

Er₂RhSi₃ Structure:

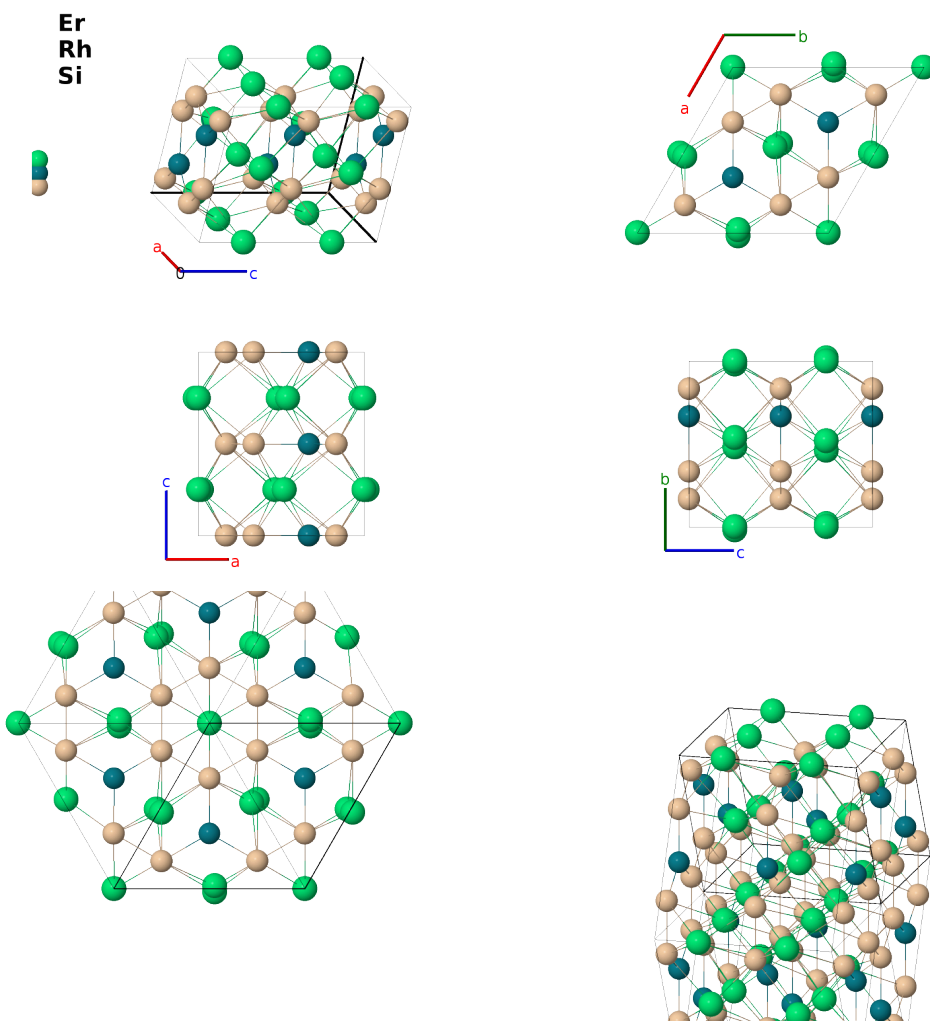
A2BC3_hP24_190_bh_f_i-001

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<https://aflow.org/prototype-encyclopedia/Z6A0>

https://aflow.org/prototype-encyclopedia/A2BC3_hP24_190_bh_f_i-001



Prototype	Er ₂ RhSi ₃
AFLOW prototype label	A2BC3_hP24_190_bh_f_i-001
ICSD	655470
CCDC	1765854
Pearson symbol	hP24
Space group number	190

Space group symbol

 $P\bar{6}2c$

AFLOW prototype command

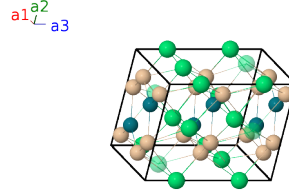
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      --params=a,c/a,z2,x3,y3,x4,y4,z4
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Other compounds with this structureCe₂NiGe₃, Ce₂RhSi₃, Ho₂RhSi₃, La₂NiGe₃, Nd₂RhSi₃, Tb₂RhSi₃, Ga₃CoLu₂

- (Gladyshevskii, 1992) put Er₂RhSi₃ in the Lu₂CoGa₃ structure and report that there is little difference between the two forms, however we find significant differences and the ICSD lists the two structures as different variants of Er₂RhSi₃. We will list the two structures under Er₂RhSi₃ (space group $P\bar{6}2c$ #190) and Lu₂CoGa₃ (space group $P6_3/mmc$ #194). The two space groups differ only in that the later group contains the inversion operator.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$

**Basis vectors**

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Er I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Er I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B}_4$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B}_5$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B}_6$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Rh I
$\mathbf{B}_7$	$= x_3\mathbf{a}_1 + y_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3)\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_8$	$= -y_3\mathbf{a}_1 + (x_3 - y_3)\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_9$	$= -(x_3 - y_3)\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_{10}$	$= y_3\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3)\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_{11}$	$= (x_3 - y_3)\mathbf{a}_1 - y_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_{12}$	$= -x_3\mathbf{a}_1 - (x_3 - y_3)\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6h)	Er II
$\mathbf{B}_{13}$	$= x_4\mathbf{a}_1 + y_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4)\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12i)	Si I
$\mathbf{B}_{14}$	$= -y_4\mathbf{a}_1 + (x_4 - y_4)\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12i)	Si I
$\mathbf{B}_{15}$	$= -(x_4 - y_4)\mathbf{a}_1 - x_4\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(12i)	Si I
$\mathbf{B}_{16}$	$= x_4\mathbf{a}_1 + y_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4)\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12i)	Si I
$\mathbf{B}_{17}$	$= -y_4\mathbf{a}_1 + (x_4 - y_4)\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12i)	Si I
$\mathbf{B}_{18}$	$= -(x_4 - y_4)\mathbf{a}_1 - x_4\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(12i)	Si I

$$\begin{aligned}
\mathbf{B}_{19} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12i) &\text{Si I} \\
\mathbf{B}_{20} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12i) &\text{Si I} \\
\mathbf{B}_{21} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12i) &\text{Si I} \\
\mathbf{B}_{22} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + &(12i) &\text{Si I} \\
&&& c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12i) &\text{Si I} \\
\mathbf{B}_{24} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + &= -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12i) &\text{Si I} \\
&& \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

References

- [1] B. Chevalier, P. Lejay, J. Etourneau, and P. Hagenmuller, *A new family of rare earth compounds, the ternary silicides RE_2RhSi_3 ($RE = Y, La, Ce, Nd, Sm, Gd, Tb, Dy, Ho, Er$) - crystal structure electrical and magnetic properties*, Solid State Commun. **49**, 753–760 (1984), doi:10.1016/0038-1098(84)90073-5.

Found in

- [1] R. E. Gladyshevskii, K. Cenxual, and E. Parthé, *Er_2RhSi_3 and R_2CoGa_3 ($R = Y, Tb, Dy, Ho, Er, Tm, Yb$) with Lu_2CoGa_3 type structure: new members of the $A1B2$ structure family*, J. Am. Chem. Soc. **189**, 221–228 (1992), doi:10.1016/0925-8388(92)90711-H.

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