

K₆Ta_{7.75}O_{17.75}F_{9.25} [1]

Structural features: Ta(O,F)₆ octahedra share vertices to form a 3D-framework; Ta(O,F)₆ trigonal prisms (partial disorder) surrounded by K atoms in large channels parallel to [001], additional K in other channels.

Boukhari A. et al. (1979) [1]

F_{18.52}K₁₂O_{35.48}Ta_{15.50}

a = 1.932, *c* = 0.3878 nm, *c/a* = 0.201, *V* = 1.2536 nm³, *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> ..	0.027	0.15	¹ / ₂		8-vertex polyhedron O ₈
M2	3 <i>k</i>	<i>m</i> ..	0.104	0.496	¹ / ₂		non-colinear Ta ₂
M3	3 <i>k</i>	<i>m</i> ..	0.15	0.313	¹ / ₂		non-colinear Ta ₂
M4	3 <i>k</i>	<i>m</i> ..	0.199	0.154	¹ / ₂		non-colinear Ta ₂
K5	3 <i>k</i>	<i>m</i> ..	0.299	0.533	¹ / ₂		10-vertex polyhedron O ₁₀
M6	3 <i>k</i>	<i>m</i> ..	0.323	0.039	¹ / ₂		non-colinear Ta ₂
M7	3 <i>k</i>	<i>m</i> ..	0.394	0.382	¹ / ₂		non-colinear Ta ₂
K8	3 <i>k</i>	<i>m</i> ..	0.416	0.24	¹ / ₂		square antiprism O ₈
K9	3 <i>k</i>	<i>m</i> ..	0.516	0.108	¹ / ₂		10-vertex polyhedron O ₁₀
M10	3 <i>k</i>	<i>m</i> ..	0.575	0.303	¹ / ₂		non-colinear Ta ₂
M11	3 <i>j</i>	<i>m</i> ..	0.01	0.393	0		non-colinear Ta ₂
M12	3 <i>j</i>	<i>m</i> ..	0.047	0.274	0		non-colinear Ta ₂
M13	3 <i>j</i>	<i>m</i> ..	0.056	0.551	0		non-colinear Ta ₂
Ta14	3 <i>j</i>	<i>m</i> ..	0.1129	0.4953	0		octahedron O ₆
M15	3 <i>j</i>	<i>m</i> ..	0.119	0.07	0		single atom Ta
Ta16	3 <i>j</i>	<i>m</i> ..	0.1641	0.3282	0		octahedron O ₆
M17	3 <i>j</i>	<i>m</i> ..	0.167	0.233	0		non-colinear Ta ₂
M18	3 <i>j</i>	<i>m</i> ..	0.176	0.439	0		non-colinear Ta ₂
M19	3 <i>j</i>	<i>m</i> ..	0.214	0.591	0		single atom Ta
Ta20	3 <i>j</i>	<i>m</i> ..	0.2265	0.1765	0		octahedron O ₆
M21	3 <i>j</i>	<i>m</i> ..	0.274	0.105	0		non-colinear Ta ₂
M22	3 <i>j</i>	<i>m</i> ..	0.281	0.389	0		non-colinear Ta ₂
Ta23	3 <i>j</i>	<i>m</i> ..	0.3227	0.0463	0		octahedron O ₆
M24	3 <i>j</i>	<i>m</i> ..	0.324	0.27	0		non-colinear Ta ₂
Ta25	3 <i>j</i>	<i>m</i> ..	0.3797	0.3859	0		octahedron O ₆
M26	3 <i>j</i>	<i>m</i> ..	0.431	0.147	0		single atom Ta
M27	3 <i>j</i>	<i>m</i> ..	0.479	0.379	0		single atom Ta
Ta28	2 <i>i</i>	3..	² / ₃	¹ / ₃	0.127	0.25	

M2 = 0.657O + 0.343F; M3 = 0.657O + 0.343F; M4 = 0.657O + 0.343F; M6 = 0.657O + 0.343F; M7 = 0.657O + 0.343F; M10 = 0.657O + 0.343F; M11 = 0.657O + 0.343F; M12 = 0.657O + 0.343F; M13 = 0.657O + 0.343F; M15 = 0.657O + 0.343F; M17 = 0.657O + 0.343F; M18 = 0.657O + 0.343F; M19 = 0.657O + 0.343F; M21 = 0.657O + 0.343F; M22 = 0.657O + 0.343F; M24 = 0.657O + 0.343F; M26 = 0.657O + 0.343F; M27 = 0.657O + 0.343F

Transformation from published data: -*y*, -*x*, -*z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.063

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] Boukhari A., Chaminade J.P., Pouchard M., Vlasse M. (1979), Acta Crystallogr. B 35, 2518-2522.