Cervantite (α-Sb_2O_4) Structure: A2B_oP24_33_4a_2a-001

This structure previously used the label(s) `A2B_oP24_33_4a_2a`. Calls to these addresses will be redirected here.

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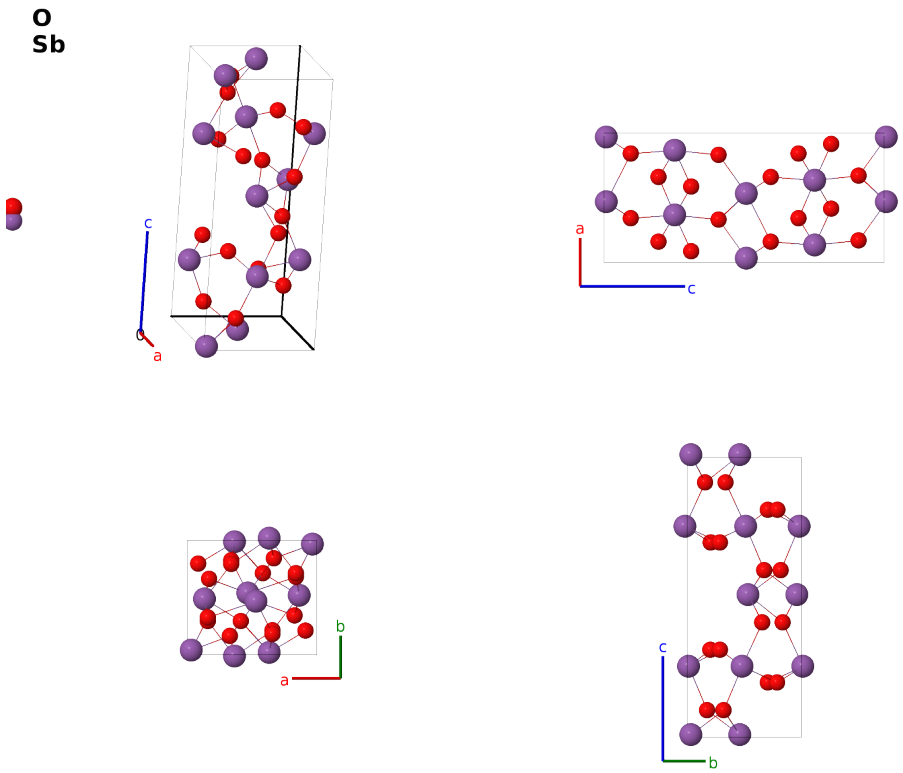
https://aflow.org/prototype-encyclopedia/49UC

https://aflow.org/prototype-encyclopedia/A2B_oP24_33_4a_2a-001



Prototype	O_2Sb
AFLOW prototype label	A2B_oP24_33_4a_2a-001
Mineral name	cervantite
ICSD	919
CCDC	1591138
Pearson symbol	oP24
Space group number	33
Space group symbol	$Pna2_1$

AFLOW prototype command `aflow --proto=A2B_oP24_33_4a_2a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

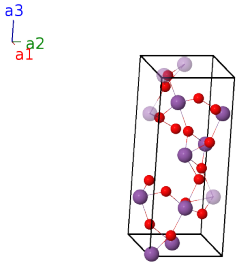
Other compounds with this structure

$BiNbO_4$, $SbNbO_4$, $SbTaO_4$ (Stibiotantalite), $Sb(Ta, Nb)O_4$ (Stibiocolumbite)

- This is *not* the $D6_2$ structure of SbO_2, which was found to be incorrect.
- There is a naturally occurring monoclinic modification of cervantite, clinocervantite (β-Sb_2O_4).

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_4}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_7}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_8}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{11}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{15}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{16}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Sb I

$$\mathbf{B_{18}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb I}$$

$$\mathbf{B_{19}} = \left(x_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb I}$$

$$\mathbf{B_{20}} = -\left(x_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb I}$$

$$\mathbf{B_{21}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb II}$$

$$\mathbf{B_{22}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb II}$$

$$\mathbf{B_{23}} = \left(x_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb II}$$

$$\mathbf{B_{24}} = -\left(x_6 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(4a)} \quad \text{Sb II}$$

References

[1] G. Thornton, *A Neutron Diffraction Study of* α-Sb_2O_3, Acta Crystallogr. Sect. B **33**, 1271–1273 (1977), doi:10.1107/S0567740877005822.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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.