CdSb (B_e) Structure: AB_oP16_61_c_c-001

This structure originally had the label `AB_oP16_61_c_c`. Calls to that address will be redirected here.

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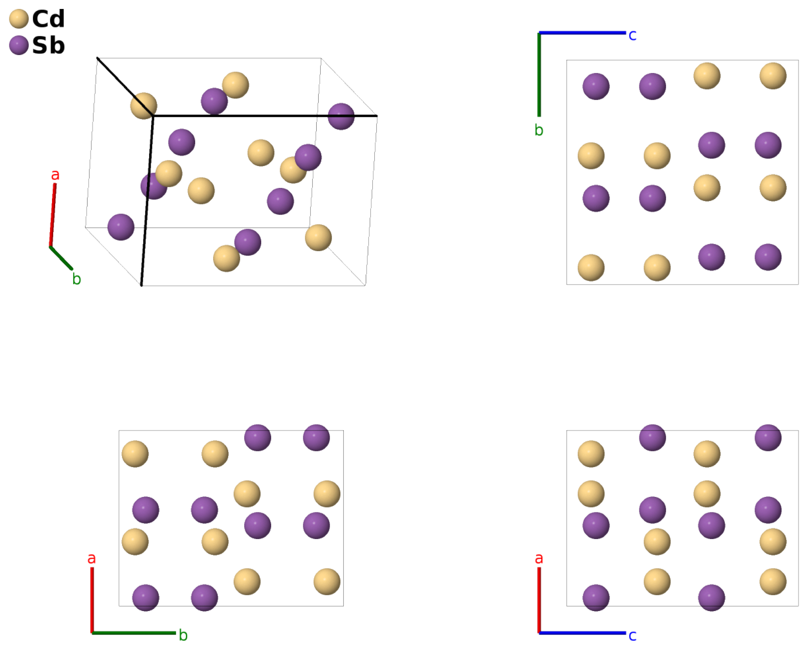
https://aflow.org/p/RL87

https://aflow.org/p/AB_oP16_61_c_c-001



Prototype	CdSb
AFLOW prototype label	AB_oP16_61_c_c-001
***Strukturbericht* designation**	B_e
ICSD	52831
Pearson symbol	oP16
Space group number	61
Space group symbol	*Pbca*
AFLOW prototype command	`aflow --proto=AB_oP16_61_c_c-001` `--params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2$

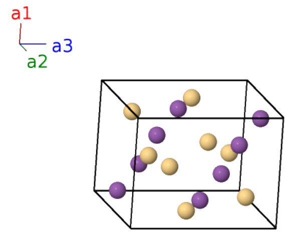
Other compounds with this structure

AsCd, AsZn, SbZn

- This structure has the same AFLOW label as solid cyanogen, $(CN)_2$. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} + cz_1\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} + c\left(z_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + b\left(y_1 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_1\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} - by_1\,\mathbf{\hat{y}} - cz_1\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + by_1\,\mathbf{\hat{y}} - c\left(z_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} - b\left(y_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_1 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_1\,\mathbf{\hat{z}}$	(8c)	Cd I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + b\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{12}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + by_2\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{15}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} - b\left(y_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Sb I
$\mathbf{B_{16}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(8c)	Sb I

References

[1] K. E. Almin, *The Crystal Structure of CdSb and ZnSb*, Acta Chem. Scand. **4**, 400–407 (1948), doi:10.3891/acta.chem.scand.02-0400.