

Clinocervantite (β -Sb₂O₄) Structure: A2B_mC24_15_2f_ae-001

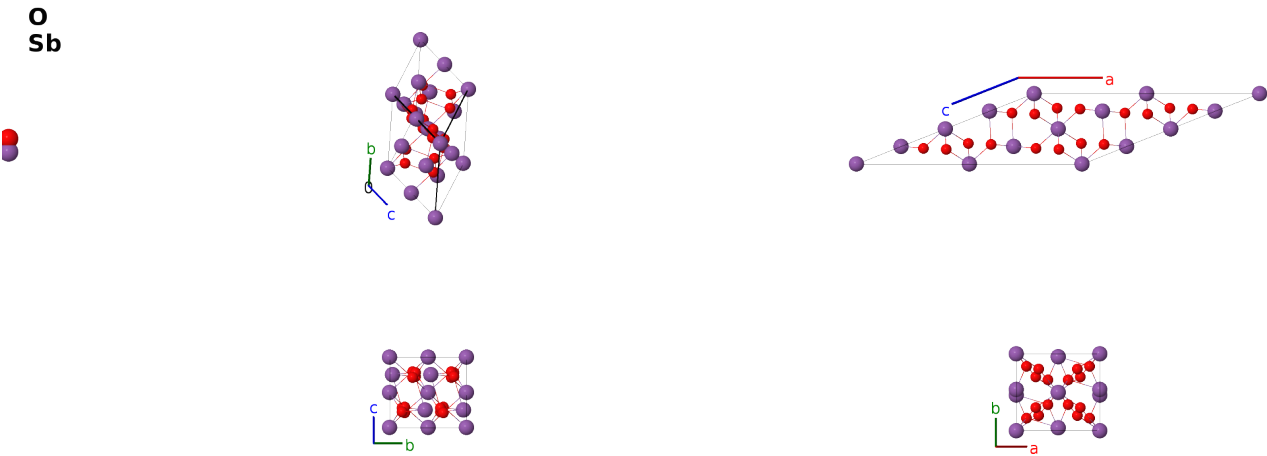
This structure previously used the label(s) **A2B_mC24_15_2f_ce**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/YM7H>

https://aflow.org/prototype-encyclopedia/A2B_mC24_15_2f_ae-001

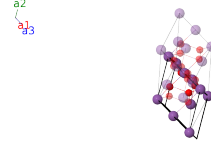


Prototype	O ₂ Sb
AFLOW prototype label	A2B_mC24_15_2f_ae-001
Mineral name	clinocervantite
ICSD	88619
CCDC	1648355
Pearson symbol	mC24
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	<code>aflow --proto=A2B_mC24_15_2f_ae-001</code> <code>--params=a, b/a, c/a, β, y_2, x_3, y_3, z_3, x_4, y_4, z_4</code>

- This is *not* the $D6_2$ structure of SbO₂, which was found erroneous. Clinocervantite is a naturally occurring monoclinic modification of cervantite (α -Sb₂O₄).

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Sb I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4a) Sb I
$\mathbf{B}_3$	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e) Sb II
$\mathbf{B}_4$	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e) Sb II
$\mathbf{B}_5$	$=$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f) O I
$\mathbf{B}_6$	$=$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f) O I
$\mathbf{B}_7$	$=$	$-(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f) O I
$\mathbf{B}_8$	$=$	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f) O I
$\mathbf{B}_9$	$=$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8f) O II
$\mathbf{B}_{10}$	$=$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f) O II
$\mathbf{B}_{11}$	$=$	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8f) O II
$\mathbf{B}_{12}$	$=$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f) O II

References

- [1] R. Basso, G. Lucchetti, L. Zefiro, and A. Palenzona, *Clinocervantite, β - Sb_2O_4 , the natural monoclinic polymorph of cervantite from the Cetine mine, Siena, Italy*, Euro. J. Mineral. **11**, 95–100 (1999), doi:10.1127/ejm/11/1/0095.

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.