

Nb₂Zr₆O₁₇ Structure: A2B17C6_oI100_46_ab_b8c_3c-001

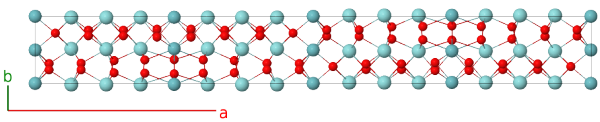
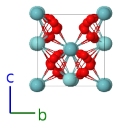
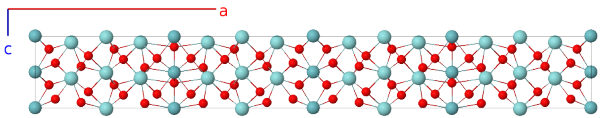
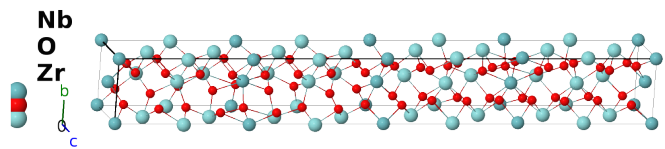
This structure previously used the label(s) **A2B17C6_oI100_46_ab_b8c_3c**. Calls to these addresses will be redirected here.

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- 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/prototype-encyclopedia/DKTF>

https://aflow.org/prototype-encyclopedia/A2B17C6_oI100_46_ab_b8c_3c-001



Prototype	Nb ₂ O ₁₇ Zr ₆
AFLOW prototype label	A2B17C6_oI100_46_ab_b8c_3c-001
ICSD	19039
CCDC	1597817
Pearson symbol	oI100
Space group number	46
Space group symbol	<i>Ima2</i>
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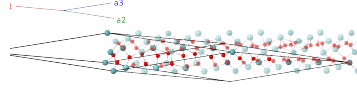
Other compounds with this structure

Nb₂Hf₆O₁₇, Nb₂Zr₆O₁₇, Ta₂Hf₆O₁₇, Ta₂Zr₆O₁₇

- 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

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_2$	$= z_1 \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$\frac{1}{2}a\hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B}_3$	$= (y_2 + z_2) \mathbf{a}_1 + (z_2 + \frac{1}{4}) \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3 =$		$\frac{1}{4}a\hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Nb II
$\mathbf{B}_4$	$= -(y_2 - z_2) \mathbf{a}_1 + (z_2 + \frac{3}{4}) \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3 =$		$\frac{3}{4}a\hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Nb II
$\mathbf{B}_5$	$= (y_3 + z_3) \mathbf{a}_1 + (z_3 + \frac{1}{4}) \mathbf{a}_2 + (y_3 + \frac{1}{4}) \mathbf{a}_3 =$		$\frac{1}{4}a\hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_6$	$= -(y_3 - z_3) \mathbf{a}_1 + (z_3 + \frac{3}{4}) \mathbf{a}_2 - (y_3 - \frac{3}{4}) \mathbf{a}_3 =$		$\frac{3}{4}a\hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_9$	$= -(y_4 - z_4) \mathbf{a}_1 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 =$		$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{10}$	$= (y_4 + z_4) \mathbf{a}_1 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 =$		$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{13}$	$= -(y_5 - z_5) \mathbf{a}_1 + (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 =$		$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{14}$	$= (y_5 + z_5) \mathbf{a}_1 + (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 =$		$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{17}$	$= -(y_6 - z_6) \mathbf{a}_1 + (x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + (x_6 - y_6 + \frac{1}{2}) \mathbf{a}_3 =$		$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	O IV

