

GeSe₂ (High Pressure) Structure: AB2_tP12_81_adg_2h-001

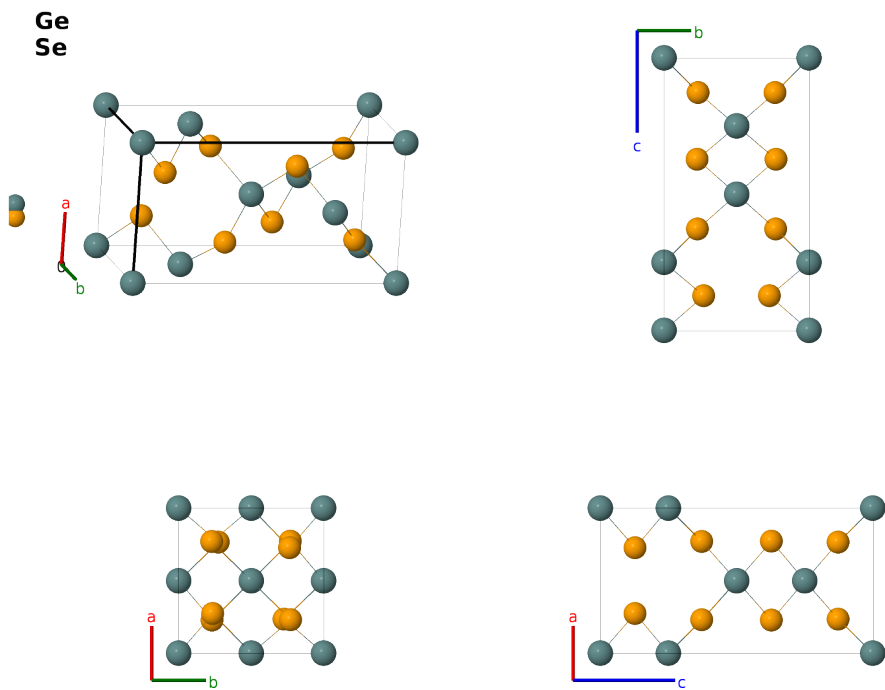
This structure previously used the label(s) **AB2_tP12_81_adg_2h**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/1L9R>

https://aflow.org/prototype-encyclopedia/AB2_tP12_81_adg_2h-001

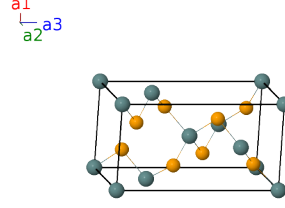


Prototype	GeSe ₂
AFLOW prototype label	AB2_tP12_81_adg_2h-001
ICSD	90957
CCDC	1650531
Pearson symbol	tP12
Space group number	81
Space group symbol	$P\bar{4}$
AFLOW prototype command	<code>aflow --proto=AB2_tP12_81_adg_2h-001</code> <code>--params=a, c/a, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

- This data was taken at $T = 698$ K with $P = 2$ GPa.
- Our original version of this structure in (Hicks, 2019) had $z_5 = 0.6373$ for the Se-II atoms. The correct value is 0.6273.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	Ge I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1d)	Ge II
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2g)	Ge III
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(2g)	Ge III
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B}_7$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B}_8$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4h)	Se II
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4h)	Se II
$\mathbf{B}_{11}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4h)	Se II
$\mathbf{B}_{12}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4h)	Se II

References

- [1] A. Grzechnik, S. St, E. Bakken, T. Grande, and M. Mezouar, *Structural Transformations in Three-Dimensional Crystalline GeSe₂ at High Pressures and High Temperatures*, J. Solid State Chem. **150**, 121–127 (2000), doi:10.1006/jssc.1999.8557.
- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

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

First cited in

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