$Nb_2Zr_6O_{17}$ Structure: A2B17C6_oI100_46_ab_b8c_3c-001

This structure originally had the label `A2B17C6_oI100_46_ab_b8c_3c`. Calls to that address will be redirected here.

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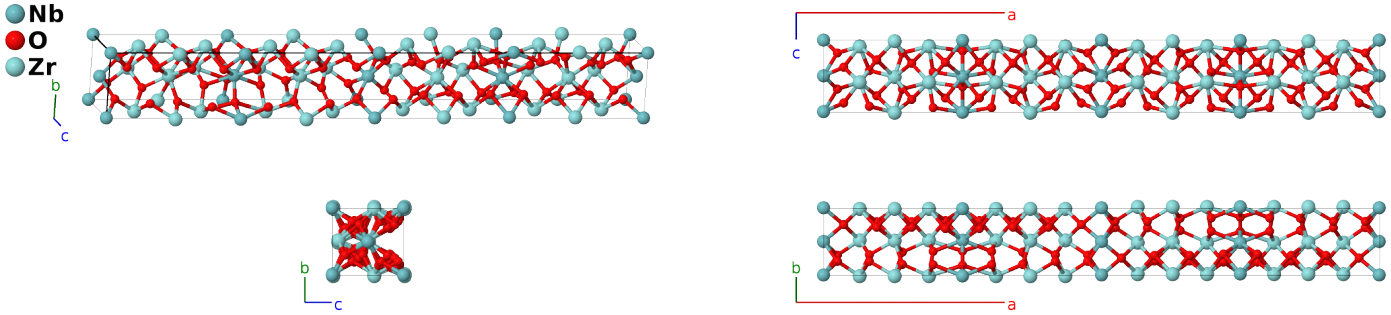
https://aflow.org/p/DKTF

https://aflow.org/p/A2B17C6_oI100_46_ab_b8c_3c-001



Prototype	$Nb_2O_{17}Zr_6$
AFLOW prototype label	A2B17C6_oI100_46_ab_b8c_3c-001
ICSD	19039
Pearson symbol	oI100
Space group number	46
Space group symbol	$Ima2$
AFLOW prototype command	`aflow --proto=A2B17C6_oI100_46_ab_b8c_3c-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

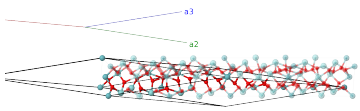
Other compounds with this structure

$Nb_2Hf_6O_{17}$, $Nb_2Zr_6O_{17}$, $Ta_2Hf_6O_{17}$, $Ta_2Zr_6O_{17}$

- Both (Galy, 1973) and (McCormack, 2019) state that the metallic atom sites are disordered, that is, for the prototype each metallic site has the average composition $Nb_{0.25}Zr_{0.75}$. We place the niobium atoms on the (2a) and (2b) sites, and the zirconium on the (4c) sites so that the different symmetries are displayed.
- (McCormack, 2019) notes that the metallic composition of these compounds can deviate from the stoichiometry shown here.

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Nb II
$\mathbf{B_4}$	=	$-(y_2 - z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Nb II
$\mathbf{B_5}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_6}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_7}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_8}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_9}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4 - y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{10}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{11}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{12}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{13}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{14}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_5 + y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{15}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_{16}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_{17}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_{18}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_{19}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B_{20}}$	=	$-(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	O V

$$\mathbf{B_{21}} = -(y_7 - z_7)\,\mathbf{a}_1 + \left(x_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8c) \quad \text{O V}$$

$$\mathbf{B_{22}} = (y_7 + z_7)\,\mathbf{a}_1 + \left(-x_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8c) \quad \text{O V}$$

$$\mathbf{B_{23}} = (y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VI}$$

$$\mathbf{B_{24}} = -(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VI}$$

$$\mathbf{B_{25}} = -(y_8 - z_8)\,\mathbf{a}_1 + \left(x_8 + z_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_8 - y_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VI}$$

$$\mathbf{B_{26}} = (y_8 + z_8)\,\mathbf{a}_1 + \left(-x_8 + z_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(-x_8 + y_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VI}$$

$$\mathbf{B_{27}} = (y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VII}$$

$$\mathbf{B_{28}} = -(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VII}$$

$$\mathbf{B_{29}} = -(y_9 - z_9)\,\mathbf{a}_1 + \left(x_9 + z_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_9 - y_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VII}$$

$$\mathbf{B_{30}} = (y_9 + z_9)\,\mathbf{a}_1 + \left(-x_9 + z_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(-x_9 + y_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VII}$$

$$\mathbf{B_{31}} = (y_{10} + z_{10})\,\mathbf{a}_1 + (x_{10} + z_{10})\,\mathbf{a}_2 + (x_{10} + y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VIII}$$

