$Ca_{11}InSb_9$ Structure: A11BC9_oI84_45_a5c_a_b4c-001

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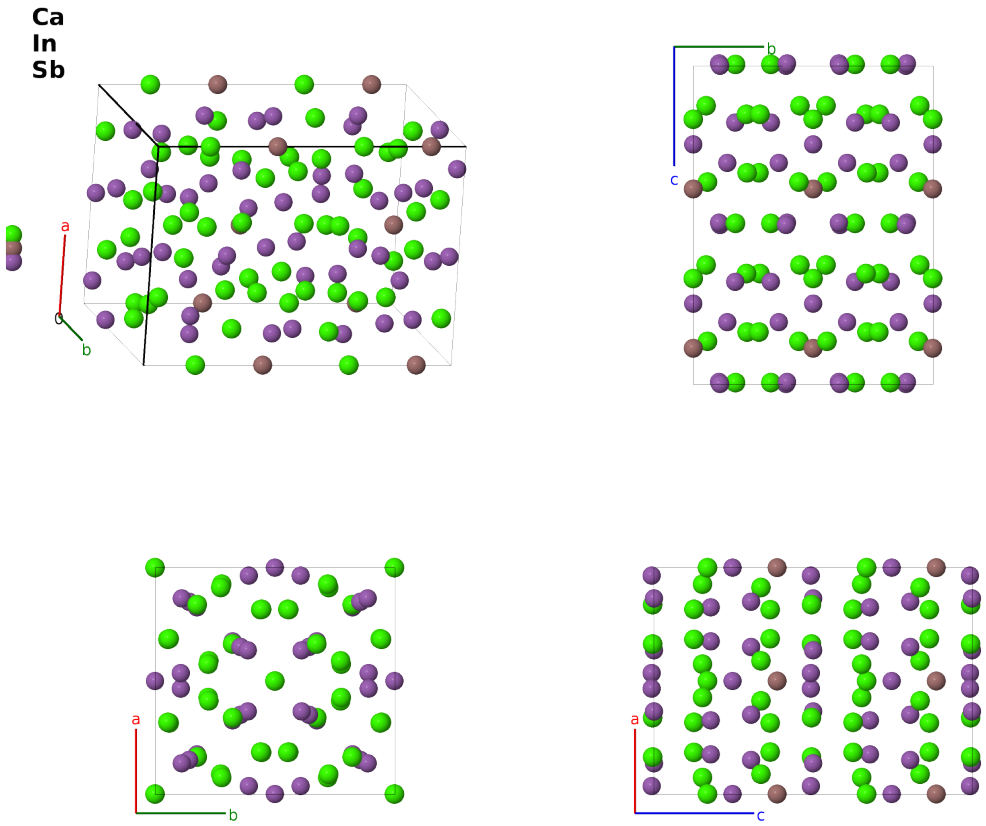
https://aflow.org/prototype-encyclopedia/DZ16

https://aflow.org/prototype-encyclopedia/A11BC9_oI84_45_a5c_a_b4c-001



Prototype	$Ca_{11}InSb_9$
AFLOW prototype label	A11BC9_oI84_45_a5c_a_b4c-001
ICSD	42371
CCDC	1612041
Pearson symbol	oI84
Space group number	45
Space group symbol	*Iba*2

AFLOW prototype command `aflow --proto=A11BC9_oI84_45_a5c_a_b4c-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

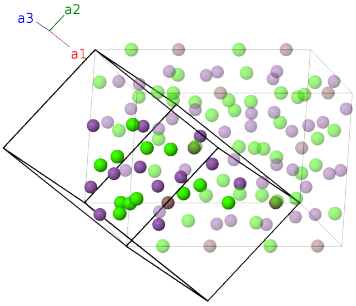
Other compounds with this structure

$Ca_{11}AlSb_9$, $Ca_{11}GaSb_9$, $Eu_{11}InSb_9$, $Yb_{11}AlSb_9$

- Space group $Iba2$ #45 allows an arbitrary placement of the z-axis origin. Here we chose it so that $z_9 = 1/2$ for the Sb-II site.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_2}$	=	$\left(z_1 + \frac{1}{2}\right)\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_2$	=	$c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	In I
$\mathbf{B_4}$	=	$\left(z_2 + \frac{1}{2}\right)\mathbf{a}_1 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_2$	=	$c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	In I
$\mathbf{B_5}$	=	$\left(z_3 + \frac{1}{2}\right)\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Sb I
$\mathbf{B_6}$	=	$z_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Sb I
$\mathbf{B_7}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B_8}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B_9}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B_{10}}$	=	$\left(y_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B_{11}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B_{12}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B_{13}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Ca III
$\mathbf{B_{14}}$	=	$\left(y_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Ca III

$$\mathbf{B_{15}} = (y_6+z_6)\,\mathbf{a}_1+(x_6+z_6)\,\mathbf{a}_2+(x_6+y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca IV}$$

$$\mathbf{B_{16}} = -(y_6-z_6)\,\mathbf{a}_1-(x_6-z_6)\,\mathbf{a}_2-(x_6+y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca IV}$$

