C-AlRuNi ($Al_{20}Ni_3Ru_5$) Structure: A23B2C6_cP31_200_cij_ab_f-001

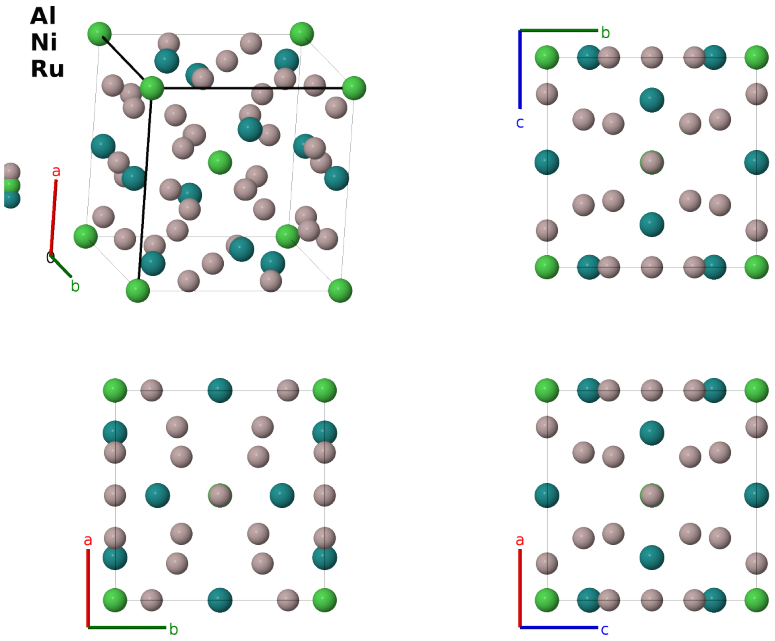
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/L1EN

https://aflow.org/prototype-encyclopedia/A23B2C6_cP31_200_cij_ab_f-001



Prototype	$Al_{20}Ni_3Ru_5$
AFLOW prototype label	A23B2C6_cP31_200_cij_ab_f-001
ICSD	230569
CCDC	2037181
Pearson symbol	cP31
Space group number	200
Space group symbol	$Pm\overline{3}$
AFLOW prototype command	`aflow --proto=A23B2C6_cP31_200_cij_ab_f-001 --params=`a, x_4, x_5, y_6, z_6

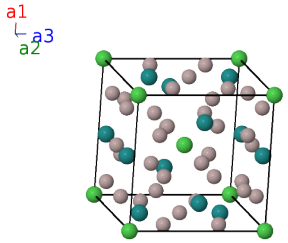
- Most of these sites are partially or contained a mixture of species. We label them by the majority species:
  - Ni-I (1a) is 79% nickel and 21% ruthenium,
  - Ni-II (1b) is 100% nickel,

- Al-I (3c) is 77% aluminum and 23% vacancies,
- Ru-I (6g) is 81.4% ruthenium and 18.6% nickel,
- Al-II (8i) is 74% aluminum and 26% vacancies, and
- Al-III (12k) is 100% aluminum.

- This gives an actual composition of $Al_{20.23}Ni_{2.906}Ru_{5.094}$, which we simplify to $Al_{20}Ni_3Ru_5$.

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= a\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Ni II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Al I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	Al I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Ru I
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Ru I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(6f)	Ru I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(6f)	Ru I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(6f)	Ru I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(6f)	Ru I
$\mathbf{B_{12}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{18}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(8i)	Al II
$\mathbf{B_{20}}$	=	$y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{21}}$	=	$-y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{22}}$	=	$y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{23}}$	=	$-y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12j)	Al III

$\mathbf{B_{24}}$	=	$z_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{25}}$	=	$z_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{26}}$	=	$-z_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{27}}$	=	$-z_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{z}}$	(12j)	Al III
$\mathbf{B_{28}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$ay_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}}$	(12j)	Al III
$\mathbf{B_{29}}$	=	$-y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$-ay_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}}$	(12j)	Al III
$\mathbf{B_{30}}$	=	$y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$ay_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}}$	(12j)	Al III
$\mathbf{B_{31}}$	=	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$-ay_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}}$	(12j)	Al III

References

[1] R. Simura, K. Sugiyama, S. Suzuki, and T. Kawamata, *Crystal Structure of the C-AlRuNi Phase*, Mater. Trans. **58**, 1101–1105 (2017), doi:10.2320/matertrans.M2017106.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.