LaOAgS Structure: ABCD_tP8_129_b_c_a_c-001

This structure originally had the label `ABCD_tP8_129_b_c_a_c`. Calls to that address will be redirected here.

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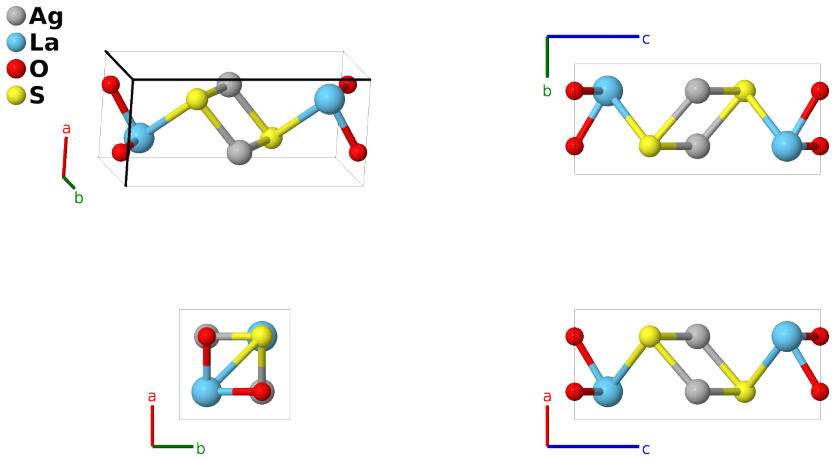
https://aflow.org/p/VCTW

https://aflow.org/p/ABCD_tP8_129_b_c_a_c-001



Prototype	AgLaOS
AFLOW prototype label	ABCD_tP8_129_b_c_a_c-001
ICSD	15530
Pearson symbol	tP8
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=ABCD_tP8_129_b_c_a_c-001 --params=`$a, c/a, z_3, z_4$

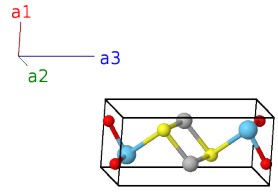
Other compounds with this structure

BaCuSeF, BiCuSeO, BiCuTeO, CeAgSeO, CeCoGeH, CeCoSiH, CeCuSeO, CeCuTeO, CeFeGeH, CeFeSiH, CeMnGeH, CeMnSiH, CeRuSiH, DyCuSeO, ErCuSeO, EuCuSeO, GdCuSeO, HoCuSeO, LaAgSO, LaAgSeO, LaAgTeO, LaCuTeO, LaRuSiH, LaiCuSeO, NdAgSeO, NdCuSeO, NdCuTeO, NdFeAsO, PrAgSeO, PrCuSeO, PrCuTeO, SmCuSeF, SmCuSeO, TbCuSeO, YCuSeO

- This structure has the same space group and Wyckoff positions as AsCuSiZr, but there is a substantial difference in the c/a ratio leading to different bonding between the layers.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ag I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ag I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	La I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	La I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2c)	S I

References

[1] M. Palazzi and S. Jaulmes, *Structure du Conducteur Ionique (LaO)AgS*, Acta Crystallogr. Sect. B **37**, 1337–1339 (1981), doi:10.1107/S0567740881005876.

Found in

[1] W. Suski and T. Palewski, *Pnictides and Chalcogenides II* (Springer-Verlag, Berlin,Heidelberg, 2003), vol. 27B5, chap. LaOAgS, doi:10.1007/10713485_89.