K_2NbF_7 ($K6_2$) Structure: A7B2C_mP40_14_7e_2e_e-001

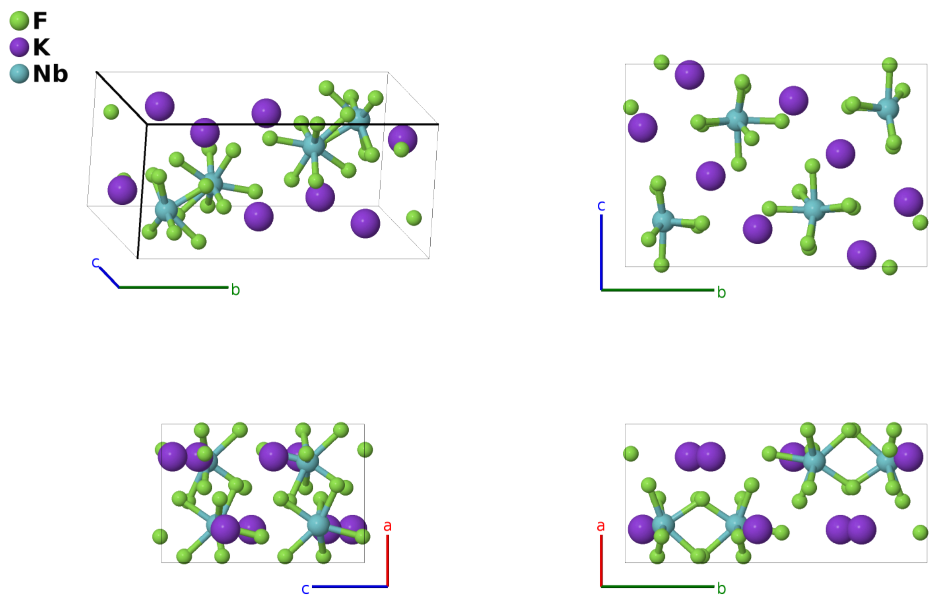
This structure originally had the label `A7B2C_mP40_14_7e_2e_e`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/p/TF3J

https://aflow.org/p/A7B2C_mP40_14_7e_2e_e-001

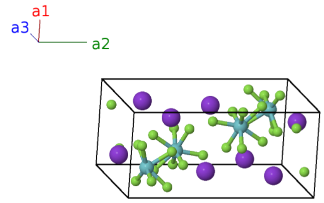


Prototype	F_7K_2Nb
AFLOW prototype label	A7B2C_mP40_14_7e_2e_e-001
***Strukturbericht* designation**	$K6_2$
ICSD	14132
Pearson symbol	mP40
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=A7B2C_mP40_14_7e_2e_e-001` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

Other compounds with this structure

K_2TaF_7

Simple Monoclinic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F V
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F V
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F V
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F V
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VI
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VI
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VI

$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VI
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VII
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VII
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VII
$\mathbf{B_{28}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F VII
$\mathbf{B_{29}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_{31}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_{32}}$	=	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_{33}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4e)	K II
$\mathbf{B_{34}}$	=	$-x_9\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9 + c\left(z_9 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	K II
$\mathbf{B_{35}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4e)	K II
$\mathbf{B_{36}}$	=	$x_9\,\mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9 + c\left(z_9 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	K II
$\mathbf{B_{37}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{38}}$	=	$-x_{10}\,\mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{10} + c\left(z_{10} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{39}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{40}}$	=	$x_{10}\,\mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{10} + c\left(z_{10} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Nb I

References

[1] G. M. Brown and L. A. Walker, *Refinement of the structure of potassium heptafluoroniobate, K_2NbF_7, from neutron-diffraction data*, Acta Cryst. **20**, 220–229 (1966), doi:10.1107/S0365110X66000458.

Found in

[1] C. C. Torardi, L. H. Brixner, and G. Blasse, *Structure and luminescence of K_2TaF_7 and K_2NbF_7*, J. Solid State Chem. **67**, 21–25 (1987), doi:10.1016/0022-4596(87)90333-1.