

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

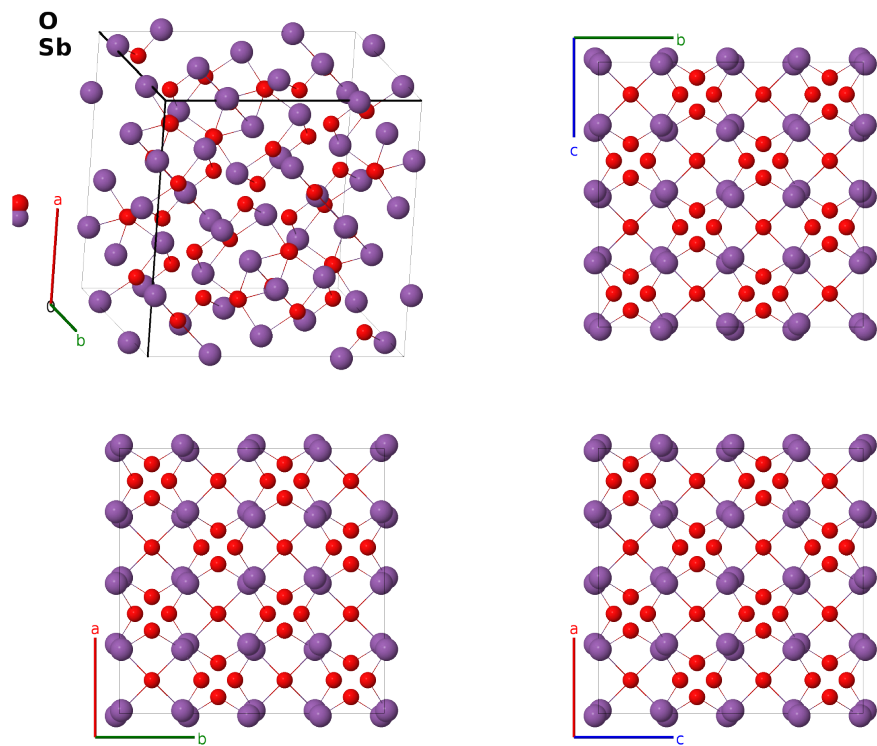
This structure previously used the label(s) **A3B2_cF80_227_f_e**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/UHQ6>

https://aflow.org/prototype-encyclopedia/A3B2_cF80_227_f_e-002



Prototype	O_3Sb_2
AFLOW prototype label	A3B2_cF80_227_f_e-002
<i>Strukturbericht</i> designation	$D6_1$
Mineral name	senarmontite
ICSD	1944
CCDC	1591903
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, x1, x2`

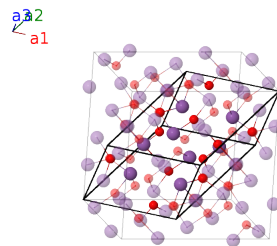
Other compounds with this structure

As₂O₃ (arsenolite)

- (Ewald, 1931) designated this as *Strukturbericht D6₁*, however (Parthé, 1993) and (Villars, 1991) label this as *Strukturbericht D5₄*, and Parthé uses As₂O₃ as the prototype. While this structure obviously fits better with the *D5* series (A₂B₃) than *D6* (A₂B₄), the *D5₄* structure was (inadvertently?) omitted from (Hermann, 1937), which jumps from *D5₃* to *D5₅*. We will follow this historical record (Ewald, 1931) here.
- This is the cubic form of Sb₂O₃. For the orthorhombic form see the valentinite (*D5₁₁*) structure.
- (Svensson, 1975) gave the atomic coordinates in setting 1 of space group *Fd3m* #227. We used FINDSYM to shift the coordinates to the standard setting 2.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(32e)	Sb I
B₂	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - (3x_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(32e)	Sb I
B₃	$x_1 \mathbf{a}_1 - (3x_1 - \frac{1}{2}) \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	Sb I
B₄	$-(3x_1 - \frac{1}{2}) \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	Sb I
B₅	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (3x_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(32e)	Sb I
B₆	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(32e)	Sb I
B₇	$-x_1 \mathbf{a}_1 + (3x_1 + \frac{1}{2}) \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	Sb I
B₈	$(3x_1 + \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	Sb I
B₉	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48f)	O I
B₁₀	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48f)	O I
B₁₁	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$\frac{1}{8}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48f)	O I
B₁₂	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{8}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48f)	O I
B₁₃	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(48f)	O I
B₁₄	$-(x_2 - \frac{1}{4}) \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48f)	O I
B₁₅	$(x_2 + \frac{3}{4}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3$	=	$\frac{3}{8}a \hat{\mathbf{x}} + a(x_2 + \frac{3}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}}$	(48f)	O I

$$\begin{aligned}
\mathbf{B}_{16} &= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3 &= \frac{3}{8}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} &(48f) &\quad \text{O I} \\
\mathbf{B}_{17} &= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_3 &= a \left(x_2 + \frac{3}{4}\right) \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} &(48f) &\quad \text{O I} \\
\mathbf{B}_{18} &= \left(x_2 + \frac{3}{4}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3 &= -ax_2 \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} &(48f) &\quad \text{O I} \\
\mathbf{B}_{19} &= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_3 &= \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} &(48f) &\quad \text{O I} \\
\mathbf{B}_{20} &= \left(x_2 + \frac{3}{4}\right) \mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3 &= \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + a \left(x_2 + \frac{3}{4}\right) \hat{\mathbf{z}} &(48f) &\quad \text{O I}
\end{aligned}$$

References

- [1] C. Svensson, *Refinement of the crystal structure of cubic antimony trioxide, Sb₂O₃*, Acta Crystallogr. Sect. B **31**, 2016–2018 (1975), doi:10.1107/S0567740875006759.
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [3] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.
- [4] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.
- [5] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.