

Ir₃Ge₇ (*D*8_{*f*}) Structure: A7B3_cI40_229_df_e-001

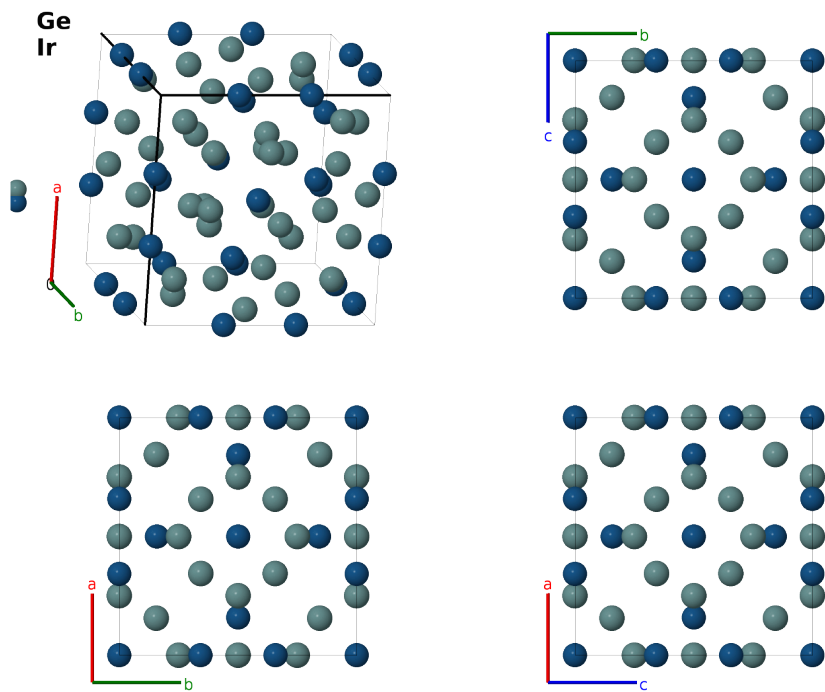
This structure previously used the label(s) **A7B3_cI40_229_df_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/9SK5>

https://aflow.org/prototype-encyclopedia/A7B3_cI40_229_df_e-001



Prototype	Ge ₇ Ir ₃
AFLOW prototype label	A7B3_cI40_229_df_e-001
<i>Strukturbericht</i> designation	<i>D</i> 8 _{<i>f</i>}
ICSD	408313
CCDC	1725540
Pearson symbol	cI40
Space group number	229
Space group symbol	<i>Im</i> $\bar{3}$ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A7B3_cI40_229_df_e-001</code> <code>--params=<i>a</i>, <i>x</i>₂, <i>x</i>₃</code>

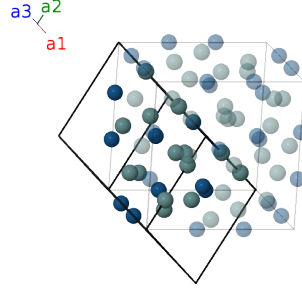
Other compounds with this structure

As₇Re₃, Ga₇Ni₃, Ga₇Pd₃, Ga₇Pt₃, In₇Pd₃, In₇Pt₃, Sb₇Mo₃, Sn₇Ir₃, Sn₇Os₃, Sn₇Ru₃

- Although (Haussermann, 1998) list the prototype for this structure as Ir₃Ge₇, that structure is not listed in the ICSD. We link to the similar Ni₃Ga₇ structure.
- The ICSD gives the prototype for this structure as Ru₃Sn₇.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B}_7$	$= x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}}$	(12e)	Ir I
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}}$	(12e)	Ir I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{y}}$	(12e)	Ir I
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{y}}$	(12e)	Ir I
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{z}}$	(12e)	Ir I
$\mathbf{B}_{12}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{z}}$	(12e)	Ir I
$\mathbf{B}_{13}$	$= 2x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{14}$	$= -2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{15}$	$= -2x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{16}$	$= -2x_3 \mathbf{a}_1$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{17}$	$= 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{18}$	$= -2x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{19}$	$= 2x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{20}$	$= 2x_3 \mathbf{a}_1$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Ge II

References

- [1] U. Häussermann, M. Elding-Pontén, C. Svensson, and S. Lidin, *Compounds with the Ir_3Ge_7 Structure Type: Interpenetrating Frameworks with Flexible Bonding Properties*, Chem. Euro. J. **4**, 1007–1015 (1998), doi:10.1002/(SICI)1521-3765(19980615)4:6<1007::AID-CHEM1007>3.0.CO;2-7.

Found in

- [1] F. Selim, J. P. Bevington, and G. S. Collins, *Diffusion of ^{111}Cd probes in Ga_7Pt_3 studied via nuclear quadrupole relaxation*, Hyperf. Int. **178**, 87–90 (2007), doi:10.1007/s10751-008-9663-3.

First cited in

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