

BaTiSi <sub>3</sub> O <sub>9</sub>	<i>hP</i> 28	(188) <i>P</i> -6 <i>c</i> 2 – 1k <sup>2</sup> ea
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**BaTiSi<sub>3</sub>O<sub>9</sub>** [2], benitoite, Strukturbericht notation S3<sub>2</sub>  
 Structural features: 3-rings of vertex-linked SiO<sub>4</sub> tetrahedra share vertices with TiO<sub>6</sub> octahedra to form a 3D-framework; Ba in channels parallel to [001]. See Fig. IV.9.

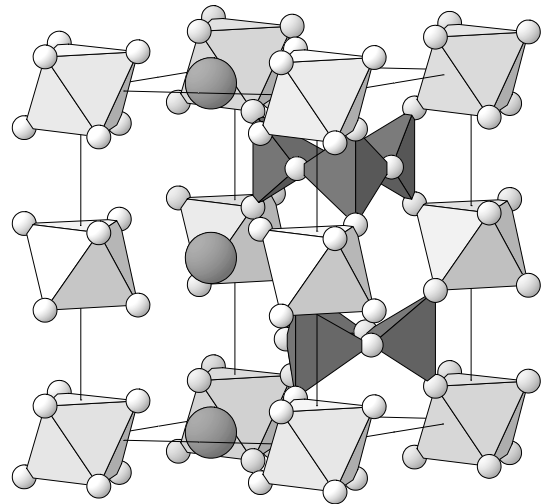


Fig. IV.9. **BaTiSi<sub>3</sub>O<sub>9</sub>**  
 Arrangement of SiO<sub>4</sub> tetrahedra (dark), TiO<sub>6</sub> octahedra (light) (O atoms small) and Ba atoms (large).

Fischer K. (1969) [1]  
 BaO<sub>9</sub>Si<sub>3</sub>Ti  
 $a = 0.6641$ ,  $c = 0.97597$  nm,  $c/a = 1.470$ ,  $V = 0.3728$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.24533	0.00886	0.11275		non-colinear SiTi
O2	6 <i>k</i>	<i>m</i> ..	0.07985	0.60592	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
Si3	6 <i>k</i>	<i>m</i> ..	0.11505	0.37726	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
Ba4	2 <i>e</i>	3.2	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0		octahedron O <sub>6</sub>
Ti5	2 <i>a</i>	3.2	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift <sup>2</sup>/<sub>3</sub> <sup>1</sup>/<sub>3</sub> 0  
 Experimental: single crystal, diffractometer, X-rays, wR = 0.045

Remarks: Natural specimen from San Benito, California.

References: [1] Fischer K. (1969), Z. Kristallogr. 129, 222-243. [2] Zachariasen W.H. (1930), Z. Kristallogr. 74, 139-146.