$$\mathbf{B_{32}} = -(y_{10} - z_{10})\,\mathbf{a}_1 - (x_{10} - z_{10})\,\mathbf{a}_2 - (x_{10} + y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VIII}$$

$$\mathbf{B_{33}} = -(y_{10} - z_{10})\,\mathbf{a}_1 + \left(x_{10} + z_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{10} - y_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VIII}$$

$$\mathbf{B_{34}} = (y_{10} + z_{10})\,\mathbf{a}_1 + \left(-x_{10} + z_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(-x_{10} + y_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O VIII}$$

$$\mathbf{B_{35}} = (y_{11} + z_{11})\,\mathbf{a}_1 + (x_{11} + z_{11})\,\mathbf{a}_2 + (x_{11} + y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O IX}$$

$$\mathbf{B_{36}} = -(y_{11} - z_{11})\,\mathbf{a}_1 - (x_{11} - z_{11})\,\mathbf{a}_2 - (x_{11} + y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O IX}$$

$$\mathbf{B_{37}} = -(y_{11} - z_{11})\,\mathbf{a}_1 + \left(x_{11} + z_{11} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{11} - y_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{11} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O IX}$$

$$\mathbf{B_{38}} = (y_{11} + z_{11})\,\mathbf{a}_1 + \left(-x_{11} + z_{11} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(-x_{11} + y_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{11} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{O IX}$$

$$\mathbf{B_{39}} = (y_{12} + z_{12})\,\mathbf{a}_1 + (x_{12} + z_{12})\,\mathbf{a}_2 + (x_{12} + y_{12})\,\mathbf{a}_3 = ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \quad (8c) \quad \text{Zr I}$$

$\mathbf{B_{40}}$	=	$-(y_{12}-z_{12})\,\mathbf{a}_1-(x_{12}-z_{12})\,\mathbf{a}_2-(x_{12}+y_{12})\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8c)	Zr I
$\mathbf{B_{41}}$	=	$-(y_{12}-z_{12})\,\mathbf{a}_1+\left(x_{12}+z_{12}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_{12}-y_{12}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8c)	Zr I
$\mathbf{B_{42}}$	=	$(y_{12}+z_{12})\,\mathbf{a}_1+\left(-x_{12}+z_{12}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(-x_{12}+y_{12}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8c)	Zr I
$\mathbf{B_{43}}$	=	$(y_{13}+z_{13})\,\mathbf{a}_1+(x_{13}+z_{13})\,\mathbf{a}_2+(x_{13}+y_{13})\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(8c)	Zr II
$\mathbf{B_{44}}$	=	$-(y_{13}-z_{13})\,\mathbf{a}_1-(x_{13}-z_{13})\,\mathbf{a}_2-(x_{13}+y_{13})\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(8c)	Zr II
$\mathbf{B_{45}}$	=	$-(y_{13}-z_{13})\,\mathbf{a}_1+\left(x_{13}+z_{13}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_{13}-y_{13}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{13}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(8c)	Zr II
$\mathbf{B_{46}}$	=	$(y_{13}+z_{13})\,\mathbf{a}_1+\left(-x_{13}+z_{13}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(-x_{13}+y_{13}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{13}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(8c)	Zr II
$\mathbf{B_{47}}$	=	$(y_{14}+z_{14})\,\mathbf{a}_1+(x_{14}+z_{14})\,\mathbf{a}_2+(x_{14}+y_{14})\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(8c)	Zr III
$\mathbf{B_{48}}$	=	$-(y_{14}-z_{14})\,\mathbf{a}_1-(x_{14}-z_{14})\,\mathbf{a}_2-(x_{14}+y_{14})\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(8c)	Zr III
$\mathbf{B_{49}}$	=	$-(y_{14}-z_{14})\,\mathbf{a}_1+\left(x_{14}+z_{14}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_{14}-y_{14}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{14}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(8c)	Zr III
$\mathbf{B_{50}}$	=	$(y_{14}+z_{14})\,\mathbf{a}_1+\left(-x_{14}+z_{14}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(-x_{14}+y_{14}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{14}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(8c)	Zr III

References

[1] J. Galy and R. S. Roth, *The Crystal Structure of $Nb_2Zr_6O_{17}$*, J. Solid State Chem. **7**, 227–285 (1973), doi:10.1016/0022-4596(73)90134-5.

Found in

[1] S. J. McCormack and W. M. Kriven, *Crystal structure solution for the $A_6B_2O_{17}$ (A = Zr, Hf; B = Nb, Ta) superstructure*, Acta Crystallogr. Sect. B **75**, 227–234 (2019), doi:10.1107/S2052520619001963.