

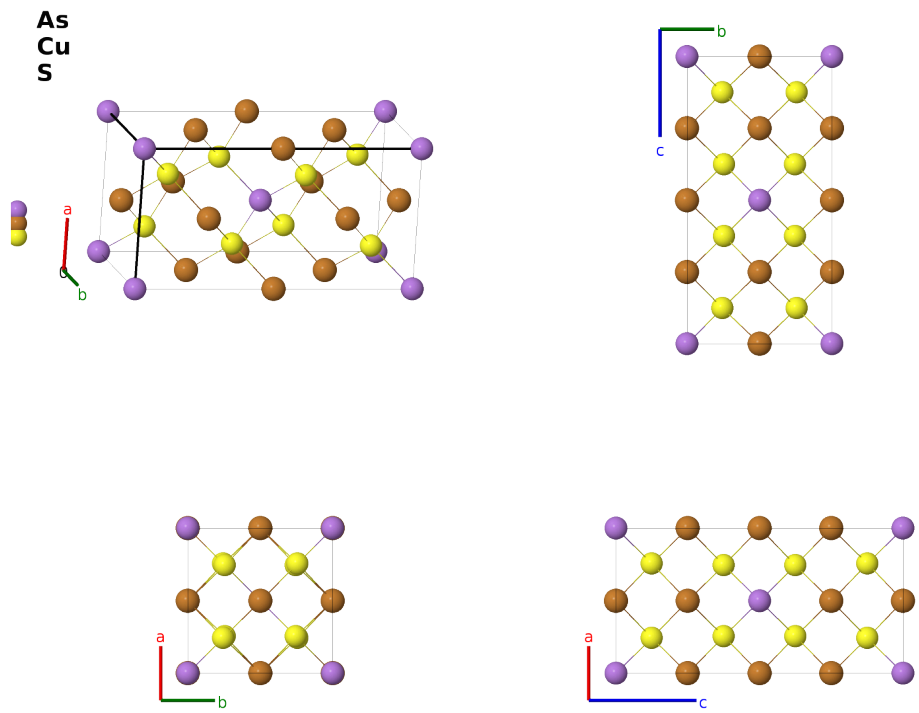
Luzonite (Cu₃AsS₄) Structure: AB3C4_tI16_121_a_bd_i-001

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<https://aflow.org/prototype-encyclopedia/3FZ9>

https://aflow.org/prototype-encyclopedia/AB3C4_tI16_121_a_bd_i-001



Prototype	AsCu ₃ S ₄
AFLOW prototype label	AB3C4_tI16_121_a_bd_i-001
Mineral name	luzonite
ICSD	26838
CCDC	1602217
Pearson symbol	tI16
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	<code>aflow --proto=AB3C4_tI16_121_a_bd_i-001 --params=a, c/a, x₄, z₄</code>

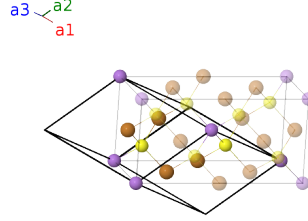
Other compounds with this structure

Ag_3VO_4 , Cu_3SbS_4 , Cu_3SbSe_4 , Cu_3AsSe_4 , Cu_3FeS_4 , Cu_3VO_4 , Si_3NiP_4

- The sample studied by (Marumo, 1967) had composition $\text{Cu}_3[\text{As}_{0.685}\text{Sb}_{0.315}]\text{S}_4$.
 - Cu_3AsS_4 can also be found as orthorhombic enargite ($H2_5$).
 - this is the ternary form of stannite ($\text{Cu}_2\text{FeS}_4\text{Sn}$), $H2_6$).
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Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	As I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Cu I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Cu II
$\mathbf{B}_5$	$= (x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B}_6$	$= -(x_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B}_7$	$= -(x_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	S I
$\mathbf{B}_8$	$= (x_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	S I

References

- [1] F. Marumo and W. Nowacki, *A refinement of the crystal structure of luzonite, Cu_3AsS_4* , Z. Kristallogr. **124**, 1–8 (1967), doi:10.1524/zkri.1967.124.16.1.

Found in

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

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