Ru₂Ge₃ Nowotny Chimney-Ladder Structure: A3B2_oP40_60_3d_2cd-001

https://aflow.org/p/EU3H

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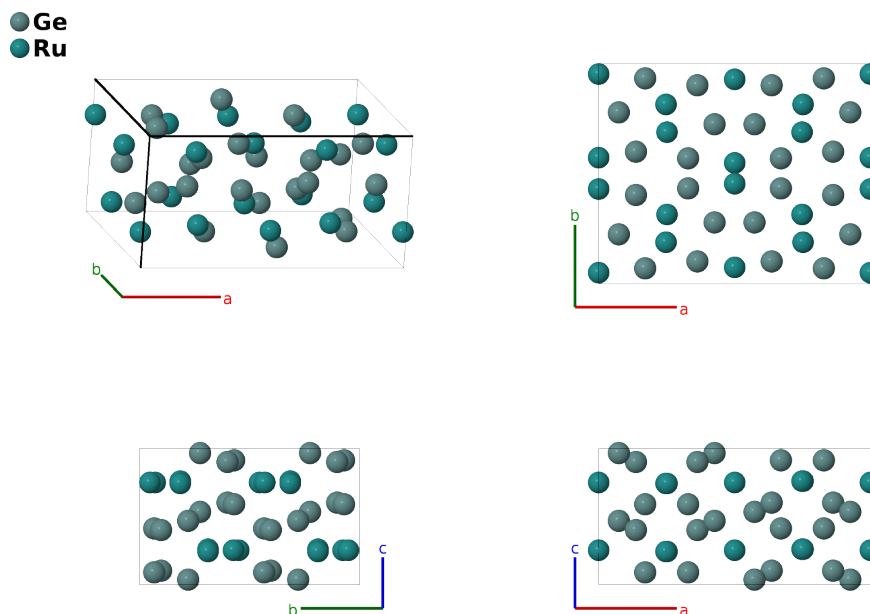
Prototype	Ge₃Ru₂
AFLOW prototype label	A3B2_oP40_60_3d_2cd-001
ICSD	637740
Pearson symbol	oP40
Space group number	60
Space group symbol	*Pbcn*
AFLOW prototype command	aflow --proto=A3B2_oP40_60_3d_2cd-001
	--params=$a, b/a, c/a, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

Ru₂Si₃

- This an example of a "Nowotny chimney-ladder structure" (Pearson, 1970), T$_n$X$_m$, where "T" is a transition metal, "X" is a row III or IV metal (or semiconductor), and $1.25 \leq m/n < 2$. The transition metal atoms are arranged similarly to the atoms in β-Sn ($A5$).
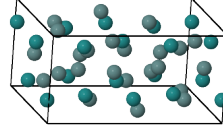
Simple Orthorhombic primitive vectors
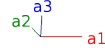
$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$y_1\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	$=$	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\,\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_3}$	$=$	$-y_1\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	$=$	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_4}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_5}$	$=$	$y_2\,\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	$=$	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru II
$\mathbf{B_6}$	$=$	$\frac{1}{2}\,\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru II
$\mathbf{B_7}$	$=$	$-y_2\,\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	$=$	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru II
$\mathbf{B_8}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ru II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{13}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{14}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{15}}$	$=$	$x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{16}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B_{17}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{18}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{19}}$	$=$	$-x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{20}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{21}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{22}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{23}}$	$=$	$x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{24}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	Ge II
$\mathbf{B_{25}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ge III

$$\mathbf{B_{26}} = -\left(x_5 - \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{27}} = -x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3} = -ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{28}} = \left(x_5 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \tfrac{1}{2}\right)\mathbf{a_2} - z_5\,\mathbf{a_3} = a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{29}} = -x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3} = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{30}} = \left(x_5 + \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3} = a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{31}} = x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3} = ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{32}} = -\left(x_5 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \tfrac{1}{2}\right)\mathbf{a_2} + z_5\,\mathbf{a_3} = -a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ge III}$$

$$\mathbf{B_{33}} = x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3} = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{34}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{35}} = -x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} = -ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{36}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3} = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{37}} = -x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{38}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{39}} = x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

$$\mathbf{B_{40}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a_2} + z_6\,\mathbf{a_3} = -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(8d)} \quad \text{Ru III}$$

References

[1] D. J. Poutcharovsky, K. Yvon, and E. Parthé, *Diffusionless phase transformations of Ru_2Si_3, Ru_2Ge_3 and Ru_2Sn_3: I. Crystal structure investigations*, J. Less-Common Met. **40**, 139–144 (1975), doi:10.1016/0022-5088(75)90189-7.

[2] W. B. Pearson, *Phases with Nowotny chimney-ladder structures considered as 'electron' phases*, Acta Crystallogr. Sect. B **26**, 1044–1046 (1970), doi:10.1107/S0567740870003564.