Ir$_3$Ge$_7$ ($D8_f$) Structure: A7B3_cI40_229_df_e-001

This structure originally had the label `A7B3_cI40_229_df_e`. Calls to that address will be redirected here.

https://aflow.org/p/9SK5

https://aflow.org/p/A7B3_cI40_229_df_e-001
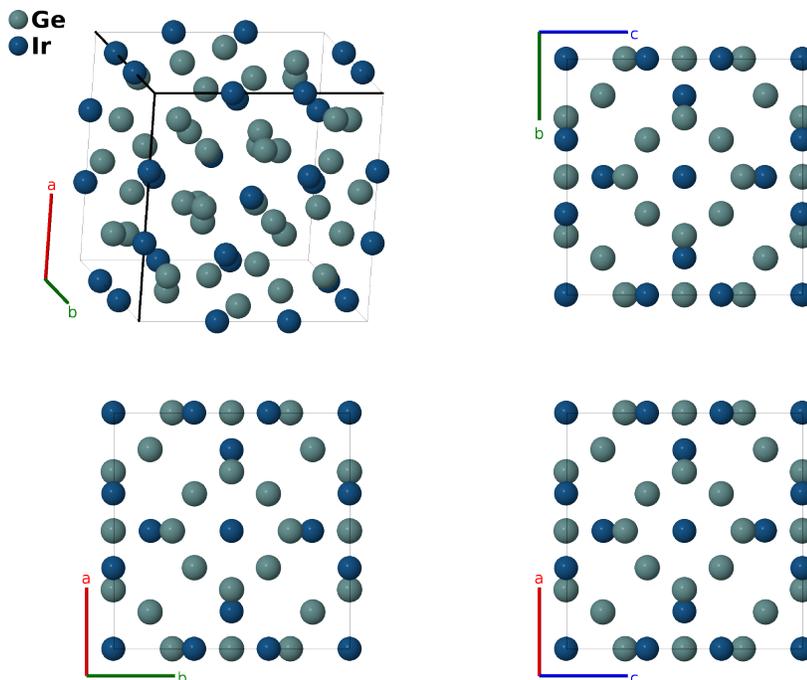
Prototype	Ge$_7$Ir$_3$
AFLOW prototype label	A7B3_cI40_229_df_e-001
***Strukturbericht* designation**	$D8_f$
ICSD	408313
Pearson symbol	cI40
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	aflow --proto=A7B3_cI40_229_df_e-001 --params=a, x_2, x_3

Other compounds with this structure

As$_7$Re$_3$, Ga$_7$Ni$_3$, Ga$_7$Pd$_3$, Ga$_7$Pt$_3$, In$_7$Pd$_3$, In$_7$Pt$_3$, Sb$_7$Mo$_3$, Sn$_7$Ir$_3$, Sn$_7$Os$_3$, Sn$_7$Ru$_3$

- Although (Haussermann, 1998) list the prototype for this structure as Ir$_3$Ge$_7$, that structure is not listed in the ICSD. We link to the similar Ni$_3$Ga$_7$ structure.

- The ICSD gives the prototype for this structure as Ru_3Sn_7.

Body-centered Cubic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
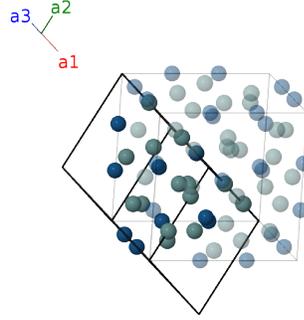
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B_3}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B_4}$	$=$	$\tfrac{3}{4}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_5}$	$=$	$\tfrac{3}{4}\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_6}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(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.