Luzonite (Cu_3AsS_4) Structure: AB3C4_tI16_121_a_bd_i-001

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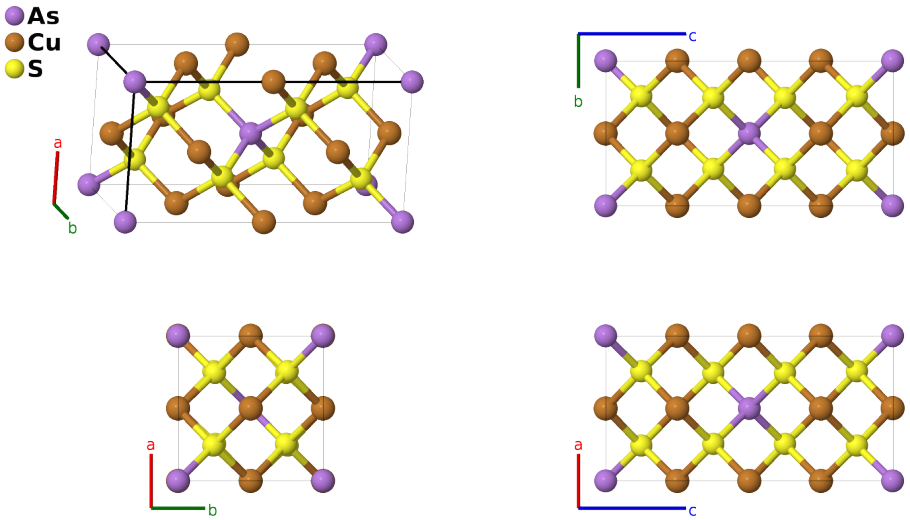
https://aflow.org/p/3FZ9

https://aflow.org/p/AB3C4_tI16_121_a_bd_i-001



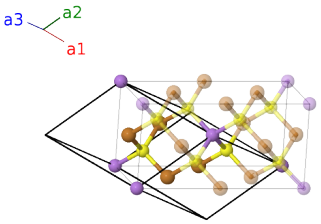
Prototype	$AsCu_3S_4$
AFLOW prototype label	AB3C4_tI16_121_a_bd_i-001
Mineral name	luzonite
ICSD	26838
Pearson symbol	tI16
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	`aflow --proto=AB3C4_tI16_121_a_bd_i-001 --params=`$a, c/a, x_4, z_4$

Other compounds with this structure
Cu_3SbS_4

- The sample studied by (Marumo, 1967) had composition $Cu_3[As_{0.685}Sb_{0.315}]S_4$.
- Cu_3AsS_4 can also be found as orthorhombic enargite ($H2_5$).
- this is the ternary form of stannite (Cu_2FeS_4Sn), $H2_6$).

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



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).