

$\text{K}_3\text{Ta}_3[\text{BO}_3]_2\text{O}_6$  $hP20$ (189)  $P-62m-jg^2fc$  **$\text{K}_3\text{Ta}_3\text{B}_2\text{O}_{12}$**  [1]

Structural features: Triple infinite chains of vertex-linked  $\text{TaO}_6$  octahedra share vertices with  $\text{BO}_3$  trigonal units to form a 3D-framework.

Abrahams S.C. et al. (1981) [1]

 $\text{B}_2\text{K}_3\text{O}_{12}\text{Ta}_3$  $a = 0.87816$ ,  $c = 0.3899$  nm,  $c/a = 0.444$ ,  $V = 0.2604$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6j	$m..$	0.1872	0.5035	0		single atom B
O2	3g	$m2m$	0.2628	0	$\frac{1}{2}$		non-colinear $\text{Ta}_2$
K3	3g	$m2m$	0.5957	0	$\frac{1}{2}$		monocapped trigonal prism $\text{O}_7$
Ta4	3f	$m2m$	0.24637	0	0		octahedron $\text{O}_6$
O5	3f	$m2m$	0.8185	0	0		non-colinear $\text{Ta}_2$
B6	2c	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle $\text{O}_3$

Transformation from published data:  $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.013$ ,  $T = 298$  K

References: [1] Abrahams S.C., Zyontz L.E., Bernstein J.L., Remeika J.P., Cooper A.S. (1981), J. Chem. Phys. 75, 5456-5460.