

GeP (High-pressure, superconducting) Structure: AB_tI4_107_a_a-001

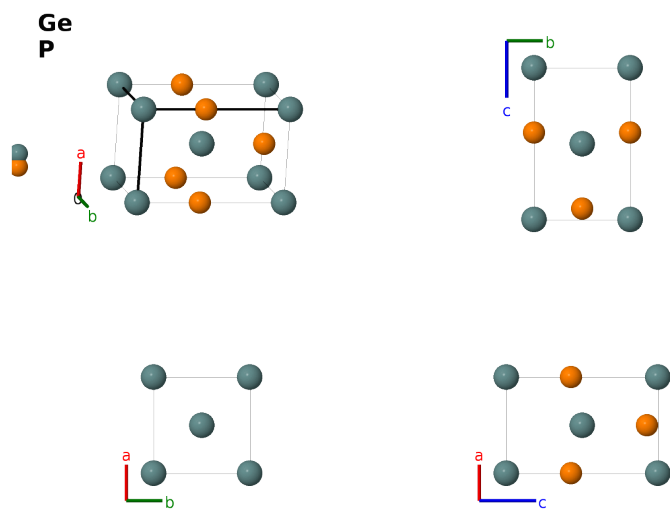
This structure previously used the label(s) **AB_tI4_107_a_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/B4LQ>

https://aflow.org/prototype-encyclopedia/AB_tI4_107_a_a-001



Prototype	GeP
AFLOW prototype label	AB.tI4_107_a_a-001
ICSD	17032
CCDC	1597527
Pearson symbol	tI4
Space group number	107
Space group symbol	$I4mm$
AFLOW prototype command	<code>aflow --proto=AB_tI4_107_a_a-001 --params=a, c/a, z₁, z₂</code>

Other compounds with this structure

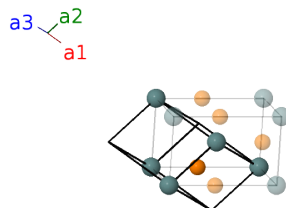
GeAs, PdSn

- We use the (Donohue, 1970) data taken at 700°C and 45 kBar.

- Space group $I4mm$ #107 allows an arbitrary placement of the origin of the z -axis. Here we set $z_1 = 0$ for the germanium atoms.

Body-centered Tetragonal primitive vectors

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



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)	Ge I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	P I

References

- [1] P. C. Donohue and H. S. Young, *Synthesis, structure, and superconductivity of new high pressure phases in the systems Ge-P and Ge-s*, J. Solid State Chem. **1**, 143–149 (1970), doi:10.1016/0022-4596(70)90005-8.

Found in

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

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