δ-GaSe Structure: AB_hP16_186_2a2b_2a2b-001

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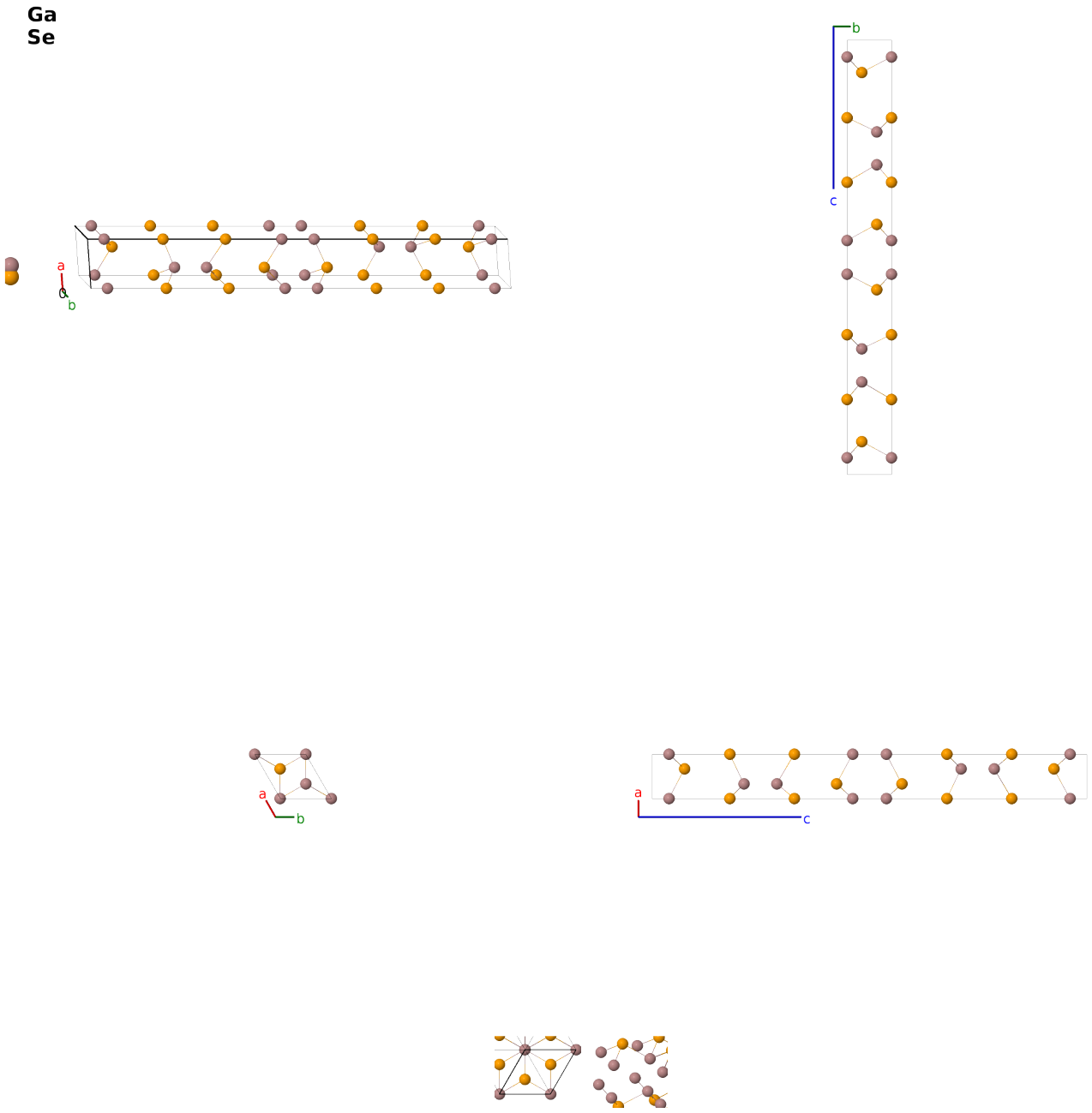
https://aflow.org/prototype-encyclopedia/W6UW

https://aflow.org/prototype-encyclopedia/AB_hP16_186_2a2b_2a2b-001



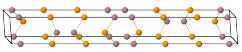
Prototype GaSe

AFLOW prototype label	AB_hP16_186_2a2b_2a2b-001
ICSD	2002
CCDC	1591958
Pearson symbol	hP16
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=AB_hP16_186_2a2b_2a2b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8$

- 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 (this structure) is in space group $P6_3mc$ #186.
  - ϵ-GaSe is in space group $P\bar{6}m2$ #187.
- The origin of the z coordinates is arbitrary in space group $P6_3mc$ #186.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ga I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ga I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Ga II
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ga II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B_6}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B_7}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	Se II
$\mathbf{B_8}$	=	$\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Se II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(2b)	Ga III
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ga III
$\mathbf{B_{11}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(2b)	Ga IV

$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ga IV
$\mathbf{B_{13}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2b)	Se III
$\mathbf{B_{14}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Se III
$\mathbf{B_{15}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(2b)	Se IV
$\mathbf{B_{16}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Se IV

References

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