

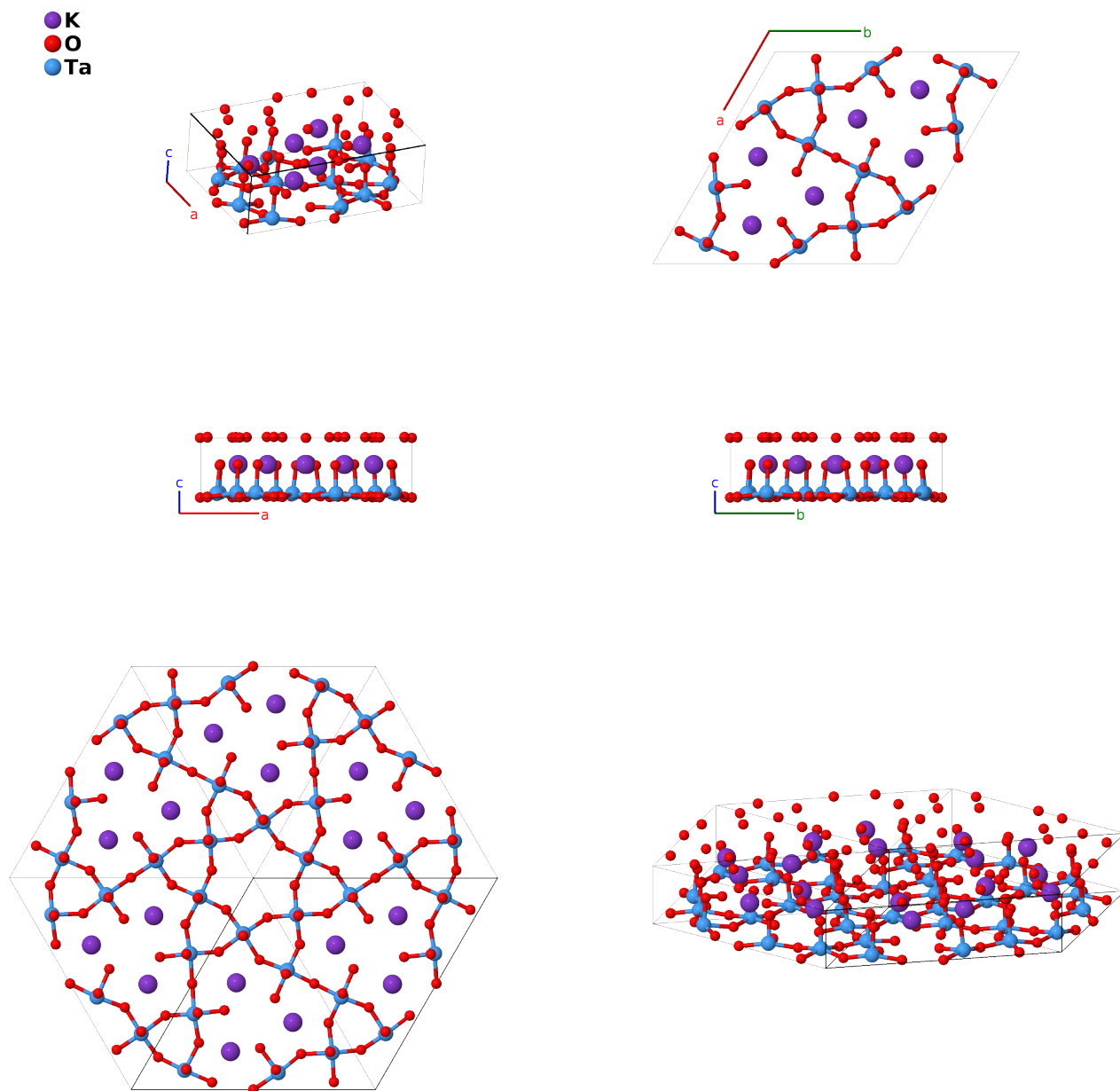
$K_2Ta_4O_9F_4$ Structure: A2B13C4_hP57_168_d_c6d_2d-001

This structure originally had the label A2B13C4_hP57_168_d_c6d_2d. Calls to that address will be redirected here.

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<https://afLOW.org/p/6140>

https://afLOW.org/p/A2B13C4_hP57_168_d_c6d_2d-001



Prototype

$F_4K_2O_9Ta_4$

AFLOW prototype label

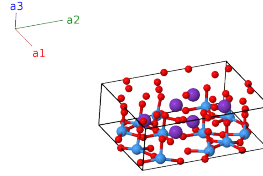
A2B13C4_hP57_168_d_c6d_2d-001

| | |
|-------------------------|--|
| ICSD | 8204 |
| Pearson symbol | hP57 |
| Space group number | 168 |
| Space group symbol | $P6$ |
| AFLOW prototype command | aflow --proto=A2B13C4_hP57_168_d_c6d_2d-001 --params= $a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$ |

- The sites we label “O” are actually 69.2% oxygen and 30.8% fluorine.
- Space group $P6$ #168 allows an arbitrary choice of the origin of the z -axis. Here we set $z_1 = 0$.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|--|-----|---|------------------|-----------|
| \mathbf{B}_1 | $= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$ | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (3c) | O I |
| \mathbf{B}_2 | $= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (3c) | O I |
| \mathbf{B}_3 | $= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$ | (3c) | O I |
| \mathbf{B}_4 | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_5 | $= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_6 | $= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_7 | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_8 | $= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_9 | $= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (6d) | K I |
| \mathbf{B}_{10} | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{11} | $= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{12} | $= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{13} | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{14} | $= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{15} | $= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (6d) | O II |
| \mathbf{B}_{16} | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (6d) | O III |
| \mathbf{B}_{17} | $= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (6d) | O III |
| \mathbf{B}_{18} | $= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (6d) | O III |
| \mathbf{B}_{19} | $= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (6d) | O III |

References

- [1] A. Boukhari, J. P. Chaminade, M. Vlasse, and M. Pouchard, *Structure cristalline de l'oxyfluorure de tantale et de potassium, $K_2Ta_4F_4O_9$* , Acta Crystallogr. Sect. B **35**, 1983–1986 (1979), doi:10.1107/S056774087900830X.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.