$$\begin{aligned}
\mathbf{B}_{18} &= \begin{pmatrix} (y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{19} &= \begin{pmatrix} (y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + \\ (x_7 + y_7) \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{20} &= \begin{pmatrix} -(y_7 - z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 - \\ (x_7 + y_7) \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{21} &= \begin{pmatrix} -(y_7 - z_7) \mathbf{a}_1 + \\ (x_7 + z_7 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_7 - y_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{22} &= \begin{pmatrix} (y_7 + z_7) \mathbf{a}_1 + \\ (-x_7 + z_7 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_7 + y_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{23} &= \begin{pmatrix} (y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + \\ (x_8 + y_8) \mathbf{a}_3 \end{pmatrix} = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{24} &= \begin{pmatrix} -(y_8 - z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 - \\ (x_8 + y_8) \mathbf{a}_3 \end{pmatrix} = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(y_8 - z_8) \mathbf{a}_1 + \\ (x_8 + z_8 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_8 - y_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{26} &= \begin{pmatrix} (y_8 + z_8) \mathbf{a}_1 + \\ (-x_8 + z_8 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{27} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{28} &= \begin{pmatrix} -(y_9 - z_9) \mathbf{a}_1 - (x_9 - z_9) \mathbf{a}_2 - \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(y_9 - z_9) \mathbf{a}_1 + \\ (x_9 + z_9 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{30} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 + \\ (-x_9 + z_9 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{31} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 + \\ (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{32} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 - \\ (x_{10} - z_{10}) \mathbf{a}_2 - (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{33} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 + \\ (x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{10} - y_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{34} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 + \\ (-x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{10} + y_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{35} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 + (x_{11} + z_{11}) \mathbf{a}_2 + \\ (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{36} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 - \\ (x_{11} - z_{11}) \mathbf{a}_2 - (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IX}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{37} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 + \\ (x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{11} - y_{11} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{11} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{38} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 + \\ (-x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{11} + y_{11} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{11} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{39} &= \begin{pmatrix} (y_{12} + z_{12}) \mathbf{a}_1 + (x_{12} + z_{12}) \mathbf{a}_2 + \\ (x_{12} + y_{12}) \mathbf{a}_3 \end{pmatrix} = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{Zr I} \\
\mathbf{B}_{40} &= \begin{pmatrix} -(y_{12} - z_{12}) \mathbf{a}_1 - \\ (x_{12} - z_{12}) \mathbf{a}_2 - (x_{12} + y_{12}) \mathbf{a}_3 \end{pmatrix} = -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{Zr I} \\
\mathbf{B}_{41} &= \begin{pmatrix} -(y_{12} - z_{12}) \mathbf{a}_1 + \\ (x_{12} + z_{12} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{12} - y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{12} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{Zr I} \\
\mathbf{B}_{42} &= \begin{pmatrix} (y_{12} + z_{12}) \mathbf{a}_1 + \\ (-x_{12} + z_{12} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{12} + y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{12} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{Zr I} \\
\mathbf{B}_{43} &= \begin{pmatrix} (y_{13} + z_{13}) \mathbf{a}_1 + (x_{13} + z_{13}) \mathbf{a}_2 + \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{Zr II} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(y_{13} - z_{13}) \mathbf{a}_1 - \\ (x_{13} - z_{13}) \mathbf{a}_2 - (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{Zr II} \\
\mathbf{B}_{45} &= \begin{pmatrix} -(y_{13} - z_{13}) \mathbf{a}_1 + \\ (x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} - y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{13} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{Zr II} \\
\mathbf{B}_{46} &= \begin{pmatrix} (y_{13} + z_{13}) \mathbf{a}_1 + \\ (-x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{13} + y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{13} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{Zr II} \\
\mathbf{B}_{47} &= \begin{pmatrix} (y_{14} + z_{14}) \mathbf{a}_1 + (x_{14} + z_{14}) \mathbf{a}_2 + \\ (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{Zr III} \\
\mathbf{B}_{48} &= \begin{pmatrix} -(y_{14} - z_{14}) \mathbf{a}_1 - \\ (x_{14} - z_{14}) \mathbf{a}_2 - (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{Zr III} \\
\mathbf{B}_{49} &= \begin{pmatrix} -(y_{14} - z_{14}) \mathbf{a}_1 + \\ (x_{14} + z_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{14} - y_{14} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{14} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{Zr III} \\
\mathbf{B}_{50} &= \begin{pmatrix} (y_{14} + z_{14}) \mathbf{a}_1 + \\ (-x_{14} + z_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{14} + y_{14} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{14} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{Zr III}
\end{aligned}$$

References

- [1] J. Galy and R. S. Roth, *The Crystal Structure of Nb₂Zr₆O₁₇*, J. Solid State Chem. **7**, 227–285 (1973), doi:10.1016/0022-4596(73)90134-5.

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