

$\text{KBa}_3\text{Ca}_4\text{Cu}_3\text{V}_7\text{O}_{28}$

$hP92$

$(186) P6_3mc - d^2c^{10}b^3a$

$\text{KBa}_3\text{Ca}_4\text{Cu}_3\text{V}_7\text{O}_{28}$ [1]

Structural features: CuO_5 square pyramids and VO_4 tetrahedra share vertices to form infinite slabs, which are interconnected via CaO_6 octahedra and CaO_6 square antiprisms to form a 3D-framework.

Postel M.V., Müller Buschbaum H. (1993) [1]

$\text{Ba}_3\text{Ca}_4\text{Cu}_3\text{VO}_{28}\text{V}_7$

$a = 1.116$, $c = 1.24283$ nm, $c/a = 1.114$, $V = 1.3405$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12d	1	0.413	0.076	0.146		non-colinear VCu
O2	12d	1	0.436	0.094	0.368		non-colinear VCu
Ba3	6c	.m.	0.14322	0.85682	0.251		icosahedron O ₁₂
O4	6c	.m.	0.184	0.816	0.038		single atom V
O5	6c	.m.	0.194	0.806	0.461		single atom V
O6	6c	.m.	0.416	0.584	0.223		single atom V
Ca7	6c	.m.	0.4645	0.5355	0.0288		square antiprism O ₈
Cu8	6c	.m.	0.5404	0.4596	0.251		square pyramid O ₅
V9	6c	.m.	0.8219	0.178	0.0882		tetrahedron O ₄
V10	6c	.m.	0.8277	0.1723	0.4065		tetrahedron O ₄
O11	6c	.m.	0.908	0.092	0.368		single atom V
O12	6c	.m.	0.91	0.09	0.114		single atom V
O13	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.038		single atom V
V14	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1814		tetrahedron O ₄
K15	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.44		non-coplanar triangle O ₃
Ca16	2a	3m.	0	0	0.0		octahedron O ₆

Transformation from published data: origin shift 0 0 0.999

Experimental: single crystal, diffractometer, X-rays, R = 0.087

Remarks: In table 1 of [1] the chemical formula is misprinted as $\text{KBa}_3\text{Ca}_4\text{CuV}_7\text{O}_{28}$ instead of $\text{KBa}_3\text{Ca}_4\text{Cu}_3\text{V}_7\text{O}_{28}$ (given elsewhere).

References: [1] Postel M.V., Müller Buschbaum H. (1993), Z. Anorg. Allg. Chem. 619, 123-127.