$NaNb_6O_{15}F$ Structure: ABC6D15_oC46_38_b_b_2a2d_2ab4d2e-001

This structure originally had the label `ABC6D15_oC46_38_b_b_2a2d_2ab4d2e`. Calls to that address will be redirected here.

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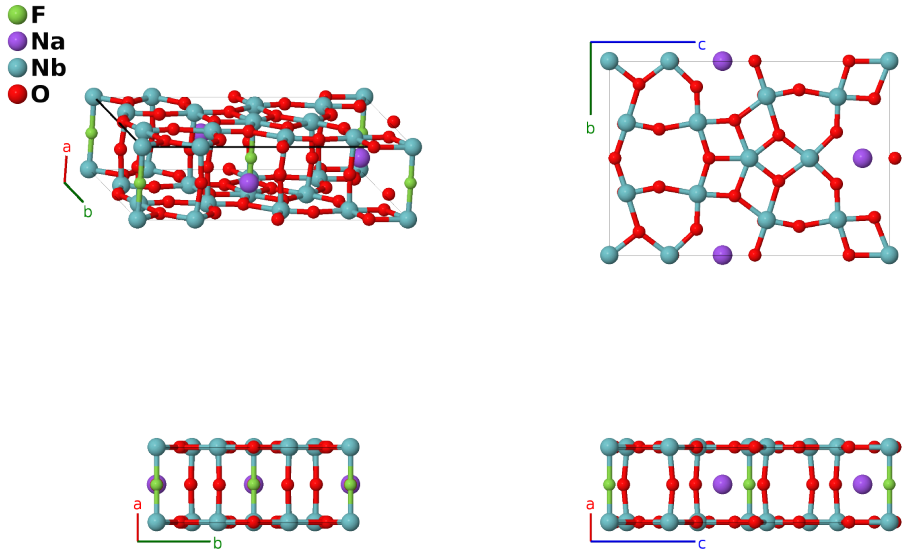
https://aflow.org/p/MYRE

https://aflow.org/p/ABC6D15_oC46_38_b_b_2a2d_2ab4d2e-001



Prototype	$FNaNb_6O_{15}$
AFLOW prototype label	ABC6D15_oC46_38_b_b_2a2d_2ab4d2e-001
ICSD	24109
Pearson symbol	oC46
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=ABC6D15_oC46_38_b_b_2a2d_2ab4d2e-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, y_8, z_8, y_9, z_9, y_{10}, z_{10}, y_{11}, z_{11}, y_{12}, z_{12}, y_{13}, z_{13}, y_{14}, z_{14}, y_{15}, z_{15}$

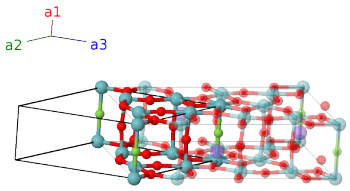
Other compounds with this structure
$NaNb_6O_{15}(OH)$

- The X-ray scattering of an F^- ion is almost identical to that of O^{-2}, and (Andersson, 1965) was not able to distinguish between them. He arbitrarily labeled the (2b) site he designated as O(1) as the location of the fluorine ion and we follow this, but in reality we have no idea if the F^- ions are located on this site, are ordered on another site, or are statistically distributed on the oxygen sites. Presumably the same considerations hold for the OH radical in $NaNb_6O_{15}(OH)$.

- Andersson sets $z_4 = 0.159$ as the coordinate of what we label as O-II and he calls O(10), but this gives an unreasonably short distance between the Nb-II and O-II atoms, and the distances between the O-II atom and the other atoms in the structure does not agree with the distances given his paper. If we assume that the first two digits were transposed when printed, so that $z_4 = 0.519$, we get within 0.1% of Andersson's distances.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a_1} &= a\,\hat{\mathbf{x}} \\ \mathbf{a_2} &= \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}} \\ \mathbf{a_3} &= \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_2}$	=	$-z_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Nb II
$\mathbf{B_3}$	=	$-z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_4}$	=	$-z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(2b)	F I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B_8}$	=	$(y_8 - z_8)\,\mathbf{a}_2 + (y_8 + z_8)\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Nb III
$\mathbf{B_9}$	=	$-(y_8 + z_8)\,\mathbf{a}_2 - (y_8 - z_8)\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	Nb III
$\mathbf{B_{10}}$	=	$(y_9 - z_9)\,\mathbf{a}_2 + (y_9 + z_9)\,\mathbf{a}_3$	=	$by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	Nb IV
$\mathbf{B_{11}}$	=	$-(y_9 + z_9)\,\mathbf{a}_2 - (y_9 - z_9)\,\mathbf{a}_3$	=	$-by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	Nb IV
$\mathbf{B_{12}}$	=	$(y_{10} - z_{10})\,\mathbf{a}_2 + (y_{10} + z_{10})\,\mathbf{a}_3$	=	$by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{13}}$	=	$-(y_{10} + z_{10})\,\mathbf{a}_2 - (y_{10} - z_{10})\,\mathbf{a}_3$	=	$-by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{14}}$	=	$(y_{11} - z_{11})\,\mathbf{a}_2 + (y_{11} + z_{11})\,\mathbf{a}_3$	=	$by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{15}}$	=	$-(y_{11} + z_{11})\,\mathbf{a}_2 - (y_{11} - z_{11})\,\mathbf{a}_3$	=	$-by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{16}}$	=	$(y_{12} - z_{12})\,\mathbf{a}_2 + (y_{12} + z_{12})\,\mathbf{a}_3$	=	$by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{17}}$	=	$-(y_{12} + z_{12})\,\mathbf{a}_2 - (y_{12} - z_{12})\,\mathbf{a}_3$	=	$-by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{18}}$	=	$(y_{13} - z_{13})\,\mathbf{a}_2 + (y_{13} + z_{13})\,\mathbf{a}_3$	=	$by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{19}}$	=	$-(y_{13} + z_{13})\,\mathbf{a}_2 - (y_{13} - z_{13})\,\mathbf{a}_3$	=	$-by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + (y_{14} - z_{14})\,\mathbf{a}_2 + (y_{14} + z_{14})\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B_{21}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - (y_{14} + z_{14})\,\mathbf{a}_2 - (y_{14} - z_{14})\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + (y_{15} - z_{15})\,\mathbf{a}_2 + (y_{15} + z_{15})\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4e)	O IX
$\mathbf{B_{23}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - (y_{15} + z_{15})\,\mathbf{a}_2 - (y_{15} - z_{15})\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4e)	O IX

References

[1] S. Andersson, *The Crystal Structure of $NaNb_6O_{15}F$ and $NaNb_6O_{15}OH$*, Acta Chem. Scand. **19**, 2285–2290 (1965), doi:10.3891/acta.chem.scand.19-2285j.