Senarmontite ($D6_1$, Sb_2O_3) Structure: A3B2_cF80_227_f_e-002

This structure originally had the label `A3B2_cF80_227_f_e`. Calls to that address will be redirected here.

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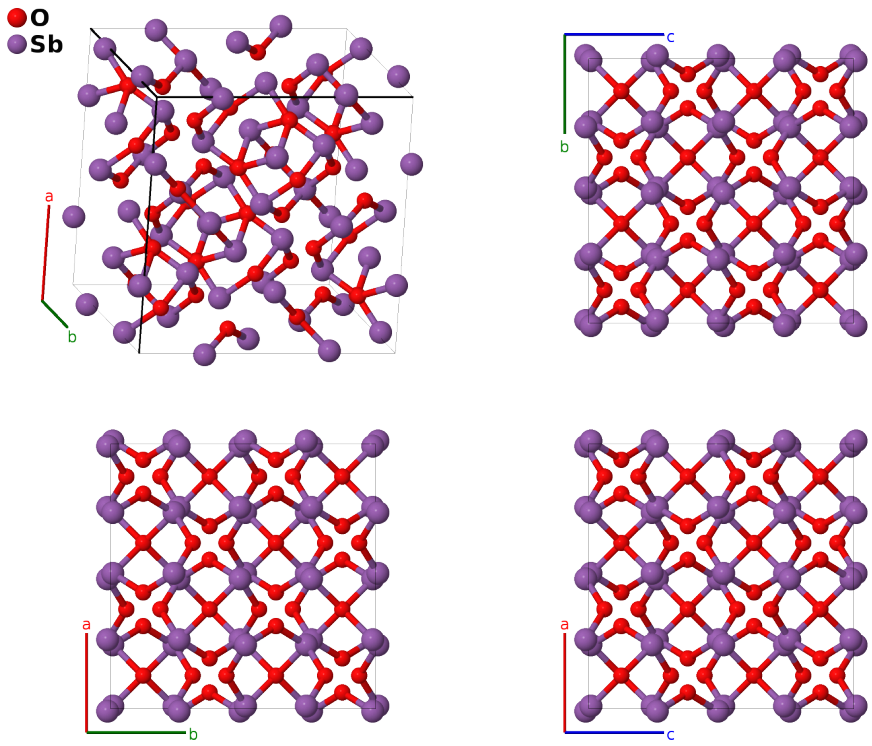
https://aflow.org/p/UHQ6

https://aflow.org/p/A3B2_cF80_227_f_e-002



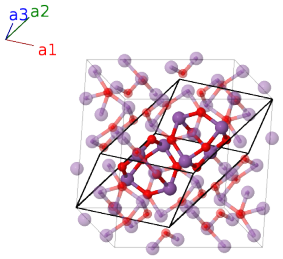
Prototype	O_3Sb_2
AFLOW prototype label	A3B2_cF80_227_f_e-002
***Strukturbericht* designation**	$D6_1$
Mineral name	senarmontite
ICSD	1944
Pearson symbol	cF80
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B2_cF80_227_f_e-002 --params=`a, x_1, x_2

Other compounds with this structure
As_2O_3 (arsenolite)

- (Ewald, 1931) designated this as *Strukturbericht* $D6_1$, however (Parthé, 1993) and (Villars, 1991) label this as *Strukturbericht* $D5_4$, and Parthé uses As_2O_3 as the prototype. While this structure obviously fits better with the $D5$ series (A_2B_3) than $D6$ (A_2B_4), the $D5_4$ structure was (inadvertently?) omitted from (Hermann, 1937), which jumps from $D5_3$ to $D5_5$. We will follow this historical record (Ewald, 1931) here.
- This is the cubic form of Sb_2O_3. For the orthorhombic form see the valentinite ($D5_{11}$) structure.
- (Svensson, 1975) gave the atomic coordinates in setting 1 of space group $Fd\bar{3}m$ #227. We used FINDSYM to shift the coordinates to the standard setting 2.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - \left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_4}$	=	$-\left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_6}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_7}$	=	$-x_1\,\mathbf{a}_1 + \left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_8}$	=	$\left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Sb I
$\mathbf{B_9}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{13}}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{14}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{15}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{16}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{17}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{18}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{19}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{20}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	O I

References

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