <i>d</i> | -6.. | ¹ / ₃ | ² / ₃ | ¹ / ₂ | | colinear Si ₂ |

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, *R* = 0.046

Remarks: In table 1 of [1] the *x*-coordinate of the Ba site is misprinted as 0.59334 instead of 0.59952 (see [3]). A refinement on X-ray powder diffraction data is reported in [2].

References: [1] Shannon J., Katz L. (1970), Acta Crystallogr. B 26, 105-109. [2] Choisnet J., Nguyen N., Groult D., Raveau B. (1976), Mater. Res. Bull. 11, 887-894. [3] Shannon J., Katz L. (1972), Acta

Crystallogr. B 28, 3438b. [4] Yamnova N.A., Pushcharovskii D.I., Voloshin A.V. (1990), Sov. Phys. Crystallogr. 35, 195-196 (Kristallografiya 35, 346-348).