

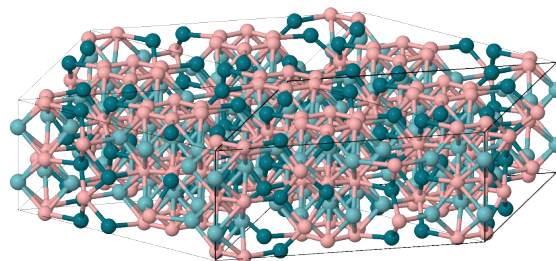
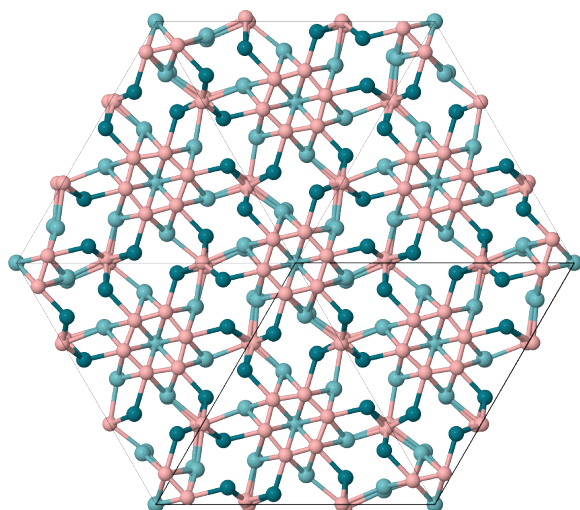
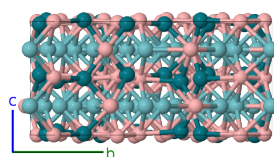
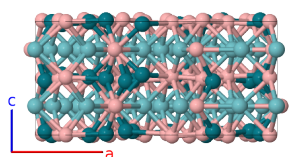
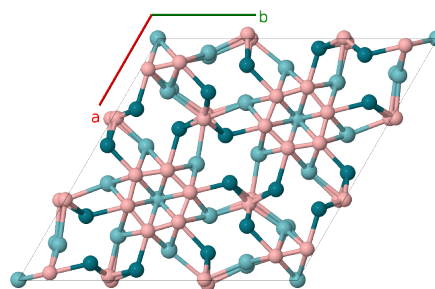
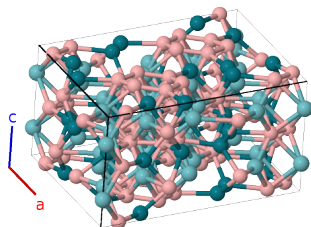
Nb₇Rh₆B₈ Structure: A8B7C6_hP126_176_2h3i_acd6h_3i-001

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<https://afLOW.org/p/01SA>

https://afLOW.org/p/A8B7C6_hP126_176_2h3i_acd6h_3i-001

● B
● Nb
● Rh



Prototype	B ₈ Nb ₇ Rh ₆
AFLOW prototype label	A8B7C6_hP126_176_2h3i_acd6h_3i-001
ICSD	263043

Pearson symbol	hP126
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	aflow --proto=A8B7C6_hP126_176_2h3i_acd6h_3i-001 --params= $a, c/a, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9, x_{10}, y_{10}, x_{11}, y_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}$

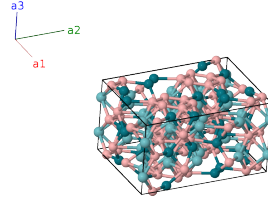
Other compounds with this structure

Ta₇Rh₆B₈

- (Zheng, 2012) place the Nb-I (their Nb3) atom on the (2b) Wyckoff position, but give the coordinates for the (2a) position. We assume that the coordinates are correct. This assessment agrees with the ICSD entry.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2a)	Nb I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Nb I
\mathbf{B}_3	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Nb II
\mathbf{B}_4	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Nb II
\mathbf{B}_5	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	Nb III
\mathbf{B}_6	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	Nb III
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_8	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_9	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_{11}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_{12}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B I
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{14}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{15}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{16}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{17}	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{18}	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	B II
\mathbf{B}_{19}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Nb IV

$$\begin{aligned}
\mathbf{B}_{113} &= \begin{matrix} -y_{16} \mathbf{a}_1 + (x_{16} - y_{16}) \mathbf{a}_2 - \\ (z_{16} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} \frac{1}{2}a(x_{16} - 2y_{16}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{16} \hat{\mathbf{y}} - \\ c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh II} \\
\mathbf{B}_{114} &= \begin{matrix} -(x_{16} - y_{16}) \mathbf{a}_1 - x_{16} \mathbf{a}_2 - \\ (z_{16} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -\frac{1}{2}a(2x_{16} - y_{16}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{16} \hat{\mathbf{y}} - \\ c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh II} \\
\mathbf{B}_{115} &= x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} + \\ cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{116} &= -y_{17} \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(x_{17} - 2y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{117} &= -(x_{17} - y_{17}) \mathbf{a}_1 - x_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \begin{matrix} -\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{118} &= -x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = \begin{matrix} -\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} + \\ c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{119} &= \begin{matrix} y_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 + \\ (z_{17} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} \frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + \\ c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{120} &= \begin{matrix} (x_{17} - y_{17}) \mathbf{a}_1 + x_{17} \mathbf{a}_2 + \\ (z_{17} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} \frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + \\ c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{121} &= -x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3 = \begin{matrix} -\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} - \\ cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{122} &= y_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{123} &= (x_{17} - y_{17}) \mathbf{a}_1 + x_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{124} &= x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} - \\ c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{125} &= \begin{matrix} -y_{17} \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 - \\ (z_{17} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} \frac{1}{2}a(x_{17} - 2y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} - \\ c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III} \\
\mathbf{B}_{126} &= \begin{matrix} -(x_{17} - y_{17}) \mathbf{a}_1 - x_{17} \mathbf{a}_2 - \\ (z_{17} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} - \\ c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} \end{matrix} & (12i) & \text{Rh III}
\end{aligned}$$

References

- [1] Q. Zheng, M. Kohout, R. Gumeniuk, N. Abramchuk, H. Borrmann, Y. Prots, U. Burkhardt, W. Schnelle, L. Akselrud, H. Gu, A. Leithe-Jasper, and Y. Grin, *TM₇TM'₆B₈* (*TM* = *Ta*, *Nb*; *TM'* = *Ru*, *Rh*, *Ir*): *New Compounds with [B₆] Ring Polyanions*, *Inorg. Chem.* **51**, 7492–7483 (2012), doi:10.1021/ic201978n.