

BaSi ₄ O ₉	<i>hP</i> 28	(188) <i>P</i> -6 <i>c</i> 2 – 1 <i>k</i> ² <i>ea</i>
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BaSi₄O₉ [1]

Structural features: 3-rings of vertex-linked SiO₄ tetrahedra share vertices with SiO₆ octahedra to form a 3D-framework; Ba in channels parallel to [001]. Ordering variant of BaTiSi₃O₉ (benitoite).

Finger L.W. et al. (1995) [1]

BaO₉Si₄

$a = 0.64953$, $c = 0.93465$ nm, $c/a = 1.439$, $V = 0.3415$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.22923	0.00127	0.1032		non-colinear Si ₂
O2	6 <i>k</i>	<i>m</i> ..	0.07103	0.58797	¹ / ₄		non-colinear Si ₂
Si3	6 <i>k</i>	<i>m</i> ..	0.12023	0.36587	¹ / ₄		tetrahedron O ₄
Ba4	2 <i>e</i>	3.2	² / ₃	¹ / ₃	0		octahedron O ₆
Si5	2 <i>a</i>	3.2	0	0	0		octahedron O ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift ²/₃ ¹/₃ 0

Experimental: powder, diffractometer, X-rays, R_B = 0.030

References: [1] Finger L.W., Hazen R.M., Fursenko B.A. (1995), J. Phys. Chem. Solids 56, 1389-1393.