β-GaSe Structure: AB_hP8_194_f_f-003

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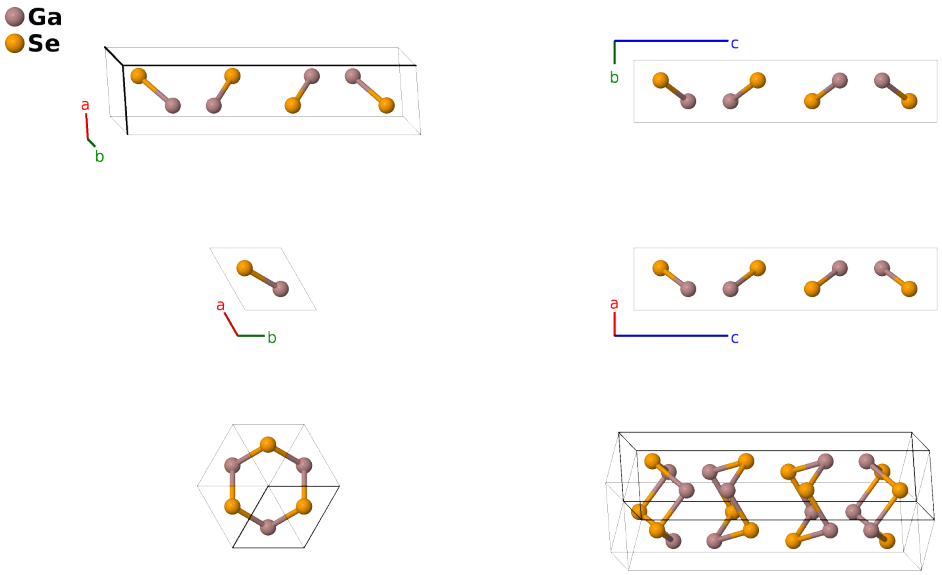
https://aflow.org/p/BDG1

https://aflow.org/p/AB_hP8_194_f_f-003



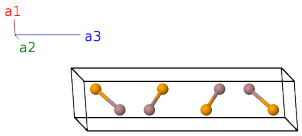
Prototype	GaSe
AFLOW prototype label	AB_hP8_194_f_f-003
ICSD	41978
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB_hP8_194_f_f-003 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure
GaS, GaTe, InSe

- GaSe takes on a variety of structures depending on the stacking of the Ga_2Se_2 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B_2}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B_3}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B_4}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_1 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_1 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Ga I
$\mathbf{B_5}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_6}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_7}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_8}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.