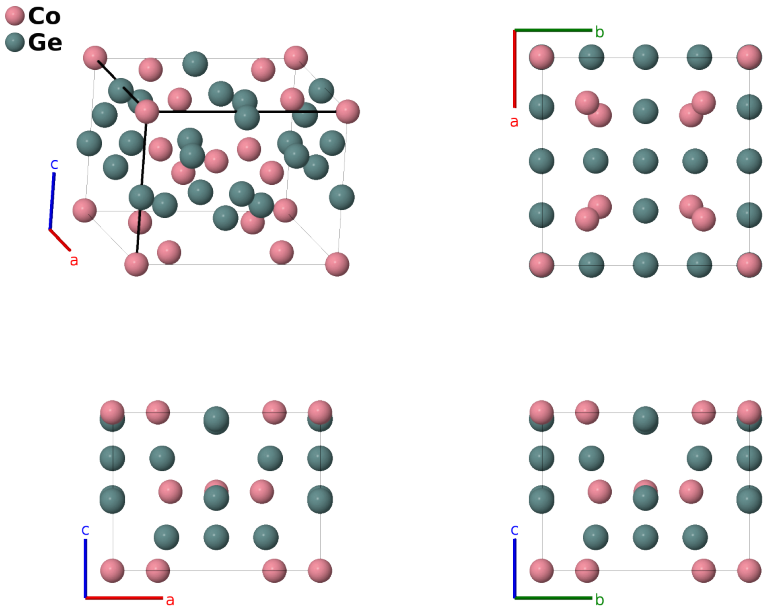
Co_5Ge_7 Structure: A5B7_tI24_107_ac_abd-001

This structure originally had the label `A5B7_tI24_107_ac_abd`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/Y7TL

https://aflow.org/p/A5B7_tI24_107_ac_abd-001



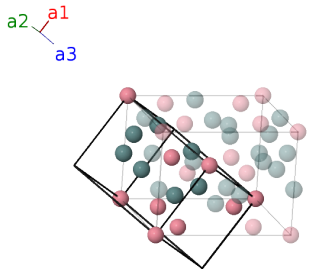
Prototype	Co_5Ge_7
AFLOW prototype label	A5B7_tI24_107_ac_abd-001
ICSD	197263
Pearson symbol	tI24
Space group number	107
Space group symbol	$I4mm$
AFLOW prototype command	`aflow --proto=A5B7_tI24_107_ac_abd-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
Ir_5Ge_7

- The origin of the z axis is arbitrary. We have chosen to place the Ge(2a) atom at the origin, taking $z_1 = 0$. (Schubert, 1960) instead set $z_4 = 0$.

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Ge I
$\mathbf{B_3}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Ge II
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Ge II
$\mathbf{B_5}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Co II
$\mathbf{B_6}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Co II
$\mathbf{B_7}$	=	$(x_4 + z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Co II
$\mathbf{B_8}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Co II
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ge III
$\mathbf{B_{10}}$	=	$z_5\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ge III
$\mathbf{B_{11}}$	=	$(x_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ge III
$\mathbf{B_{12}}$	=	$-(x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ge III

References

[1] K. Schubert, T. R. Anantharaman, H. O. K. Ata, H. G. Meissner, M. Pötzschke, W. Rossteutscher, and E. Stolz, *Einige strukturelle Ergebnisse an metallischen Phasen (6)*, Naturwissenschaften **47**, 512 (1960), doi:10.1007/BF00641115.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.