

KNa₉Ba₆Ca₂Ti₆Mn₆Si₃₆B₁₂O₁₂₃[OH]₂

hP203

(175) $P6/m - 1^{13}k^4j^2gfdca$ **KNa₉Ba₆Ca₂(Mn,Fe)₆(Ti,Nb,Ta)₆Si₃₆B₁₂O₁₁₄O₉(OH)₂** [1], tienshanite

Structural features: Branched 6-rings formed by eighteen vertex-linked SiO₄ tetrahedra are interconnected via TiO₆ octahedra and rings of edge-linked MnO₅ square pyramids on one side and units of two vertex-linked BO₄ tetrahedra on the other side to form a 3D-framework; K, Na and Ca in the layers containing the O atoms belonging to two BO₄ tetrahedra, Ba and OH in the TiMn layers.

Malinovskii I.A. et al. (1977) [1]

B₁₂Ba₆Ca₂H₂KMn₆Na₉O₁₂₅Si₃₆Ti₆ $a = 1.6772$, $c = 1.0434$ nm, $c/a = 0.622$, $V = 2.5419$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	12l	1	0.015	0.363	0.215		tetrahedron O ₄
O2	12l	1	0.021	0.372	0.363		non-colinear SiTi
O3	12l	1	0.027	0.187	0.366		single atom Si
Si4	12l	1	0.029	0.192	0.221		tetrahedron O ₄
O5	12l	1	0.044	0.288	0.16		non-colinear Si ₂
O6	12l	1	0.076	0.459	0.138		non-colinear BSi
B7	12l	1	0.176	0.512	0.121		tetrahedron O ₄
O8	12l	1	0.178	0.068	0.154		non-colinear Si ₂
O9	12l	1	0.22	0.485	0.235		non-colinear BSi
O10	12l	1	0.414	0.09	0.16		non-colinear Si ₂
Si11	12l	1	0.505	0.18	0.23		tetrahedron O ₄
O12	12l	1	0.514	0.153	0.369		non-colinear SiTi
O13	12l	1	0.594	0.207	0.138		non-colinear BSi
Ba14	6k	<i>m</i> ..	0.1856	0.5067	1/2		pseudo Frank-Kasper (OH)O ₁₀
Mn15	6k	<i>m</i> ..	0.2207	0.0844	1/2		square pyramid O ₅
O16	6k	<i>m</i> ..	0.358	0.131	1/2		non-colinear TiMn
Ti17	6k	<i>m</i> ..	0.4206	0.0707	1/2		octahedron O ₆
O18	6j	<i>m</i> ..	0.208	0.501	0		non-colinear B ₂
Na19	6j	<i>m</i> ..	0.342	0.155	0		monocapped trigonal prism O ₇
O20	3g	2/ <i>m</i> ..	1/2	0	1/2		colinear Ti ₂
Na21	3f	2/ <i>m</i> ..	1/2	0	0		coplanar square O ₄
(OH)22	2d	-6..	1/3	2/3	1/2		coplanar triangle Ba ₃
Ca23	2c	-6..	1/3	2/3	0		tricapped trigonal prism O ₉
K24	1a	6/ <i>m</i> ..	0	0	0		hexagonal prism O ₁₂

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.083

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Splitting of the Na site in Wyckoff position 3f and the Ti site is reported in [2].

References: [1] Malinovskii I.A., Pobedinskaya E.A., Belov N.V. (1977), Dokl. Akad. Nauk SSSR 236, 863-865. [2] Cooper M.A., Hawthorne F.C., Grew E.S. (1998), Can. Mineral. 36, 1305-1310.