

$\text{K}_6\text{Ta}_{6.5}(\text{O}_{0.6}\text{F}_{0.4})_{24}$  $hP41$  $(174) P-6 - k^6j^7g$  $\text{K}_6\text{Ta}_{6.5}\text{O}_{14.5}\text{F}_{9.5}$  [1]

Structural features:  $\text{Ta}(\text{O},\text{F})_6$  octahedra share vertices to form a 3D-framework; infinite columns of base-linked  $\text{Ta}(\text{O},\text{F})_6$  trigonal prisms (partial disorder) surrounded by K atoms in channels parallel to [001].

Vlasse M. et al. (1979) [1]

 $\text{F}_{9.50}\text{K}_6\text{O}_{14.50}\text{Ta}_{6.50}$  $a = 1.3109$ ,  $c = 0.388$  nm,  $c/a = 0.296$ ,  $V = 0.5774$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
K1	3 <i>k</i>	<i>m</i> ..	0.08497	0.31933	$\frac{1}{2}$		bicapped square prism O <sub>10</sub>
M2	3 <i>k</i>	<i>m</i> ..	0.11567	0.13133	$\frac{1}{2}$	0.5	
M3	3 <i>k</i>	<i>m</i> ..	0.13567	0.08533	$\frac{1}{2}$	0.5	
M4	3 <i>k</i>	<i>m</i> ..	0.34147	0.51053	$\frac{1}{2}$		non-colinear Ta <sub>2</sub>
K5	3 <i>k</i>	<i>m</i> ..	0.35227	0.26503	$\frac{1}{2}$		
M6	3 <i>k</i>	<i>m</i> ..	0.49897	0.13073	$\frac{1}{2}$		non-colinear Ta <sub>2</sub>
M7	3 <i>j</i>	<i>m</i> ..	0.00187	0.49713	0		non-colinear Ta <sub>2</sub>
M8	3 <i>j</i>	<i>m</i> ..	0.21777	0.53733	0		non-colinear Ta <sub>2</sub>
M9	3 <i>j</i>	<i>m</i> ..	0.26297	0.35113	0		single atom Ta
M10	3 <i>j</i>	<i>m</i> ..	0.35107	0.08703	0		single atom Ta
Ta11	3 <i>j</i>	<i>m</i> ..	0.36817	0.52663	0		octahedron O <sub>6</sub>
Ta12	3 <i>j</i>	<i>m</i> ..	0.52697	0.15363	0		octahedron O <sub>6</sub>
M13	3 <i>j</i>	<i>m</i> ..	0.53177	0.30213	0		non-colinear Ta <sub>2</sub>
Ta14	2 <i>g</i>	3..	0	0	0.129	0.25	

M2 = 0.604O + 0.396F; M3 = 0.604O + 0.396F; M4 = 0.604O + 0.396F; M6 = 0.604O + 0.396F; M7 = 0.604O + 0.396F; M8 = 0.604O + 0.396F; M9 = 0.604O + 0.396F; M10 = 0.604O + 0.396F; M13 = 0.604O + 0.396F

Transformation from published data:  $y, x, z$ ; origin shift  $\frac{1}{3} \frac{2}{3} \frac{1}{2}$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.061

Remarks: No attempt was made to distinguish F and O in the refinement; we assigned an approximate value to the F/O ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Vlasse M., Boukhari A., Chaminade J.P., Pouchard M. (1979), Mater. Res. Bull. 14, 101-108.