γ-GaSe Structure: AB_hR4_160_2a_2a-001

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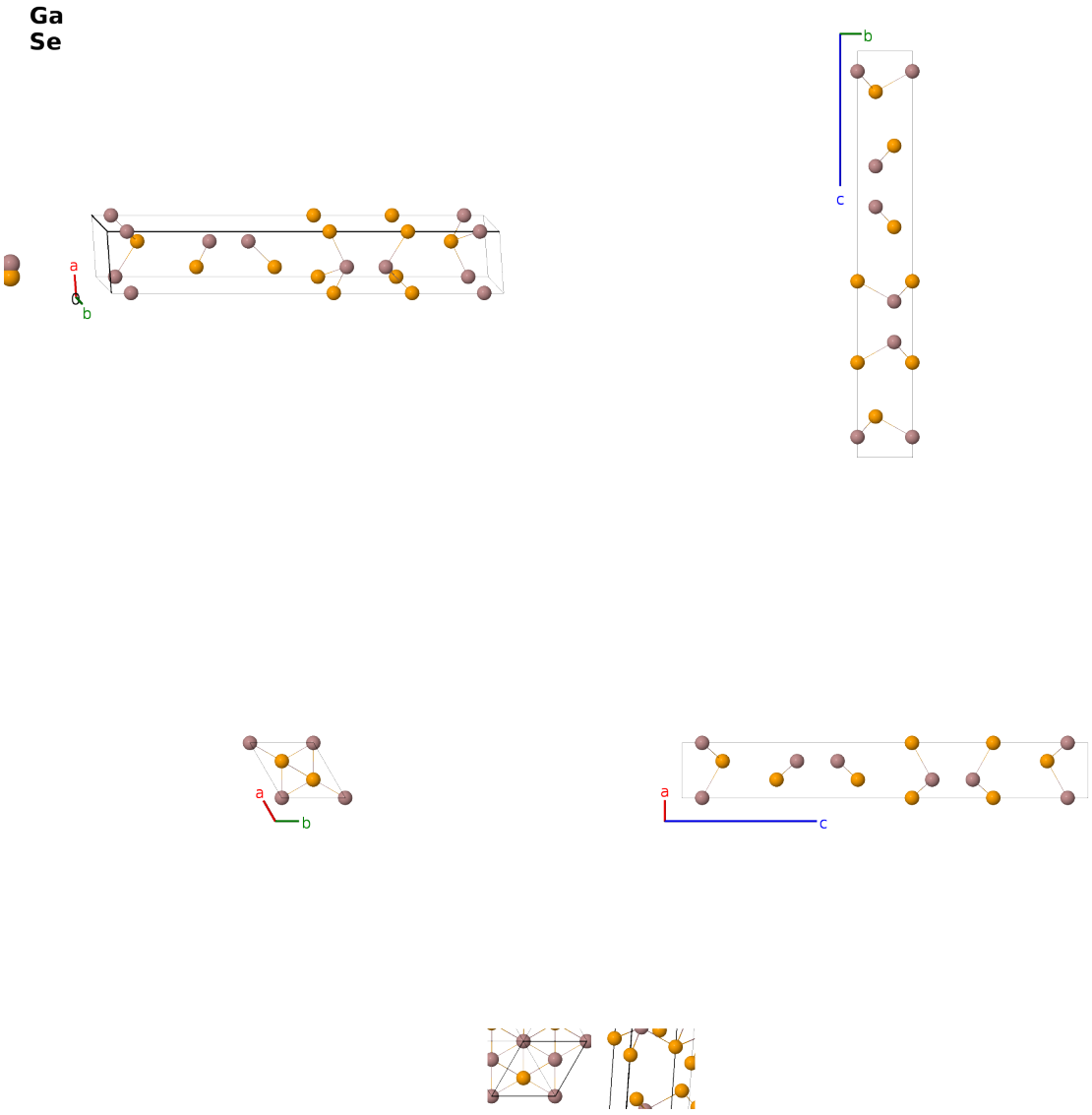
https://aflow.org/prototype-encyclopedia/M3V5

https://aflow.org/prototype-encyclopedia/AB_hR4_160_2a_2a-001



Prototype	GaSe
AFLOW prototype label	AB_hR4_160_2a_2a-001
ICSD	73388
CCDC	1634184

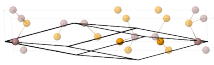
Pearson symbol	hR4
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB_hR4_160_2a_2a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4$

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 (this structure) 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.
- There is no ICSD entry for (Kuhn, 1975), so we use the earlier work of (Schubert, 1955).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Ga I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	Ga II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	Se I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	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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