$$\mathbf{B_{17}} = \left(-y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_2+(x_6-y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca IV}$$

$$\mathbf{B_{18}} = \left(y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_2-(x_6-y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca IV}$$

$$\mathbf{B_{19}} = (y_7+z_7)\,\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+(x_7+y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca V}$$

$$\mathbf{B_{20}} = -(y_7-z_7)\,\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-(x_7+y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca V}$$

$$\mathbf{B_{21}} = \left(-y_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_2+(x_7-y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca V}$$

$$\mathbf{B_{22}} = \left(y_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_2-(x_7-y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca V}$$

$$\mathbf{B_{23}} = (y_8+z_8)\,\mathbf{a}_1+(x_8+z_8)\,\mathbf{a}_2+(x_8+y_8)\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca VI}$$

$$\mathbf{B_{24}} = -(y_8-z_8)\,\mathbf{a}_1-(x_8-z_8)\,\mathbf{a}_2-(x_8+y_8)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (8c) \quad \text{Ca VI}$$

$$\mathbf{B_{25}} = \left(-y_8+z_8+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_8+z_8+\tfrac{1}{2}\right)\mathbf{a}_2+(x_8-y_8)\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca VI}$$

$$\mathbf{B_{26}} = \left(y_8+z_8+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_8+z_8+\tfrac{1}{2}\right)\mathbf{a}_2-(x_8-y_8)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Ca VI}$$

$$\mathbf{B_{27}} = (y_9+z_9)\,\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+(x_9+y_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb II}$$

$$\mathbf{B_{28}} = -(y_9-z_9)\,\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-(x_9+y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb II}$$

$$\mathbf{B_{29}} = \left(-y_9+z_9+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_9+z_9+\tfrac{1}{2}\right)\mathbf{a}_2+(x_9-y_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Sb II}$$

$$\mathbf{B_{30}} = \left(y_9+z_9+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_9+z_9+\tfrac{1}{2}\right)\mathbf{a}_2-(x_9-y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Sb II}$$

$$\mathbf{B_{31}} = (y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}+z_{10})\,\mathbf{a}_2+(x_{10}+y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb III}$$

$$\mathbf{B_{32}} = -(y_{10}-z_{10})\,\mathbf{a}_1-(x_{10}-z_{10})\,\mathbf{a}_2-(x_{10}+y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb III}$$

$$\mathbf{B_{33}} = \left(-y_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_2+(x_{10}-y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Sb III}$$

$$\mathbf{B_{34}} = \left(y_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_{10}+z_{10}+\tfrac{1}{2}\right)\mathbf{a}_2-(x_{10}-y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8c) \quad \text{Sb III}$$

$$\mathbf{B_{35}} = (y_{11}+z_{11})\,\mathbf{a}_1+(x_{11}+z_{11})\,\mathbf{a}_2+(x_{11}+y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb IV}$$

$$\mathbf{B_{36}} = -(y_{11}-z_{11})\,\mathbf{a}_1-(x_{11}-z_{11})\,\mathbf{a}_2-(x_{11}+y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (8c) \quad \text{Sb IV}$$

$\mathbf{B_{37}}$	=	$\left(-y_{11}+z_{11}+\frac{1}{2}\right)\mathbf{a}_1+\left(x_{11}+z_{11}+\frac{1}{2}\right)\mathbf{a}_2+\left(x_{11}-y_{11}\right)\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{38}}$	=	$\left(y_{11}+z_{11}+\frac{1}{2}\right)\mathbf{a}_1+\left(-x_{11}+z_{11}+\frac{1}{2}\right)\mathbf{a}_2-\left(x_{11}-y_{11}\right)\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{39}}$	=	$\left(y_{12}+z_{12}\right)\mathbf{a}_1+\left(x_{12}+z_{12}\right)\mathbf{a}_2+\left(x_{12}+y_{12}\right)\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8c)	Sb V
$\mathbf{B_{40}}$	=	$-\left(y_{12}-z_{12}\right)\mathbf{a}_1-\left(x_{12}-z_{12}\right)\mathbf{a}_2-\left(x_{12}+y_{12}\right)\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8c)	Sb V
$\mathbf{B_{41}}$	=	$\left(-y_{12}+z_{12}+\frac{1}{2}\right)\mathbf{a}_1+\left(x_{12}+z_{12}+\frac{1}{2}\right)\mathbf{a}_2+\left(x_{12}-y_{12}\right)\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Sb V
$\mathbf{B_{42}}$	=	$\left(y_{12}+z_{12}+\frac{1}{2}\right)\mathbf{a}_1+\left(-x_{12}+z_{12}+\frac{1}{2}\right)\mathbf{a}_2-\left(x_{12}-y_{12}\right)\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8c)	Sb V

References

[1] G. Cordier, H. Schäfer, and M. Stelter, *$Ca_{11}InSb_9$, eine Zintlphase mit diskreten $InSb_4^{9-}$-Anionen*, Z. Naturforsch. B **40**, 868–871 (1985), doi:10.1515/znb-1985-0703.

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