

Sulvanite ($\text{Cu}_3\text{S}_4\text{V}$, $H2_4$) Structure: A3B4C_cP8_215_c_e_b-001

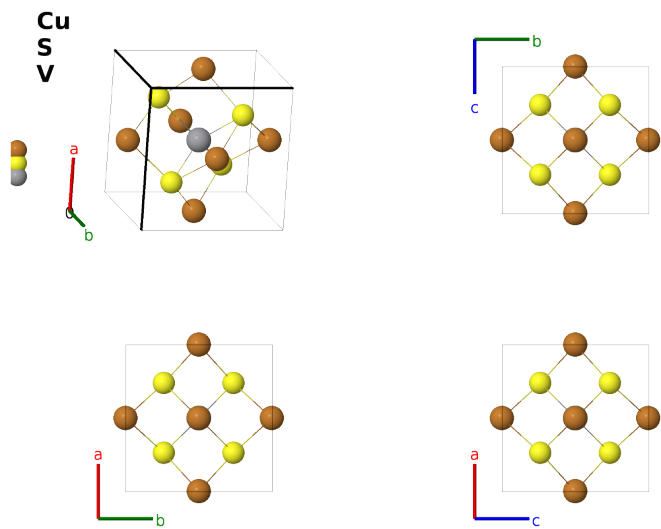
This structure previously used the label(s) **A3B4C_cP8_215_d_e_a**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A3B4C_cP8_215_c_e_b-001



Prototype	$\text{Cu}_3\text{S}_4\text{V}$
AFLOW prototype label	A3B4C_cP8_215_c_e_b-001
<i>Strukturbericht</i> designation	$H2_4$
Mineral name	sulvanite
ICSD	15490
CCDC	1596234
Pearson symbol	cP8
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A3B4C_cP8_215_c_e_b-001</code> <code>--params=a, x_3</code>

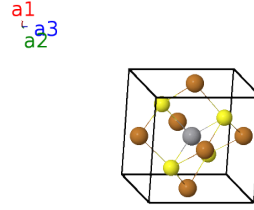
Other compounds with this structure

$\text{Cu}_3\text{S}_4\text{Nb}$, $\text{Cu}_3\text{S}_4\text{Ta}$, $\text{Cu}_3\text{Se}_4\text{Nb}$, $\text{Cu}_3\text{Se}_4\text{Ta}$, $\text{Cu}_3\text{Se}_4\text{V}$, $\text{Cu}_3\text{Te}_4\text{Nb}$, $\text{Cu}_3\text{Te}_4\text{Ta}$, $\text{Cu}_3\text{Te}_4\text{V}$

- This structure is very similar to lazarevičite (AsCu_3S_4), except that in this case the copper atoms are on the cubic edges [the (3d) sites] rather than the cubic faces [the (3c) sites].

Simple Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(1b)	V I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(3c)	Cu I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(3c)	Cu I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(3c)	Cu I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4e)	S I

References

- [1] F. J. Trojer, *Refinement of the Structure of Sulfanite*, Am. Mineral. **51**, 890–894 (1966).

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

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