

$\text{K}_6\text{Ta}_{6.5}\text{O}_{15.75}\text{F}_{6.75}$  $hP48$  $(175) P6/m - \text{Ik}^2_3\text{J}^3\text{Fea}$  $\text{K}_6\text{Ta}_{6.5}\text{O}_{15+x}\text{F}_{6+y}$  [1]

Structural features:  $\text{Ta}(\text{O}_5\text{F})$  octahedra share vertices to form a 3D-framework;  $\text{Ta}(\text{F},\text{O})_6$  octahedra (or trigonal prisms; disorder) surrounded by K atoms in channels parallel to [001].

Arakcheeva A.V. et al. (2001) [1]

 $\text{F}_{6.75}\text{K}_6\text{O}_{15.75}\text{Ta}_{6.48}$  $a = 1.3118$ ,  $c = 0.3862$  nm,  $c/a = 0.294$ ,  $V = 0.5755$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	12l	1	0.038	0.131	0.329	0.125	single atom F
O2	6k	$m..$	0.1497	0.5056	$\frac{1}{2}$		non-colinear $\text{Ta}_2$
K3	6k	$m..$	0.3436	0.0866	$\frac{1}{2}$		non-colinear $\text{F}_2$
F4	6j	$m..$	0.0885	0.346	0		single atom Ta
Ta5	6j	$m..$	0.15603	0.52558	0		octahedron $\text{O}_5\text{F}$
O6	6j	$m..$	0.5327	0.2214	0		non-colinear $\text{Ta}_2$
O7	3f	$2/m..$	$\frac{1}{2}$	0	0		colinear $\text{Ta}_2$
Ta8	2e	$6..$	0	0	0.2197	0.013	
Ta9	1a	$6/m..$	0	0	0	0.45	

 $\text{M1} = 0.5\text{F} + 0.5\text{O}$ Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.029$ 

Remarks: Short interatomic distances for partly occupied site(s). A refinement ignoring the Ta site in Wyckoff position 2e is reported in [2].

References: [1] Arakcheeva A.V., Grinevich V.V., Mitin A.V., Lubman G.U., Shamrai V.F. (2001), Crystallogr. Rep. 46, 182-189 (Kristallografiya 46, 221-229). [2] Arakcheeva A.V., Chapuis G., Grinevich V.V., Shamrai V.F. (2004), Crystallogr. Rep. 49, 70-85 (Kristallografiya 49, 75-91).