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

This structure originally had the label `A2B_cF96_227_abf_cd`. Calls to that address will be redirected here.

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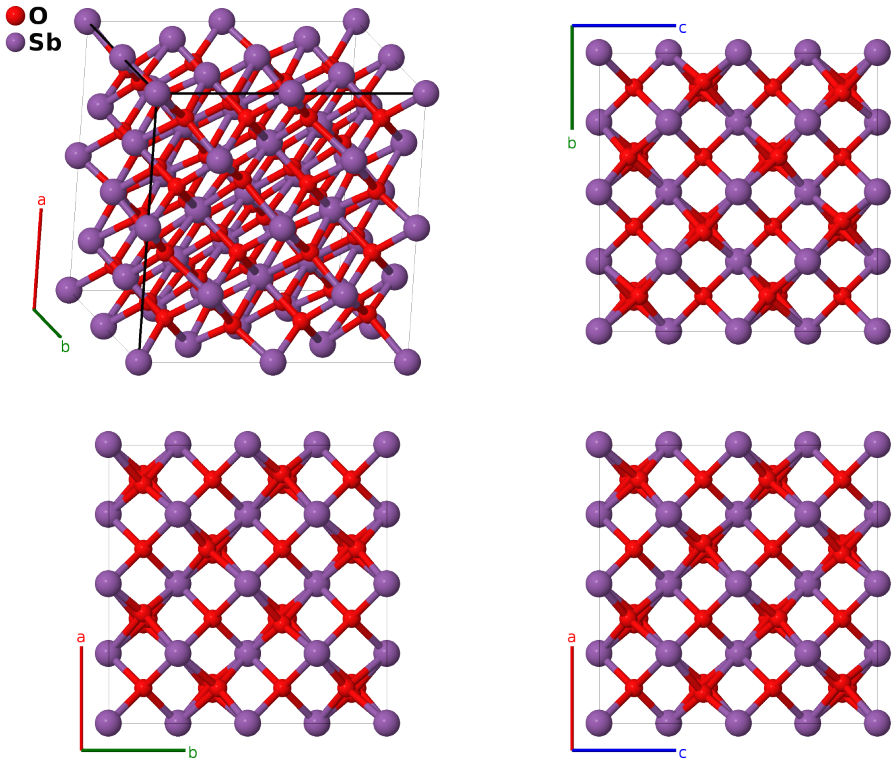
https://aflow.org/p/UGWY

https://aflow.org/p/A2B_cF96_227_abf_cd-001



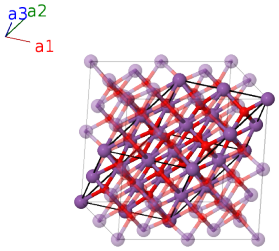
Prototype	O_2Sb
AFLOW prototype label	A2B_cF96_227_abf_cd-001
***Strukturbericht* designation**	$D6_2$
ICSD	24244
Pearson symbol	cF96
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B_cF96_227_abf_cd-001 --params=`a, x_5

- 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

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