$AlPS_4$ Structure: ABC4_oP12_16_ae_bd_2u-001

This structure originally had the label `ABC4_oP12_16_ag_cd_2u`. Calls to that address will be redirected here.

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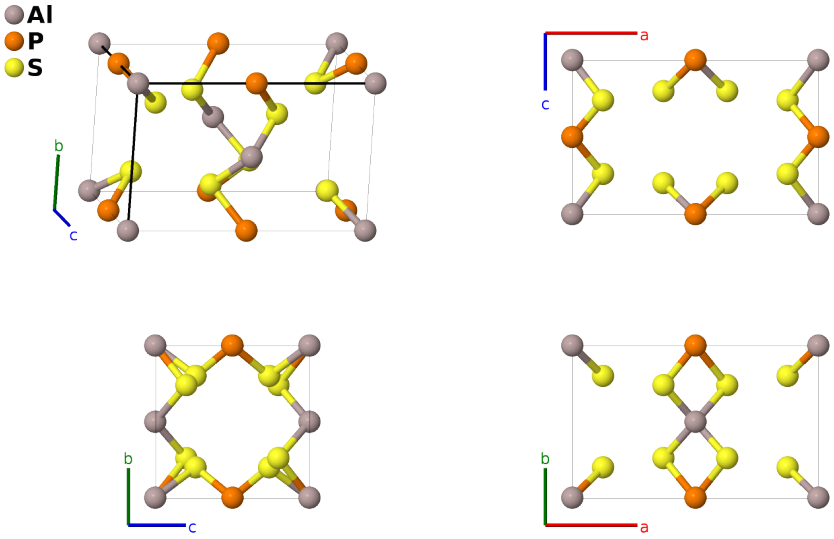
https://aflow.org/p/8PL6

https://aflow.org/p/ABC4_oP12_16_ae_bd_2u-001

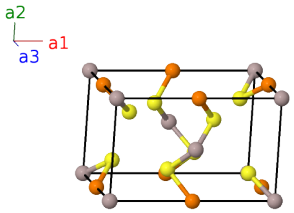


Prototype	$AlPS_4$
AFLOW prototype label	ABC4_oP12_16_ae_bd_2u-001
ICSD	15910
Pearson symbol	oP12
Space group number	16
Space group symbol	$P222$
AFLOW prototype command	`aflow --proto=ABC4_oP12_16_ae_bd_2u-001 --params=`$a, b/a, c/a, x_5, y_5, z_5, x_6, y_6, z_6$

- Our original publication of this structure (Mehl, 2017) had numerous errors dating back to the original NRL website. We have corrected these errors here. This changed the AFLOW label from ABC4_oP12_16_ag_cd_2u to ABC4_oP12_16_ae_bd_2u. The old AFLOW link will redirect to this page.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(1b)	P I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	P II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(1e)	Al II
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4u)	S I
$\mathbf{B_6}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4u)	S I
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4u)	S I
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4u)	S I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4u)	S II
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4u)	S II
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4u)	S II
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4u)	S II

References

[1] A. Weiss and H. Schäfer, *Zur Kenntnis vo Aluminiumthiophosphat $AlPS_4$*, Naturwissenschaften **47**, 495 (1960), doi:10.1007/BF00631053.

[2] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.