

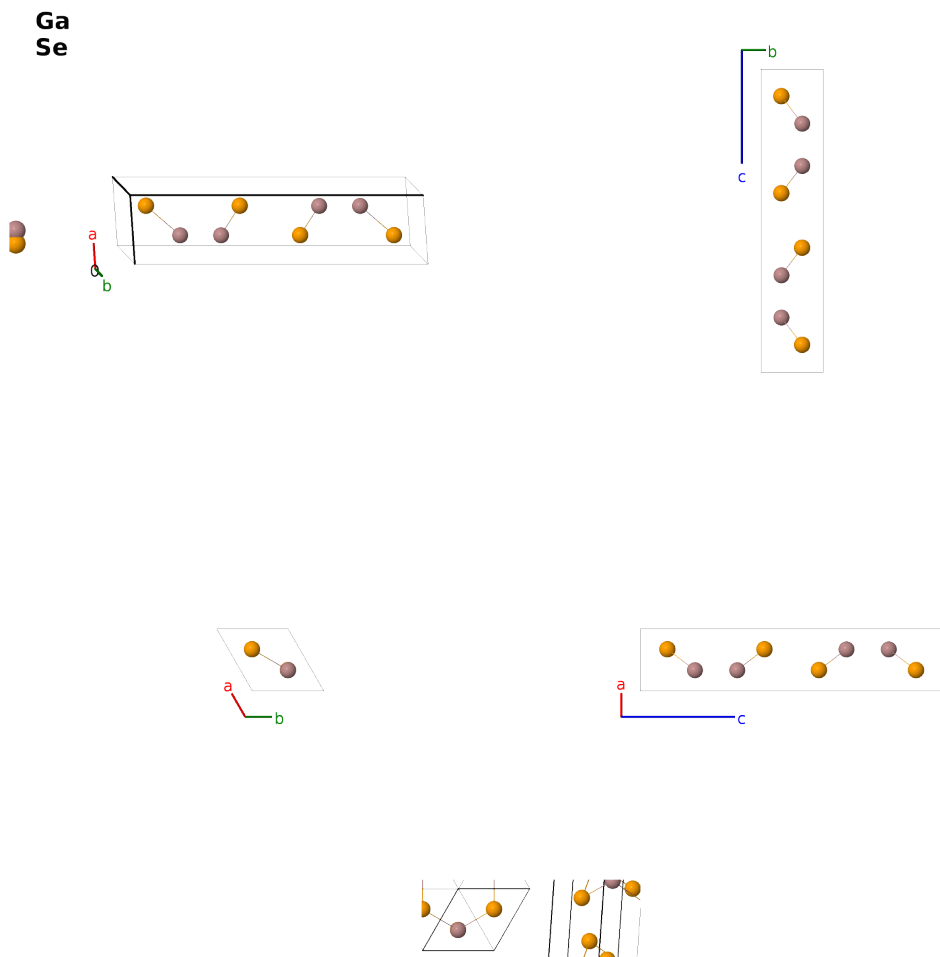
β -GaSe Structure: AB_hP8_194_f_f-003

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<https://aflow.org/prototype-encyclopedia/BDG1>

https://aflow.org/prototype-encyclopedia/AB_hP8_194_f_f-003



Prototype	GaSe
AFLOW prototype label	AB_hP8_194_f_f-003
ICSD	41978
CCDC	1611699
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$

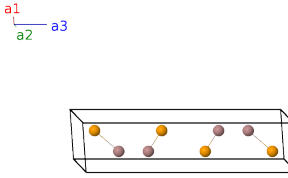
AFLOW prototype command `aflow --proto=AB_hP8_194_f_f-003`
 `--params=a, c/a, z1, z2`

Other compounds with this structure

GaS, GaTe, InSe

- GaSe takes on a variety of structures depending on the stacking of the Ga₂Se₂ layers:
 - β -GaSe (this structure) 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 is in space group $P\bar{6}m2$ #187.

Hexagonal primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B}_3$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B}_4$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Se I

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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