Ru$_2$Sn$_3$ Structure: A2B3_tP20_116_adi_ej-001

This structure originally had the label `A2B3_tP20_116_bci_fj`. Calls to that address will be redirected here.

https://aflow.org/p/RJFD

https://aflow.org/p/A2B3_tP20_116_adi_ej-001
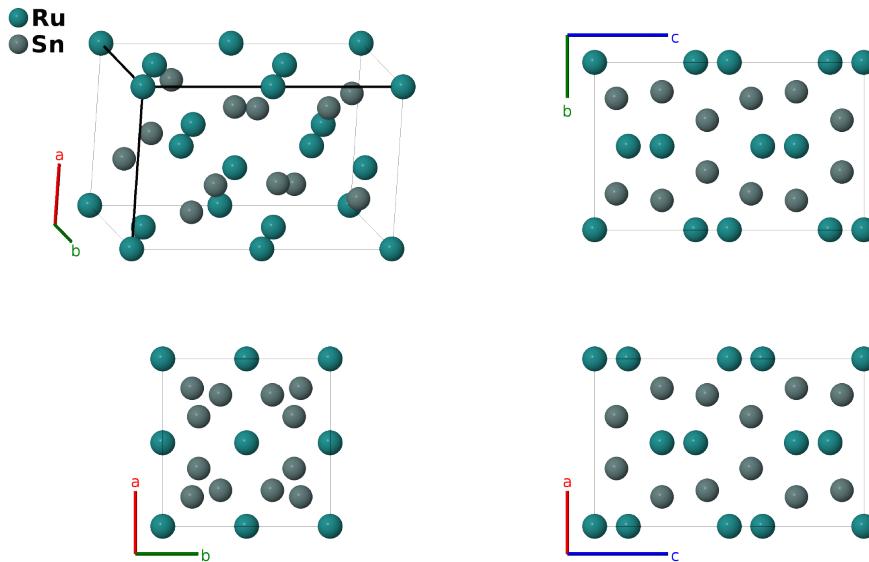
Prototype	Ru$_2$Sn$_3$
AFLOW prototype label	A2B3_tP20_116_adi_ej-001
ICSD	105994
Pearson symbol	tP20
Space group number	116
Space group symbol	$P\overline{4}c2$
AFLOW prototype command	aflow --proto=A2B3_tP20_116_adi_ej-001
	--params=$a, c/a, x_3, z_4, x_5, y_5, z_5$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
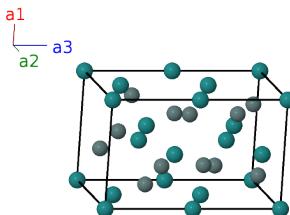
Basis vectors

		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

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