ϵ-GaSe Structure: AB_hP8_187_gh_gh-001

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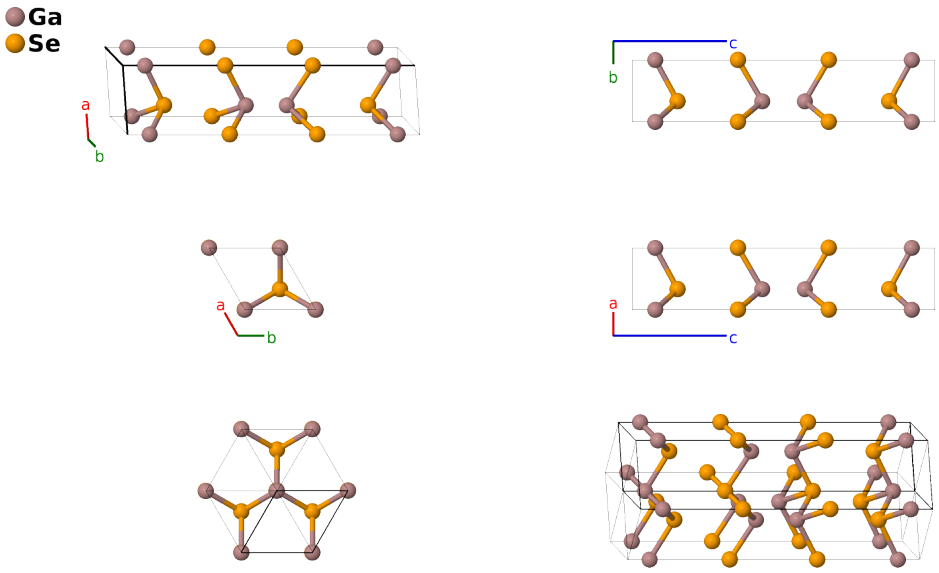
https://aflow.org/p/M3JC

https://aflow.org/p/AB_hP8_187_gh_gh-001



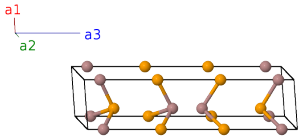
Prototype	GaSe
AFLOW prototype label	AB_hP8_187_gh_gh-001
ICSD	none
Pearson symbol	hP8
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=AB_hP8_187_gh_gh-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

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.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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.