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

This structure originally had the label `AB_tI4_107_a_a`. Calls to that address will be redirected here.

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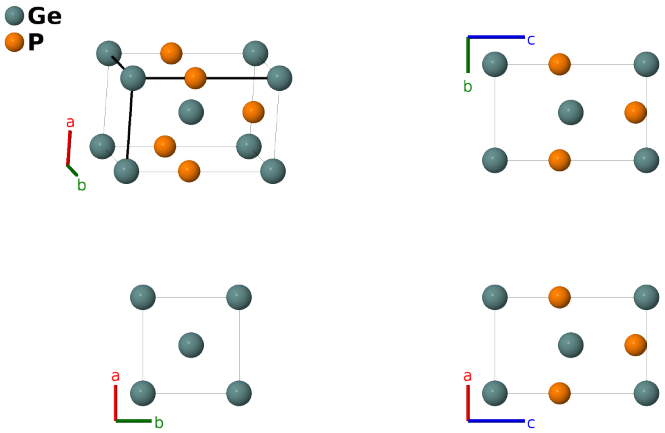
https://aflow.org/p/B4LQ

https://aflow.org/p/AB_tI4_107_a_a-001



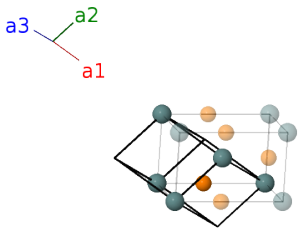
Prototype	GeP
AFLOW prototype label	AB_tI4_107_a_a-001
ICSD	17032
Pearson symbol	tI4
Space group number	107
Space group symbol	$I4mm$
AFLOW prototype command	`aflow --proto=AB_tI4_107_a_a-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure
GeAs, PdSn

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

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



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.