

Ba₂₄CaTi₁₂Fe₄Si₁₂[Si₂O₇]₆Cl₆O₄₂[OH]₂₄[H₂O]₁₄ *hP*193 (187) *P*-6*m*2 – o⁶n¹⁰ml³k⁶j⁴ihdba

Ba₂₄CaFe₄Ti₁₂[Si₁₂O₃₆](Si₂O₇)₆(O,OH)₃₀Cl₆·14H₂O [1], traskite

Structural features: 12-rings of vertex-linked SiO₄ tetrahedra and Si₂O₇ units (two vertex-linked SiO₄ tetrahedra) share vertices with Ti(O₅[OH]) octahedra, Fe(O₃[OH]₃) octahedra and CaO₆ trigonal prisms to form a 3D-framework; H₂O in large channels formed by the 12-rings.

Malinovskii I.A. et al. (1976) [1]

Ba₂₄CaCl₆Fe₄H₅₂O₁₂₂Si₂₄Ti₁₂

a = 1.789, *c* = 1.233 nm, *c/a* = 0.689, *V* = 3.4175 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ti1	12 <i>o</i>	1	0.0055	0.4062	0.203		octahedron O ₅ (OH)
(OH)2	12 <i>o</i>	1	0.013	0.302	0.286		single atom Ti
O3	12 <i>o</i>	1	0.089	0.466	0.315		non-colinear SiTi
O4	12 <i>o</i>	1	0.1	0.418	0.105		non-colinear SiTi
O5	12 <i>o</i>	1	0.403	0.092	0.115		non-colinear SiTi
O6	12 <i>o</i>	1	0.472	0.095	0.321		single atom Si
Ba7	6 <i>n</i>	. <i>m</i> .	0.2034	0.7966	0.262		square antiprism O ₄ (OH) ₃ Cl
(OH)8	6 <i>n</i>	. <i>m</i> .	0.285	0.715	0.112		single atom Fe
O9	6 <i>n</i>	. <i>m</i> .	0.387	0.613	0.364		single atom Si
Si10	6 <i>n</i>	. <i>m</i> .	0.44	0.56	0.372		tetrahedron O ₄
O11	6 <i>n</i>	. <i>m</i> .	0.509	0.491	0.139		non-colinear Ti ₂
Si12	6 <i>n</i>	. <i>m</i> .	0.569	0.431	0.361		tetrahedron O ₄
O13	6 <i>n</i>	. <i>m</i> .	0.617	0.383	0.328		non-colinear SiFe
(OH)14	6 <i>n</i>	. <i>m</i> .	0.715	0.285	0.118		single atom Fe
Ba15	6 <i>n</i>	. <i>m</i> .	0.7793	0.2207	0.257		tricapped trigonal prism (OH)O ₆ Cl(OH ₂)
(OH ₂)16	6 <i>n</i>	. <i>m</i> .	0.878	0.122	0.254		4-vertex polyhedron (OH) ₂ Ba(OH ₂)
Ba17	6 <i>m</i>	<i>m</i> ..	0.0103	0.3618	1/2		square antiprism O ₅ (OH) ₂ Cl
Si18	6 <i>l</i>	<i>m</i> ..	0.092	0.358	0		tetrahedron O ₄
O19	6 <i>l</i>	<i>m</i> ..	0.272	0.005	0		non-colinear Si ₂
Si20	6 <i>l</i>	<i>m</i> ..	0.362	0.098	0		tetrahedron O ₄
(OH ₂)21	3 <i>k</i>	<i>mm</i> 2	0.088	0.912	1/2		colinear (OH ₂)Cl
Cl22	3 <i>k</i>	<i>mm</i> 2	0.185	0.815	1/2		square pyramid Ba ₄ (OH ₂)
O23	3 <i>k</i>	<i>mm</i> 2	0.447	0.553	1/2		non-colinear Si ₂
O24	3 <i>k</i>	<i>mm</i> 2	0.571	0.429	1/2		non-colinear Si ₂
Cl25	3 <i>k</i>	<i>mm</i> 2	0.791	0.209	1/2		single atom (OH ₂)
(OH ₂)26	3 <i>k</i>	<i>mm</i> 2	0.864	0.136	1/2		single atom Cl
O27	3 <i>j</i>	<i>mm</i> 2	0.169	0.831	0		non-colinear Si ₂
Ba28	3 <i>j</i>	<i>mm</i> 2	0.4222	0.5778	0		square prism (cube) (OH) ₄ O ₄
Ba29	3 <i>j</i>	<i>mm</i> 2	0.5694	0.4306	0		non-colinear O ₂
O30	3 <i>j</i>	<i>mm</i> 2	0.833	0.167	0		non-colinear Si ₂
Fe31	2 <i>i</i>	3 <i>m</i> .	2/3	1/3	0.229		octahedron O ₃ (OH) ₃
Fe32	2 <i>h</i>	3 <i>m</i> .	1/3	2/3	0.26		octahedron O ₃ (OH) ₃
Ca33	1 <i>d</i>	-6 <i>m</i> 2	1/3	2/3	1/2		trigonal prism O ₆
(OH ₂)34	1 <i>b</i>	-6 <i>m</i> 2	0	0	1/2		coplanar triangle (OH ₂) ₃
(OH ₂)35	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		anticuboctahedron O ₆ (OH ₂) ₆

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.120

Remarks: General formula Ba₂₄A₂B₂CD₁₂[Si₁₂O₃₆][Si₂O₇]₆(O,OH)₃₀Cl₆·14H₂O. Natural specimen from Fresno County, California. 27.30 wt.% SiO₂, 0.45 wt.% Al₂O₃, 5.71 wt.% TiO₂, 4.46 wt.% FeO, 1.35 wt.% MnO, 0.32 wt.% MgO, 0.89 wt.% CaO, 53.50 wt.% BaO, 0.35 wt.% SrO, 3.50 wt.% Cl, and

2.52 wt.% H₂O found by chemical analysis [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Malinovskii I.A., Pobedinskaya E.A., Belov N.V. (1976), Dokl. Akad. Nauk SSSR 229, 1101-1104. [2] Alfors J.T., Stinson M.C., Matthews R.A., Pabst A. (1965), Am. Mineral. 50, 314-340.