

Nb₇Ru₆B₈ Structure: A8B7C6_hP21_175_ck_aj_k-001

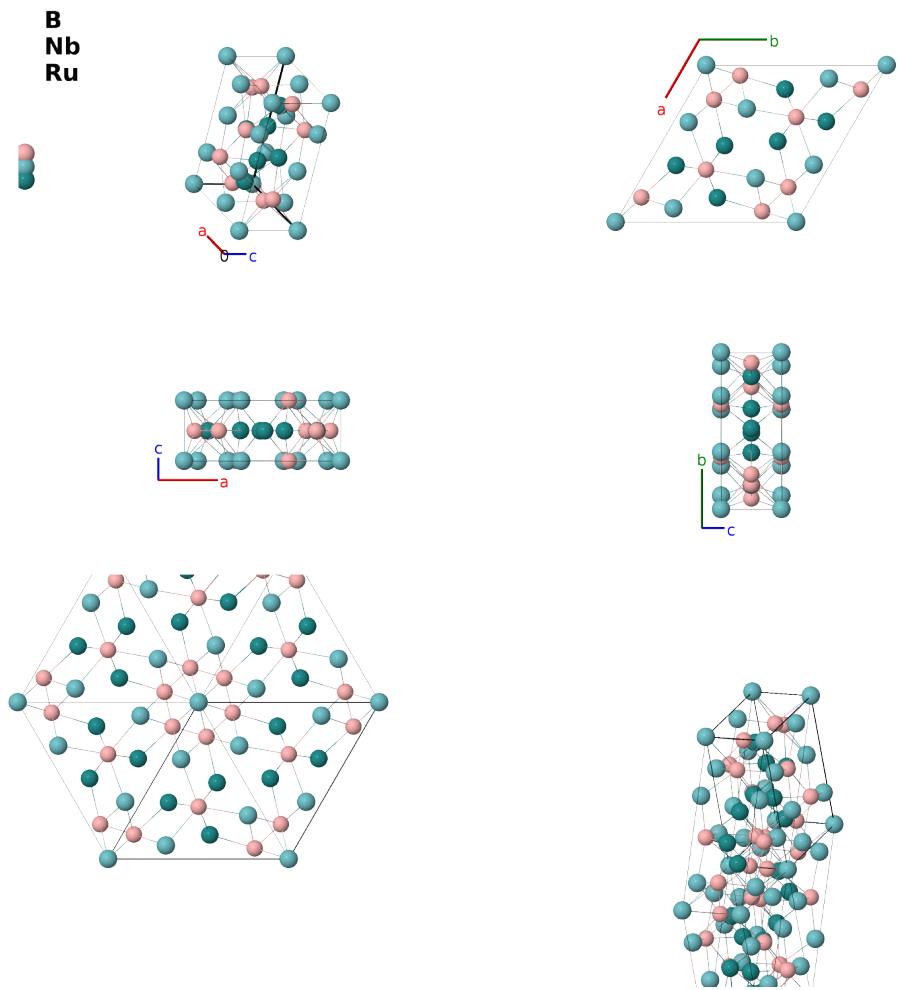
This structure previously used the label(s) **A8B7C6_hP21_175_ck_aj_k**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/F86A>

https://aflow.org/prototype-encyclopedia/A8B7C6_hP21_175_ck_aj_k-001



Prototype	B ₈ Nb ₇ Ru ₆
AFLOW prototype label	A8B7C6_hP21_175_ck_aj_k-001
ICSD	263041
CCDC	1720598
Pearson symbol	hP21

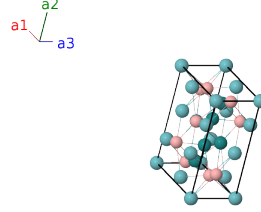
Space group number 175
Space group symbol $P6/m$
AFLOW prototype command `aflow --proto=A8B7C6_hP21_175_ck_aj_k-001`
--params= $a, c/a, x_3, y_3, x_4, y_4, x_5, y_5$

Other compounds with this structure

Ta₇Ru₆B₈

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
$\mathbf{B}_1$	$=$	0	$=$	0	(1a) Nb I
$\mathbf{B}_2$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c) B I
$\mathbf{B}_3$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c) B I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_6$	$=$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_7$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_8$	$=$	$y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_9$	$=$	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}}$	(6j) Nb II
$\mathbf{B}_{10}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{11}$	$=$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{12}$	$=$	$-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{13}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{14}$	$=$	$y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{15}$	$=$	$(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) B II
$\mathbf{B}_{16}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I
$\mathbf{B}_{17}$	$=$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I
$\mathbf{B}_{18}$	$=$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I
$\mathbf{B}_{19}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I
$\mathbf{B}_{20}$	$=$	$y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I
$\mathbf{B}_{21}$	$=$	$(x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k) Ru I

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.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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