

BaCa[SiO₄]*hP*56(186) *P*6₃*mc* – dc⁶b³a**BaCaSiO₄** [1]

Structural features: Single SiO₄ tetrahedra share atoms with distorted CaO₆ octahedra and CaO₆O₃ tricapped trigonal prisms.

Il'inets A.M., Bikbau M.Y. (1989) [1]

BaCaO₄Si $a = 1.10189$, $c = 0.70164$ nm, $c/a = 0.637$, $V = 0.7378$ nm³, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.092	0.417	0.311		single atom Si
O2	6 <i>c</i>	. <i>m</i> .	0.085	0.915	0.269		single atom Si
Si3	6 <i>c</i>	. <i>m</i> .	0.1678	0.8321	0.2302		tetrahedron O ₄
O4	6 <i>c</i>	. <i>m</i> .	0.196	0.804	0.011		single atom Si
Ca5	6 <i>c</i>	. <i>m</i> .	0.4826	0.5174	0.005		tricapped trigonal prism O ₉
O6	6 <i>c</i>	. <i>m</i> .	0.593	0.407	0.166		single atom Si
Ba7	6 <i>c</i>	. <i>m</i> .	0.832	0.168	0.1884		single atom O
O8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.003		single atom Si
Ba9	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3342		10-vertex polyhedron O ₁₀
Si10	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.778		tetrahedron O ₄
Ca11	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		octahedron O ₆

Transformation from published data: origin shift 0 0 0.283

Experimental: single crystal, diffractometer, X-rays, R = 0.051

References: [1] Il'inets A.M., Bikbau M.Y. (1989), Sov. Phys. Crystallogr. 34, 677-679 (Kristallografiya 34, 1123-1126).