$Yb_3Rh_4Sn_{13}$ Structure: A4B13C3_cP40_223_e_ak_c-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.

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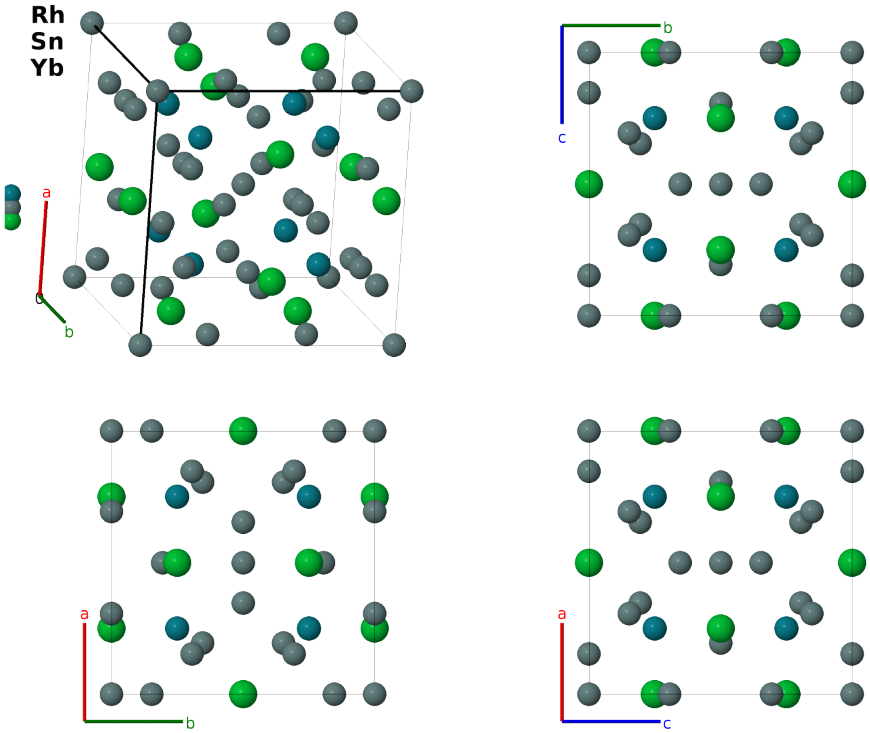
https://aflow.org/prototype-encyclopedia/GYST

https://aflow.org/prototype-encyclopedia/A4B13C3_cP40_223_e_ak_c-001



Prototype	$Rh_4Sn_{13}Yb_3$
AFLOW prototype label	A4B13C3_cP40_223_e_ak_c-001
ICSD	105936
CCDC	1663802
Pearson symbol	cP40
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	`aflow --proto=A4B13C3_cP40_223_e_ak_c-001 --params=`a, y_4, z_4

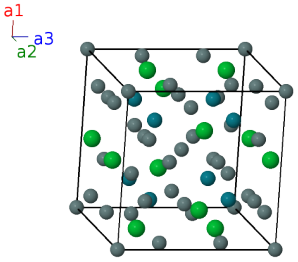
Other compounds with this structure

$Ca_3Co_4Ge_{13}$, $Ca_3Ir_4Ge_{13}$, $Ca_3Os_4Ge_{13}$, $Ca_3Rh_4Ge_{13}$, $Ca_3Ru_4Ge_{13}$, $Ce_3Rh_4Sn_{13}$, $Gd_3Co_4Ge_{13}$, $Gd_3Ir_4Ge_{13}$, $Gd_3Os_4Ge_{13}$, $Gd_3Rh_4Ge_{13}$, $Gd_3Ru_4Ge_{13}$, $La_3Rh_4Sn_{13}$, $Pr_3Rh_4Sn_{13}$, $Sn_3Rh_4Sn_{13}$, $U_3Co_4Ge_{13}$, $U_3Ir_4Ge_{13}$, $U_3Os_4Ge_{13}$, $U_3Rh_4Ge_{13}$, $U_3Ru_4Ge_{13}$, $Y_3Co_4Ge_{13}$, $Y_3Ir_4Ge_{13}$, $Y_3Os_4Ge_{13}$, $Y_3Rh_4Ge_{13}$, $Y_3Ru_4Ge_{13}$, $Yb_3Co_4Ge_{13}$, $Yb_3Ir_4Ge_{13}$, $Yb_3Os_4Ge_{13}$, $Yb_3Rh_4Ge_{13}$, $Yb_3Ru_4Ge_{13}$

- (Bordet, 1991) refers to this as "phase I" of structures with the formula $M_3Rh_4Sn_{13}$, with the "phase I'" structure represented by the non-centrosymmetric $La_3Rh_4Sn_{13}$ phase.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Yb I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Yb I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(6c)	Yb I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(6c)	Yb I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	Yb I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	Yb I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{13}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{14}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{15}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{16}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8e)	Rh I
$\mathbf{B_{17}}$	=	$y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{18}}$	=	$-y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{19}}$	=	$y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{20}}$	=	$-y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{21}}$	=	$z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{22}}$	=	$z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{23}}$	=	$-z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{24}}$	=	$-z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24k)	Sn II
$\mathbf{B_{25}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}}$	(24k)	Sn II
$\mathbf{B_{26}}$	=	$-y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}}$	(24k)	Sn II

$$\mathbf{B_{27}} = y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 = a y_4\,\hat{\mathbf{x}} - a z_4\,\hat{\mathbf{y}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{28}} = -y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 = -a y_4\,\hat{\mathbf{x}} - a z_4\,\hat{\mathbf{y}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{29}} = \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 - \left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{30}} = -\left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 - \left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{31}} = \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{32}} = -\left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{33}} = \tfrac{1}{2}\,\mathbf{a}_1 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{34}} = \tfrac{1}{2}\,\mathbf{a}_1 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{35}} = \tfrac{1}{2}\,\mathbf{a}_1 - \left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{36}} = \tfrac{1}{2}\,\mathbf{a}_1 - \left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{37}} = \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{38}} = \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = a\left(z_4+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{39}} = -\left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

$$\mathbf{B_{40}} = -\left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -a\left(z_4-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad \text{(24k)} \quad \text{Sn II}$$

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[2] P. Bordet, D. E. Cox, G. P. Espinosa, J. L. Hodeau, and M. Marezio, *Synchrotron X-ray powder diffraction study of the phase I' compound: $SnLa_3Rh_4Sn_{12}$*, Solid State Commun. **78**, 359–366 (1991), doi:10.1016/0038-1098(91)90684-N.

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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.