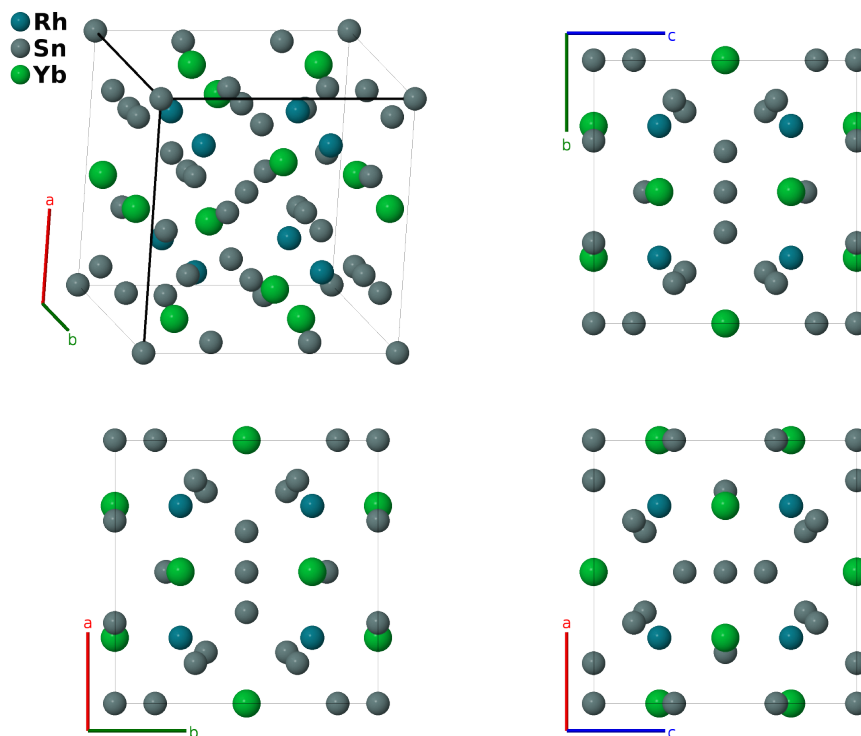


Yb₃Rh₄Sn₁₃ Structure: A4B13C3_cP40_223_e_ak_c-001

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<https://aflow.org/p/GYST>

https://aflow.org/p/A4B13C3_cP40_223_e_ak_c-001



Prototype	Rh ₄ Sn ₁₃ Yb ₃
AFLOW prototype label	A4B13C3_cP40_223_e_ak_c-001
ICSD	105936
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= <i>a</i> , <i>y</i> ₄ , <i>z</i> ₄

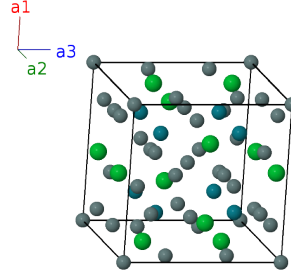
Other compounds with this structure

Ca₃Co₄Ge₁₃, Ca₃Ir₄Ge₁₃, Ca₃Os₄Ge₁₃, Ca₃Rh₄Ge₁₃, Ca₃Ru₄Ge₁₃, Ce₃Rh₄Sn₁₃, Gd₃Co₄Ge₁₃, Gd₃Ir₄Ge₁₃, Gd₃Os₄Ge₁₃, Gd₃Rh₄Ge₁₃, Gd₃Ru₄Ge₁₃, La₃Rh₄Sn₁₃, Pr₃Rh₄Sn₁₃, Sn₃Rh₄Sn₁₃, U₃Co₄Ge₁₃, U₃Ir₄Ge₁₃, U₃Os₄Ge₁₃, U₃Rh₄Ge₁₃, U₃Ru₄Ge₁₃, Y₃Co₄Ge₁₃, Y₃Ir₄Ge₁₃, Y₃Os₄Ge₁₃, Y₃Rh₄Ge₁₃, Y₃Ru₄Ge₁₃, Yb₃Co₄Ge₁₃, Yb₃Ir₄Ge₁₃, Yb₃Os₄Ge₁₃, Yb₃Rh₄Ge₁₃, Yb₃Ru₄Ge₁₃

- (Bordet, 1991) refers to this as “phase I” of structures with the formula M₃Rh₄Sn₁₃, with the “phase I” structure represented by the non-centrosymmetric La₃Rh₄Sn₁₃ phase.

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	(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}	$y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24k)	Sn II
\mathbf{B}_{28}	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24k)	Sn II

$$\begin{aligned}
\mathbf{B}_{29} &= (y_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{30} &= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = -a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{31} &= (y_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{32} &= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = -a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{33} &= \frac{1}{2} \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{34} &= \frac{1}{2} \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{35} &= \frac{1}{2} \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{y}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{36} &= \frac{1}{2} \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2} a \hat{\mathbf{x}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{37} &= (z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a (z_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{38} &= (z_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a (z_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{39} &= -(z_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a (z_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24k) & \text{Sn II} \\
\mathbf{B}_{40} &= -(z_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a (z_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24k) & \text{Sn II}
\end{aligned}$$

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