

Ba₆Nb₁₄Si₄O₄₇*hP142*(185) *P6₃cm – d⁴c¹³b⁴***Ba₆Nb₁₄Si₄O₄₇** [1]

Structural features: NbO₆ octahedra are interconnected via common edges and vertices and Si₂O₇ units (two vertex-linked SiO₄ tetrahedra) to form a 3D-framework.

Serra D.L., Hwu S.J. (1992) [1]

Ba₆Nb₁₄O₄₇Si₄*a* = 0.9022, *c* = 2.789 nm, *c/a* = 3.091, *V* = 1.9660 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.169	0.479	0.2337		non-colinear Nb ₂
O2	12 <i>d</i>	1	0.184	0.488	0.3619		non-colinear SiNb
O3	12 <i>d</i>	1	0.306	0.487	0.0233		non-colinear SiNb
O4	12 <i>d</i>	1	0.313	0.486	0.1464		non-colinear Nb ₂
O5	6 <i>c</i>	.. <i>m</i>	0.177	0	0.8769		non-colinear Nb ₂
O6	6 <i>c</i>	.. <i>m</i>	0.18	0	0.0061		non-colinear Nb ₂
O7	6 <i>c</i>	.. <i>m</i>	0.186	0	0.161		non-coplanar triangle Nb ₃
Nb8	6 <i>c</i>	.. <i>m</i>	0.2159	0	0.23497		octahedron O ₆
O9	6 <i>c</i>	.. <i>m</i>	0.217	0	0.3013		non-colinear Nb ₂
O10	6 <i>c</i>	.. <i>m</i>	0.217	0	0.5822		non-colinear Nb ₂
O11	6 <i>c</i>	.. <i>m</i>	0.235	0	0.725		non-coplanar triangle Nb ₃
Nb12	6 <i>c</i>	.. <i>m</i>	0.2363	0	0.37509		octahedron O ₆
Nb13	6 <i>c</i>	.. <i>m</i>	0.238	0	0.50745		octahedron O ₆
Nb14	6 <i>c</i>	.. <i>m</i>	0.255	0	0.64704		octahedron O ₆
O15	6 <i>c</i>	.. <i>m</i>	0.281	0	0.4429		non-colinear Nb ₂
Ba16	6 <i>c</i>	.. <i>m</i>	0.3999	0	0.0826		12-vertex polyhedron O ₁₂
Ba17	6 <i>c</i>	.. <i>m</i>	0.5847	0	0.29987		pseudo Frank-Kasper O ₁₃
Si18	4 <i>b</i>	3..	¹ / ₃	² / ₃	0.0		tetrahedron O ₄
Nb19	4 <i>b</i>	3..	¹ / ₃	² / ₃	0.19761		octahedron O ₆
Si20	4 <i>b</i>	3..	¹ / ₃	² / ₃	0.3839		tetrahedron O ₄
O21	4 <i>b</i>	3..	¹ / ₃	² / ₃	0.4421		colinear Si ₂

Transformation from published data: origin shift 0 0 0.7145

Experimental: single crystal, diffractometer, X-rays, R = 0.025, T = 296 K

References: [1] Serra D.L., Hwu S.J. (1992), J. Solid State Chem. 101, 32-40.