

Cubic Lazarevićite (AsCu_3S_4) Structure: AB3C4_cP8_215_a_c_e-001

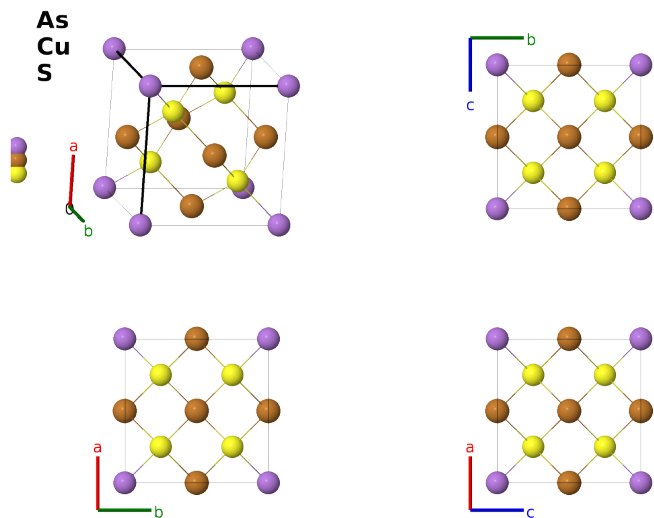
This structure previously used the label(s) **AB3C4_cP8_215_a_c_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/31D9>

https://aflow.org/prototype-encyclopedia/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
CCDC	1612176
Pearson symbol	cP8
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=AB3C4_cP8_215_a_c_e-001 --params=a, x_3</code>

- This structure is very similar to sylvanite ($H2_4$), 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 $\text{Cu}_3(\text{As}_{0.65}\text{Cu}_{0.20}\text{Fe}_{0.13})\text{S}_4$. 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.

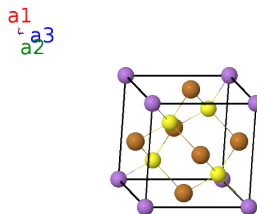
- After much searching we finally obtained the original article for this structure from the Internet Archive. We thank them for making these documents available.

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 Sulfide from Bor, Yugoslavia*, 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 · Cu₃AsS₄* (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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017