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

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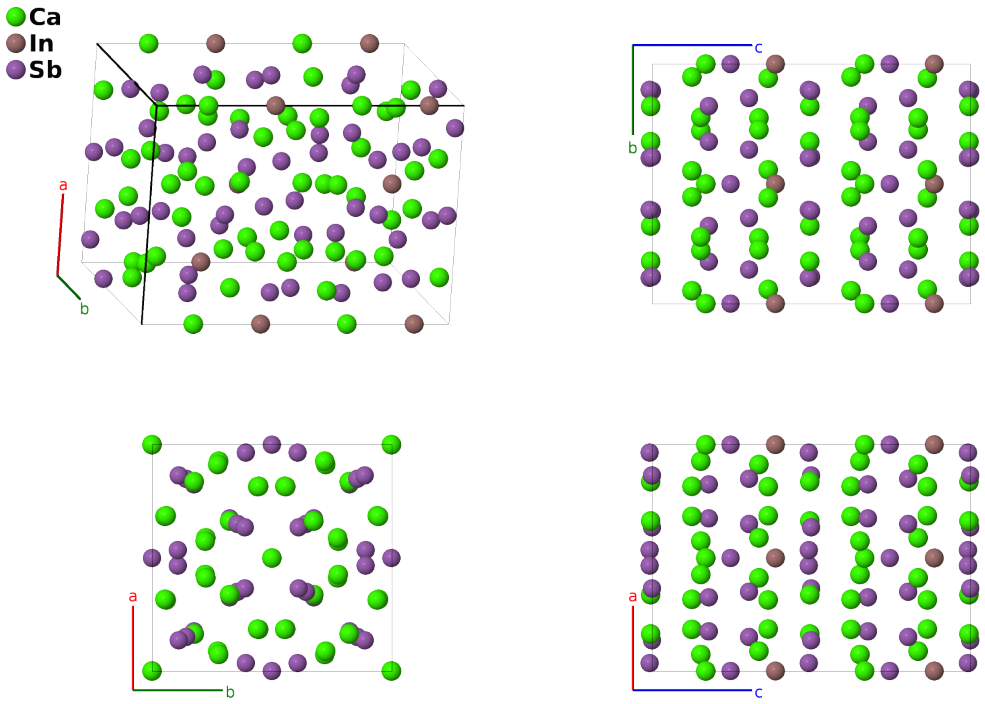
https://aflow.org/p/DZ16

https://aflow.org/p/A11BC9_oI84_45_a5c_a_b4c-001



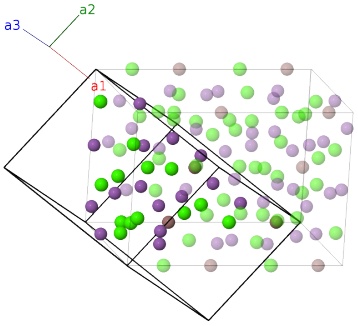
Prototype	$Ca_{11}InSb_9$
AFLOW prototype label	A11BC9_oI84_45_a5c_a_b4c-001
ICSD	42371
Pearson symbol	oI84
Space group number	45
Space group symbol	$Iba2$
AFLOW prototype command	`aflow --proto=A11BC9_oI84_45_a5c_a_b4c-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

Other compounds with this structure
$Ca_{11}AlSb_9$, $Ca_{11}GaSb_9$, $Eu_{11}InSb_9$

- 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
$\mathbf{B_{15}}$	=	$(y_6+z_6)\,\mathbf{a}_1 + (x_6+z_6)\,\mathbf{a}_2 + (x_6+y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B_{16}}$	=	$-(y_6-z_6)\,\mathbf{a}_1 - (x_6-z_6)\,\mathbf{a}_2 - (x_6+y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B_{17}}$	=	$\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_6-y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B_{18}}$	=	$\left(y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2 - (x_6-y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca IV
$\mathbf{B_{19}}$	=	$(y_7+z_7)\,\mathbf{a}_1 + (x_7+z_7)\,\mathbf{a}_2 + (x_7+y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Ca V

$\mathbf{B_{20}}$	$=$	$-(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Ca V
$\mathbf{B_{21}}$	$=$	$\left(-y_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca V
$\mathbf{B_{22}}$	$=$	$\left(y_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca V
$\mathbf{B_{23}}$	$=$	$(y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3$	$=$	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8c)	Ca VI
$\mathbf{B_{24}}$	$=$	$-(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3$	$=$	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8c)	Ca VI
$\mathbf{B_{25}}$	$=$	$\left(-y_8 + z_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 + z_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3$	$=$	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca VI
$\mathbf{B_{26}}$	$=$	$\left(y_8 + z_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_8 + z_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3$	$=$	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ca VI
$\mathbf{B_{27}}$	$=$	$(y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3$	$=$	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8c)	Sb II
$\mathbf{B_{28}}$	$=$	$-(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3$	$=$	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8c)	Sb II
$\mathbf{B_{29}}$	$=$	$\left(-y_9 + z_9 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_9 + z_9 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_9 - y_9)\,\mathbf{a}_3$	$=$	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb II
$\mathbf{B_{30}}$	$=$	$\left(y_9 + z_9 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_9 + z_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3$	$=$	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb II
$\mathbf{B_{31}}$	$=$	$(y_{10} + z_{10})\,\mathbf{a}_1 + (x_{10} + z_{10})\,\mathbf{a}_2 + (x_{10} + y_{10})\,\mathbf{a}_3$	$=$	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8c)	Sb III
$\mathbf{B_{32}}$	$=$	$-(y_{10} - z_{10})\,\mathbf{a}_1 - (x_{10} - z_{10})\,\mathbf{a}_2 - (x_{10} + y_{10})\,\mathbf{a}_3$	$=$	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8c)	Sb III
$\mathbf{B_{33}}$	$=$	$\left(-y_{10} + z_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_{10} + z_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_{10} - y_{10})\,\mathbf{a}_3$	$=$	$ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb III
$\mathbf{B_{34}}$	$=$	$\left(y_{10} + z_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_{10} + z_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_{10} - y_{10})\,\mathbf{a}_3$	$=$	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb III
$\mathbf{B_{35}}$	$=$	$(y_{11} + z_{11})\,\mathbf{a}_1 + (x_{11} + z_{11})\,\mathbf{a}_2 + (x_{11} + y_{11})\,\mathbf{a}_3$	$=$	$ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{36}}$	$=$	$-(y_{11} - z_{11})\,\mathbf{a}_1 - (x_{11} - z_{11})\,\mathbf{a}_2 - (x_{11} + y_{11})\,\mathbf{a}_3$	$=$	$-ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{37}}$	$=$	$\left(-y_{11} + z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_{11} + z_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_{11} - y_{11})\,\mathbf{a}_3$	$=$	$ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{38}}$	$=$	$\left(y_{11} + z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_{11} + z_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_{11} - y_{11})\,\mathbf{a}_3$	$=$	$-ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb IV
$\mathbf{B_{39}}$	$=$	$(y_{12} + z_{12})\,\mathbf{a}_1 + (x_{12} + z_{12})\,\mathbf{a}_2 + (x_{12} + y_{12})\,\mathbf{a}_3$	$=$	$ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(8c)	Sb V
$\mathbf{B_{40}}$	$=$	$-(y_{12} - z_{12})\,\mathbf{a}_1 - (x_{12} - z_{12})\,\mathbf{a}_2 - (x_{12} + y_{12})\,\mathbf{a}_3$	$=$	$-ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(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.