

ϵ-GaSe Structure:

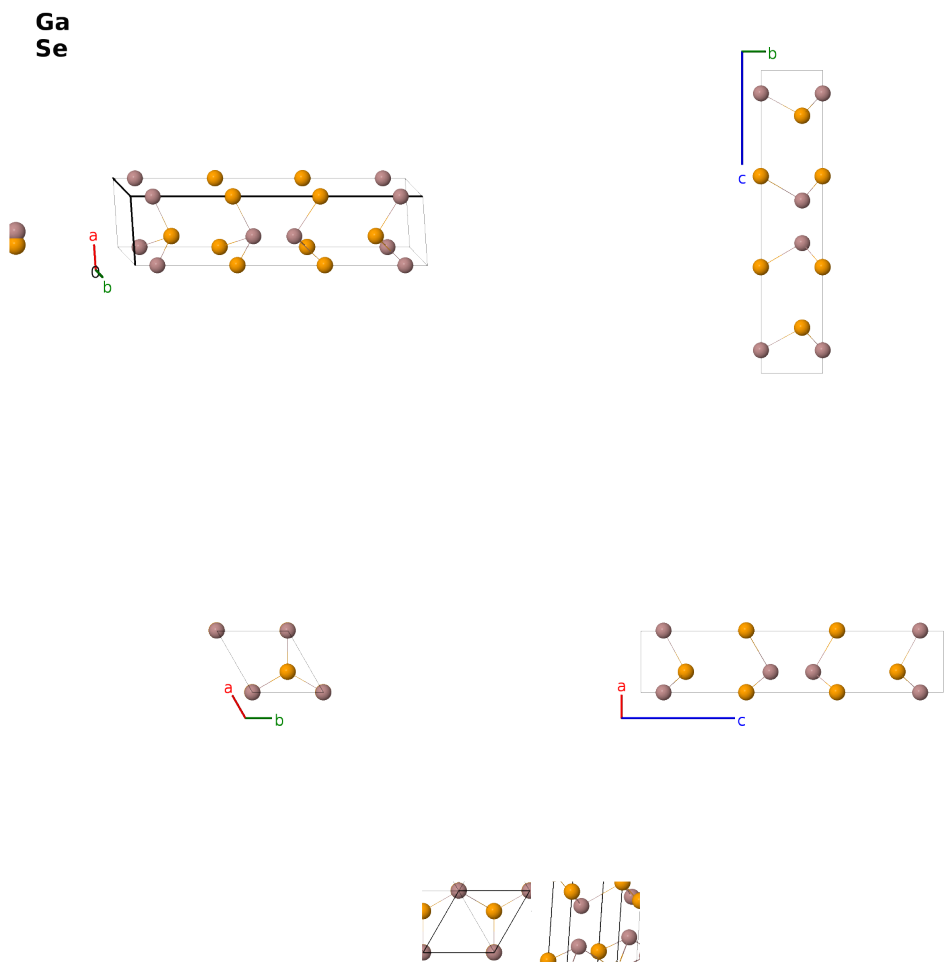
AB_hP8_187_gh_gh-001

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<https://aflow.org/prototype-encyclopedia/M3JC>

https://aflow.org/prototype-encyclopedia/AB_hP8_187_gh_gh-001



Prototype	GaSe
AFLOW prototype label	AB_hP8_187_gh_gh-001
Pearson symbol	hP8
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	<code>aflow --proto=AB_hP8_187_gh_gh-001</code> <code>--params=$a, c/a, z_1, z_2, z_3, z_4$</code>

Other compounds with this structure

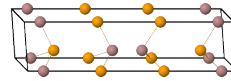
InSe

- GaSe takes on a variety of structures depending on the stacking of the Ga_2Se_2 layers:
 - β -GaSe is in space group $P6_3/mmc$ #194.
 - γ -GaSe is in space group $R3m$ #160.
 - δ -GaSe is in space group $P6_3mc$ #186.
 - ϵ -GaSe (this structure) is in space group $P\bar{6}m2$ #187.
 - We have rotated the cell to move the published (2i) Wyckoff positions to the (2h) Wyckoff sites.
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Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$

a1
a2 a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2g)	Ga I
$\mathbf{B}_2$	$= -z_1 \mathbf{a}_3$	$=$	$-cz_1 \hat{\mathbf{z}}$	(2g)	Ga I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2g)	Se I
$\mathbf{B}_4$	$= -z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(2g)	Se I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2h)	Ga II
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2h)	Ga II
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2h)	Se II
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2h)	Se II

References

- [1] A. Kuhn, A. Chevy, and R. Chevalier, *Crystal Structure and Interatomic Distances in GaSe*, phys. stat. sol. (a) **31**, 469–475 (1975), doi:10.1002/pssa.2210310216.
- [2] K. Schubert, E. Dörre, and M. Kluge, *Zur Kristallchemie der B-Metalle. III. Kristallstruktur von GaSe und InTe*, Z. Metallkd. **46**, 216–224 (1955), doi:10.1515/ijmr-1955-460312.

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