CsV_8Sb_{12} Structure: AB12C8_oF84_69_a_2g2n_fgl-001

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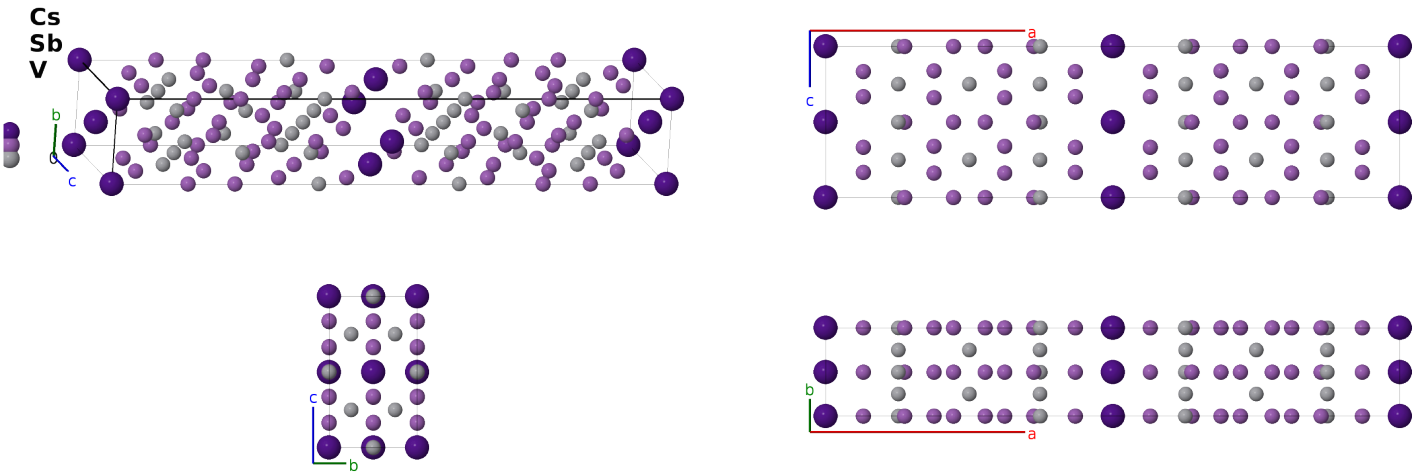
https://aflow.org/prototype-encyclopedia/GP6W

https://aflow.org/prototype-encyclopedia/AB12C8_oF84_69_a_2g2n_fgl-001

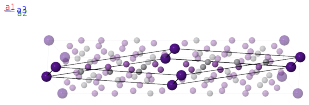


Prototype	CsV_8Sb_{12}
AFLOW prototype label	AB12C8_oF84_69_a_2g2n_fgl-001
Pearson symbol	oF84
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=AB12C8_oF84_69_a_2g2n_fgl-001 --params=`$a, b/a, c/a, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8$

- The AFLOW prototype label protocol rotates the reported axes, taking → b → c → a.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cs I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	V I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	V I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8g)	Sb I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8g)	Sb I
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(8g)	Sb II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(8g)	Sb II
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(8g)	V II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}$	(8g)	V II
$\mathbf{B_{10}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	V III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	V III
$\mathbf{B_{12}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	V III
$\mathbf{B_{13}}$	=	$-x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	V III
$\mathbf{B_{14}}$	=	$-\left(x_7 - z_7\right)\,\mathbf{a}_1 + \left(x_7 + z_7\right)\,\mathbf{a}_2 + \left(x_7 - z_7\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(16n)	Sb III
$\mathbf{B_{15}}$	=	$\left(x_7 + z_7\right)\,\mathbf{a}_1 - \left(x_7 - z_7\right)\,\mathbf{a}_2 - \left(x_7 + z_7\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(16n)	Sb III
$\mathbf{B_{16}}$	=	$\left(x_7 - z_7\right)\,\mathbf{a}_1 - \left(x_7 + z_7\right)\,\mathbf{a}_2 - \left(x_7 - z_7\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(16n)	Sb III
$\mathbf{B_{17}}$	=	$-\left(x_7 + z_7\right)\,\mathbf{a}_1 + \left(x_7 - z_7\right)\,\mathbf{a}_2 + \left(x_7 + z_7\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(16n)	Sb III
$\mathbf{B_{18}}$	=	$-\left(x_8 - z_8\right)\,\mathbf{a}_1 + \left(x_8 + z_8\right)\,\mathbf{a}_2 + \left(x_8 - z_8\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sb IV
$\mathbf{B_{19}}$	=	$\left(x_8 + z_8\right)\,\mathbf{a}_1 - \left(x_8 - z_8\right)\,\mathbf{a}_2 - \left(x_8 + z_8\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sb IV
$\mathbf{B_{20}}$	=	$\left(x_8 - z_8\right)\,\mathbf{a}_1 - \left(x_8 + z_8\right)\,\mathbf{a}_2 - \left(x_8 - z_8\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sb IV
$\mathbf{B_{21}}$	=	$-\left(x_8 + z_8\right)\,\mathbf{a}_1 + \left(x_8 - z_8\right)\,\mathbf{a}_2 + \left(x_8 + z_8\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sb IV

References

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