$SmSb_2$ Structure: A2B_oC24_64_ef_f-001

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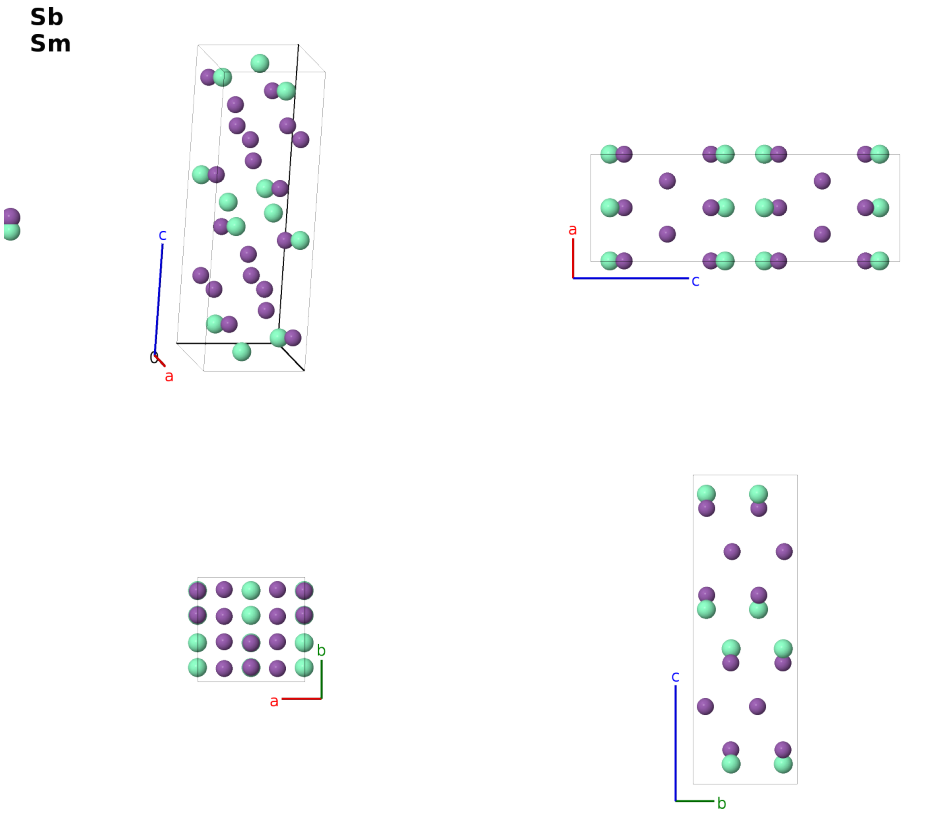
https://aflow.org/prototype-encyclopedia/370K

https://aflow.org/prototype-encyclopedia/A2B_oC24_64_ef_f-001

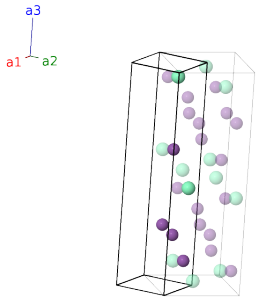


Prototype	Sb_2Sm
AFLOW prototype label	A2B_oC24_64_ef_f-001
ICSD	43029
CCDC	1612624
Pearson symbol	oC24
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=A2B_oC24_64_ef_f-001 --params=`$a, b/a, c/a, y_1, y_2, z_2, y_3, z_3$

Other compounds with this structure
$CeSb_2$, $LaSb_2$, $NbSb_2$, $NdSb_2$, $PrSb_2$, $TbSb_2$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-\left(y_1-\frac{1}{4}\right)\mathbf{a}_1+\left(y_1+\frac{1}{4}\right)\mathbf{a}_2+\frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Sb I
$\mathbf{B_2}$	=	$\left(y_1+\frac{1}{4}\right)\mathbf{a}_1-\left(y_1-\frac{1}{4}\right)\mathbf{a}_2+\frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Sb I
$\mathbf{B_3}$	=	$\left(y_1+\frac{3}{4}\right)\mathbf{a}_1-\left(y_1-\frac{3}{4}\right)\mathbf{a}_2+\frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Sb I
$\mathbf{B_4}$	=	$-\left(y_1-\frac{3}{4}\right)\mathbf{a}_1+\left(y_1+\frac{3}{4}\right)\mathbf{a}_2+\frac{1}{4}\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Sb I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8f)	Sb II
$\mathbf{B_6}$	=	$\left(y_2+\frac{1}{2}\right)\mathbf{a}_1-\left(y_2-\frac{1}{2}\right)\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Sb II
$\mathbf{B_7}$	=	$-\left(y_2-\frac{1}{2}\right)\mathbf{a}_1+\left(y_2+\frac{1}{2}\right)\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Sb II
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(8f)	Sb II
$\mathbf{B_9}$	=	$-y_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(8f)	Sm I
$\mathbf{B_{10}}$	=	$\left(y_3+\frac{1}{2}\right)\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Sm I
$\mathbf{B_{11}}$	=	$-\left(y_3-\frac{1}{2}\right)\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8f)	Sm I
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(8f)	Sm I

References

[1] R. Wang and H. Steinfink, *The crystal chemistry of selected AB_2 rare earth compounds with selenium, tellurium, and antimony*, Inorg. Chem. **6**, 1685–1692 (1967), doi:10.1021/ic50055a017.

Found in

[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Antimony-Samarium Binary Phase Diagram (1994 Okamoto H.). Copyright ©2006-2018 ASM International.

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