

Columbite (FeNb_2O_6 , $E5_1$) Structure: AB2C6_oP36_60_c_d_3d-001

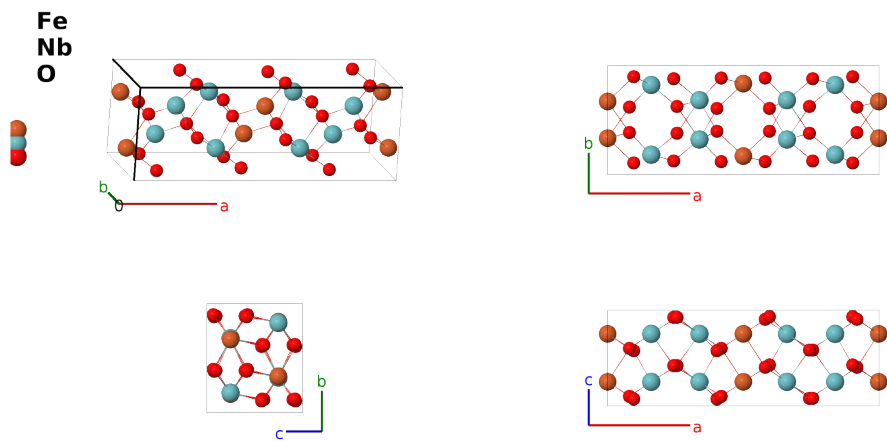
This structure previously used the label(s) AB2C6_oP36_60_c_d_3d. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/ZB5U>

https://aflow.org/prototype-encyclopedia/AB2C6_oP36_60_c_d_3d-001



Prototype	FeNb_2O_6
AFLOW prototype label	AB2C6_oP36_60_c_d_3d-001
<i>Strukturbericht</i> designation	$E5_1$
Mineral name	columbite
ICSD	201962
CCDC	1706576
Pearson symbol	oP36
Space group number	60
Space group symbol	$Pbcn$
AFLOW prototype command	<code>aflow --proto=AB2C6_oP36_60_c_d_3d-001</code> <code>--params=a,b/a,c/a,y1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5</code>

Other compounds with this structure

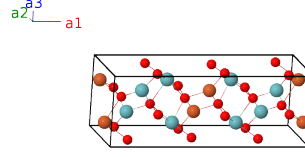
CaNb_2O_6 (fermsmite), CdNb_2O_6 , CoNb_2O_6 , CuNb_2O_6 , MnNb_2O_6 , MoNb_2O_6 , NiNb_2O_6 , SnNb_2O_6 , ZnNb_2O_6 , $\text{Zr}_5\text{Ti}_7\text{O}_{24}$

- The original *Strukturbericht* reference uses $(\text{Fe,Mn})\text{Nb}_2\text{O}_6$ as the prototype for $E5_1$ columbite.

- FeNb₂O₄ can also be found in a tetragonal structure.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_{10}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{16}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{17}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{18}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{19}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{20}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{21}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{22}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{23}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{24}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8d)	O II

$$\begin{aligned}
\mathbf{B}_{25} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{26} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - &= a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
&\quad \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{27} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{28} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
&\quad z_4 \mathbf{a}_3 \\
\mathbf{B}_{29} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{30} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
&\quad \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{31} &= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{32} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{33} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{34} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - &= a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
&\quad \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O III} \\
\mathbf{B}_{36} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8d) & \text{O III} \\
&\quad z_5 \mathbf{a}_3
\end{aligned}$$

References

- [1] P. Bordet, A. McHale, A. Santoro, and R. S. Roth, *Powder neutron diffraction study of ZrTiO_4 , $\text{Zr}_5\text{Ti}_7\text{O}_{24}$, and FeNb_2O_6* , J. Solid State Chem. **64**, 30–46 (1986), doi:10.1016/0022-4596(86)90119-2.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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.