$D6_2$ (Sb_2O_4, *Obsolete*) Structure: A2B_cF96_227_abf_cd-001

This structure previously used the label(s) `A2B_cF96_227_abf_cd`. Calls to these addresses will be redirected here.

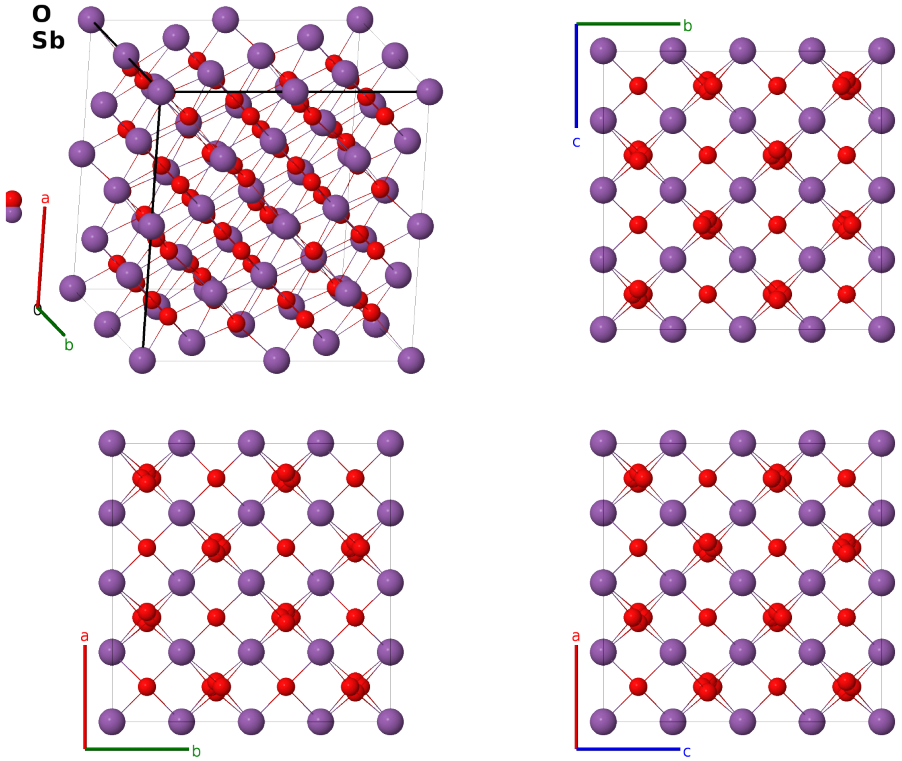
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/UGWY

https://aflow.org/prototype-encyclopedia/A2B_cF96_227_abf_cd-001

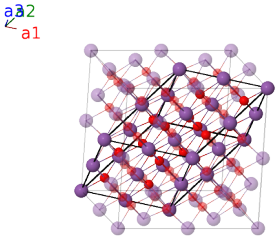


Prototype	O_2Sb
AFLOW prototype label	A2B_cF96_227_abf_cd-001
***Strukturbericht* designation**	$D6_2$
ICSD	24244
CCDC	1600290
Pearson symbol	cF96
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B_cF96_227_abf_cd-001 --params=`a, x_5

- Shortly after (Gottfried, 1937) gave this compound the *Strukturbericht* designation $D6_2$, (Dihiström, 1937) showed that they were actually determining the structure of Sb_3O_6OH, making this structure obsolete. Indeed, (Herrman, 1943) formally withdraws this from the *Strukturbericht* list, saying "The type and description [in (Gottfried, 1937)] should be deleted, as the radiographs were not based on the supposed substance." We present it for its historical interest.
- Modern experiments have determined that SbO_2 appears as cervantite (α-Sb_2O_4) or clinocervantite (β-Sb_2O_4).

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
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_4}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_5}$	=	0	=	0	(16c)	Sb I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Sb I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Sb II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Sb II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Sb II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Sb II
$\mathbf{B_{13}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{16}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{19}}$	=	$\left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_5 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{20}}$	=	$-x_5\,\mathbf{a}_1 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O III

$\mathbf{B_{21}}$	$=$	$-x_5\,\mathbf{a}_1+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{22}}$	$=$	$\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{23}}$	$=$	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(48f)	O III
$\mathbf{B_{24}}$	$=$	$\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_1+\left(x_5+\frac{3}{4}\right)\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+a\left(x_5+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	O III

References

[1] G. Natta and M. Baccaredda, *Tetrossido di antimonio e antimoniati*, Z. Kristallogr. **85**, 271–296 (1933), doi:10.1524/zkri.1933.85.1.271.

[2] K. Dihlström and A. Westgren, *Über den Bau des sogenannten Antimontetroxyds und der damit isomorphen Verbindung* $BiTa_2O_6F$, Z. Anorganische und Allgemeine Chemie **235**, 153–160 (1937), doi:10.1002/zaac.19372350121.

[3] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).

Found in

[1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (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.