Cubic Lazarevićite ($AsCu_3S_4$) Structure: AB3C4_cP8_215_a_c_e-001

This structure originally had the label `AB3C4_cP8_215_a_c_e`. Calls to that address will be redirected here.

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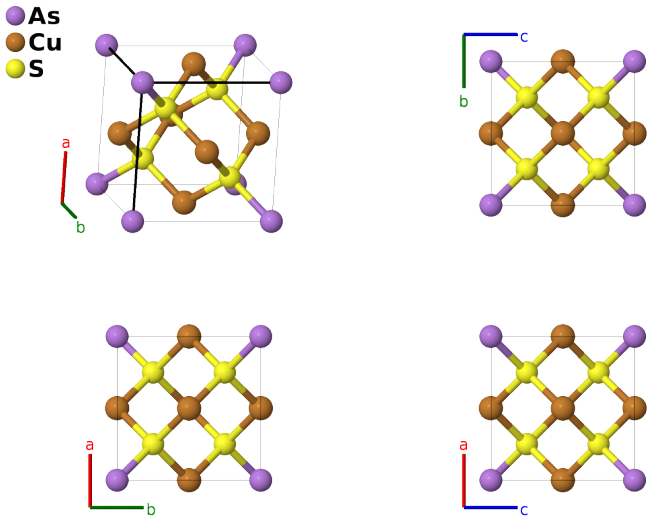
https://aflow.org/p/31D9

https://aflow.org/p/AB3C4_cP8_215_a_c_e-001

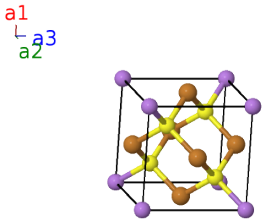


Prototype	$AsCu_3S_4$
AFLOW prototype label	AB3C4_cP8_215_a_c_e-001
Mineral name	lazarevićite
ICSD	42516
Pearson symbol	cP8
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB3C4_cP8_215_a_c_e-001 --params=`a, x_3

- This structure is very similar to sulvanite ($H2_4$), except that in this case the copper atoms are on the cubic faces [the (3c) sites] rather than the cubic edges [the (3d) sites]. The actual composition of the sample under study is $Cu_3(As_{0.65}Cu_{0.20}Fe_{0.13})S_4$. We will ignore the alloying on the arsenic site here.
- (Sclar, 1960) set $x_3 = 1/4$, but that is not required by symmetry and there is undoubtedly some relaxation.
- After much searching we finally obtained the original article for this structure from the Internet Archive. We thank them for making these documents available.

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	As 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] C. B. Sclar and M. Drovenik, *Lazarevićite, A New Cubic Copper-Arsenic Sulfied from Bor, Jugoslavia*, Bull. Geo. Soc. Am. **71**, 1970 (1960).

[2] M. Fleischer, *New Mineral Names*, Am. Mineral. **46**, 464–468 (1961).

[3] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, S. Stoiko, and L. Sysa, *Structure Types. Part 2: Space Groups (218) P-43n - (195) P23 · Cu_3AsS_4* (2005), doi:10.1007/10920473_223. Springer-Verlag Berlin Heidelberg.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.