

$\text{Ba}_3\text{Ta}_6[\text{Si}_2\text{O}_7]_2\text{O}_9$ $hP36$ (189) $P-62m - \text{li}^2\text{hgfc}$ **Ba₃Ta₆Si₄O₂₃** [1]

Structural features: TaO₅ square pyramids and units of two vertex-linked SiO₄ tetrahedra share vertices to form approximately planar slabs; Ba in channels of pentagonal cross-section parallel to [001].

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

 $\text{Ba}_3\text{O}_{23}\text{Si}_4\text{Ta}_6$ $a = 0.8997$, $c = 0.7745$ nm, $c/a = 0.861$, $V = 0.5429$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12l	1	0.1773	0.4939	0.2802		non-colinear SiTa
Ta2	6i	$\bar{3}m$	0.2384	0	0.2428		square pyramid O ₅
O3	6i	$\bar{3}m$	0.8191	0	0.2363		non-colinear Ta ₂
Si4	4h	3 $\bar{2}$	$\frac{1}{3}$	$\frac{2}{3}$	0.2046		tetrahedron O ₄
Ba5	3g	$m2m$	0.6016	0	$\frac{1}{2}$		trigonal prism O ₆
O6	3f	$m2m$	0.2919	0	0		non-colinear Ta ₂
O7	2c	$\bar{6}$	$\frac{1}{3}$	$\frac{2}{3}$	0		colinear Si ₂

Experimental: single crystal, diffractometer, X-rays, R = 0.077

References: [1] Shannon J., Katz L. (1970), J. Solid State Chem. 1, 399-408.