

K₂Ta₄O₉F₄ Structure: A2B13C4_hP57_168_d_c6d_2d-001

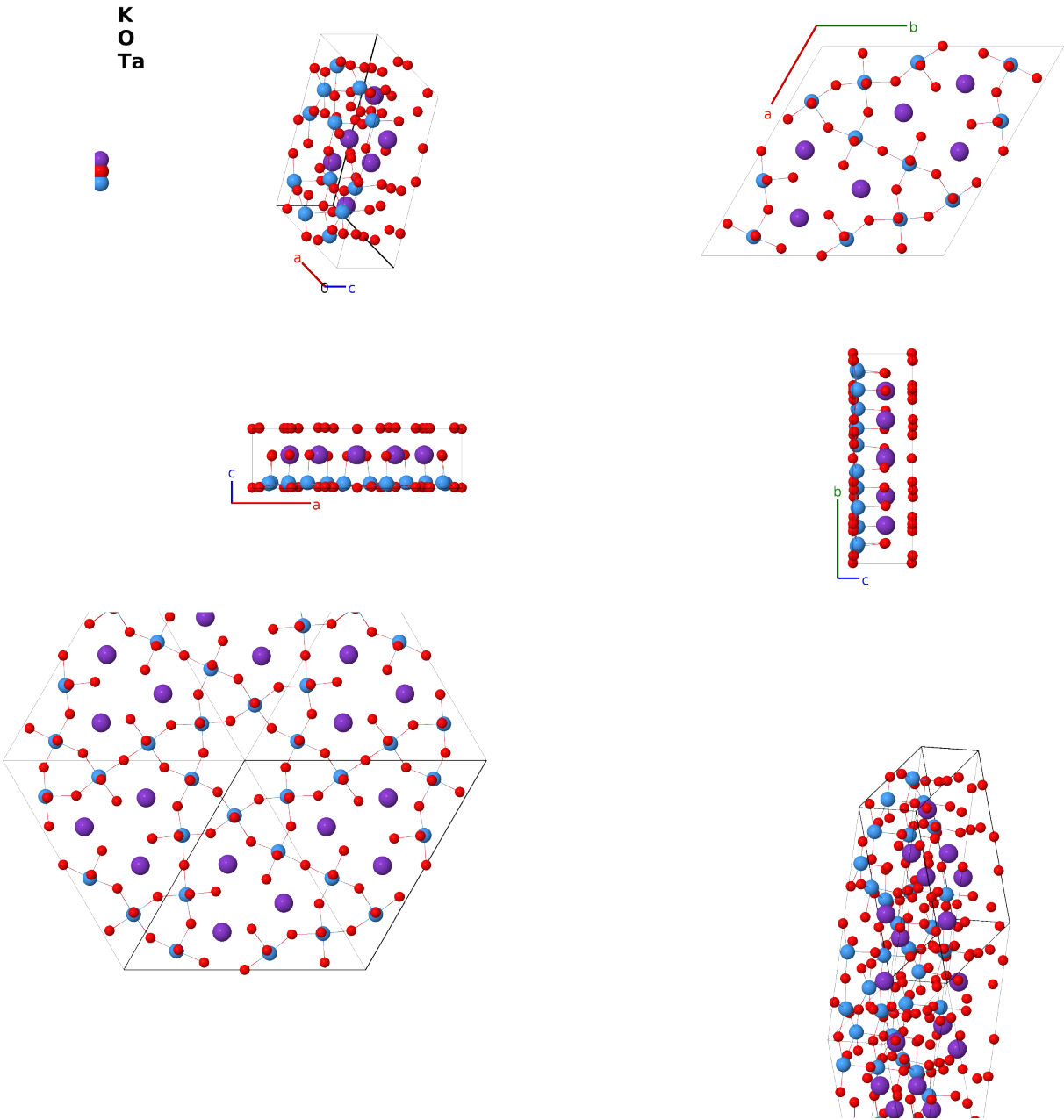
This structure previously used the label(s) **A2B13C4_hP57_168_d_c6d_2d**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/6140>

https://aflow.org/prototype-encyclopedia/A2B13C4_hP57_168_d_c6d_2d-001

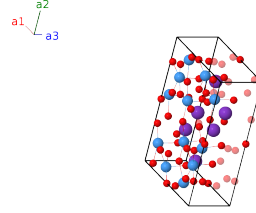


Prototype	$\text{F}_4\text{K}_2\text{O}_9\text{Ta}_4$
AFLOW prototype label	A2B13C4_hP57_168_d_c6d_2d-001
ICSD	8204
CCDC	1593988
Pearson symbol	hP57
Space group number	168
Space group symbol	$P6$
AFLOW prototype command	<pre>aflow --proto=A2B13C4_hP57_168_d_c6d_2d-001 --params=a,c/a,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8, z8,x9,y9,z9,x10,y10,z10</pre>

- 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
$\mathbf{B}_{20} =$	$y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{21} =$	$(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O III
$\mathbf{B}_{22} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{23} =$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{24} =$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{25} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{26} =$	$y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{27} =$	$(x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6d)	O IV
$\mathbf{B}_{28} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{29} =$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{30} =$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{31} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{32} =$	$y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{33} =$	$(x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6d)	O V
$\mathbf{B}_{34} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{35} =$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{36} =$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{37} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{38} =$	$y_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{39} =$	$(x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6d)	O VI
$\mathbf{B}_{40} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6d)	O VII
$\mathbf{B}_{41} =$	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\$		

$$\mathbf{B}_{56} = y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} \quad (6d) \quad \text{Ta II}$$

$$\mathbf{B}_{57} = (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} \quad (6d) \quad \text{Ta II}$$

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.

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- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043