

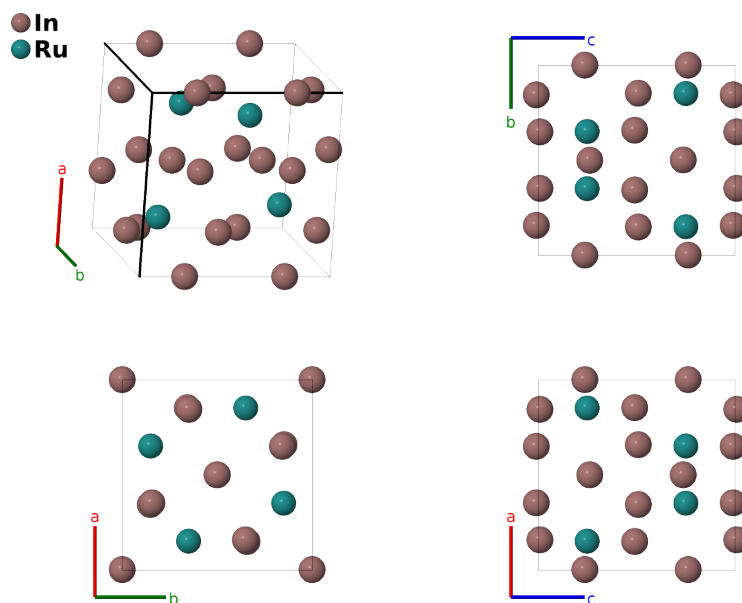
# RuIn<sub>3</sub> Structure: A3B\_tP16\_118\_ei\_f-001

This structure originally had the label `A3B_tP16_118_ei_f`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/0ZUR>

[https://aflow.org/p/A3B\\_tP16\\_118\\_ei\\_f-001](https://aflow.org/p/A3B_tP16_118_ei_f-001)



Prototype	In <sub>3</sub> Ru
AFLOW prototype label	A3B_tP16_118_ei_f-001
ICSD	59518
Pearson symbol	tP16
Space group number	118
Space group symbol	$P\bar{4}n2$
AFLOW prototype command	<code>aflow --proto=A3B_tP16_118_ei_f-001 --params=a, c/a, z<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></code>

---

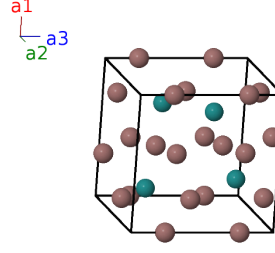
## Other compounds with this structure

CoGa<sub>3</sub>

---

## Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	=	$c z_1 \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_2$	$= -z_1 \mathbf{a}_3$	=	$-c z_1 \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	In I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$a x_2 \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Ru I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-a x_2 \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4f)	Ru I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Ru I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4f)	Ru I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{11}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{12}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{13}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{15}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	In II
$\mathbf{B}_{16}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	In II

## References

- [1] R. B. Roof, Z. Fisk, and J. L. Smith, *Crystal Data for RuIn<sub>3</sub>*, Powder Diff. **1**, 20–21 (1986), doi:10.1017/S0885715600011234.

## Found in

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