

Ru₂Sn₃ Structure:

A2B3_tP20_116_adi_ej-001

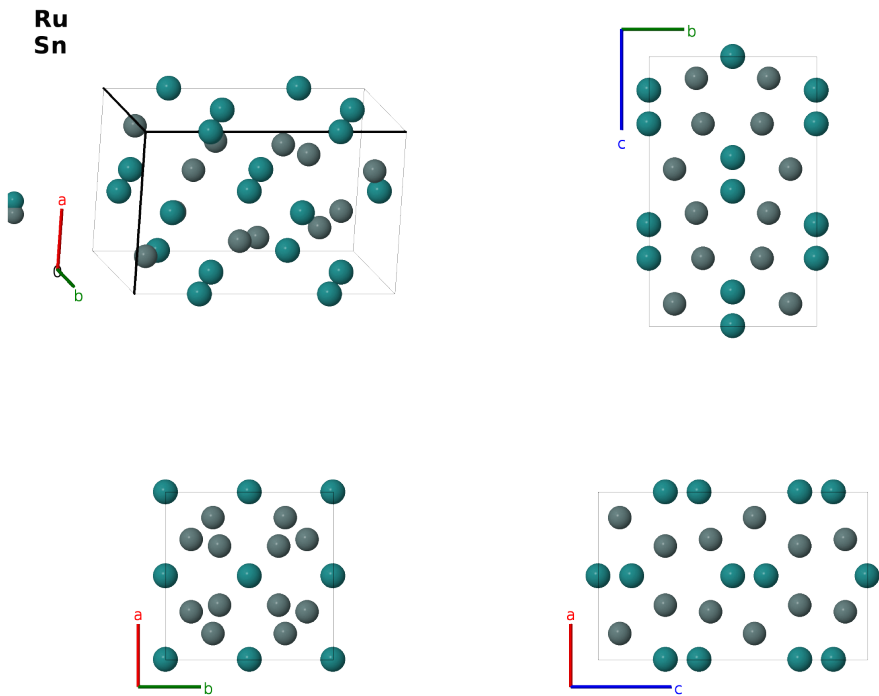
This structure previously used the label(s) **A2B3_tP20_116_bci_fj**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A2B3_tP20_116_adi_ej-001



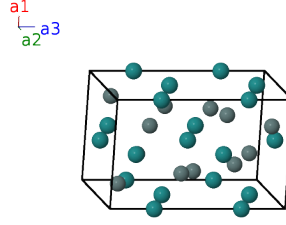
Prototype	Ru ₂ Sn ₃
AFLOW prototype label	A2B3_tP20_116_adi_ej-001
ICSD	105994
CCDC	1663856
Pearson symbol	tP20
Space group number	116
Space group symbol	$P\bar{4}c2$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_116_adi_ej-001</code> <code>--params=a, c/a, x₃, z₄, x₅, y₅, z₅</code>

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



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)	Ru I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Ru I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2d)	Ru II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2d)	Ru II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4e)	Sn I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4e)	Sn I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4e)	Sn I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4e)	Sn I
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4i)	Ru III
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_4 \hat{\mathbf{z}}$	(4i)	Ru III
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4i)	Ru III
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4i)	Ru III
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{15}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{16}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{19}$	$= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Sn II
$\mathbf{B}_{20}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Sn II

References

- [1] O. Schwomma, H. Nowotny, and A. Wittmann, *Untersuchungen im System: Ru-Sn*, Monatsh. Chem. **95** (1964), doi:10.1007/BF00901709.

Found in

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First cited in

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