

K₆Ta_{6.27}O₁₅F_{7.4}*hP46*(175) *P6/m – 1k²j³fa***K₆Ta_{6.27}O₁₅F_{7.4}** [1]

Structural features: Ta(O₅F) octahedra share vertices to form a 3D-framework; TaF₆ octahedra (or trigonal prisms; disorder) surrounded by K atoms in channels parallel to [001].

Arakcheeva A.V. et al. (2004) [1]

F_{7.36}K₆O₁₅Ta_{6.27}*a* = 1.311, *c* = 0.38625 nm, *c/a* = 0.295, *V* = 0.5749 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>l</i>	1	0.037	0.111	0.4	0.113	
O2	6 <i>k</i>	<i>m</i> ..	0.1506	0.5041	¹ / ₂		non-colinear Ta ₂
K3	6 <i>k</i>	<i>m</i> ..	0.3416	0.0872	¹ / ₂		
F4	6 <i>j</i>	<i>m</i> ..	0.0873	0.3453	0		single atom Ta
Ta5	6 <i>j</i>	<i>m</i> ..	0.15546	0.52532	0		octahedron O ₅ F
O6	6 <i>j</i>	<i>m</i> ..	0.5333	0.2233	0		non-colinear Ta ₂
O7	3 <i>f</i>	2/ <i>m</i> ..	¹ / ₂	0	0		colinear Ta ₂
Ta8	1 <i>a</i>	6/ <i>m</i> ..	0	0	0	0.271	hexagonal prism F ₁₂

Transformation from published data: origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.027

Remarks: Short interatomic distances for partly occupied site(s). An additional Ta site in Wyckoff position 2*e* with occ. = 0.013 is reported in [2].

References: [1] Arakcheeva A.V., Chapuis G., Grinevich V.V., Shamrai V.F. (2004), Crystallogr. Rep. 49, 70-85 (Kristallografiya 49, 75-91). [2] 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).