

AlPS₄ Structure: ABC4_oP12_16_ae_bd_2u-001

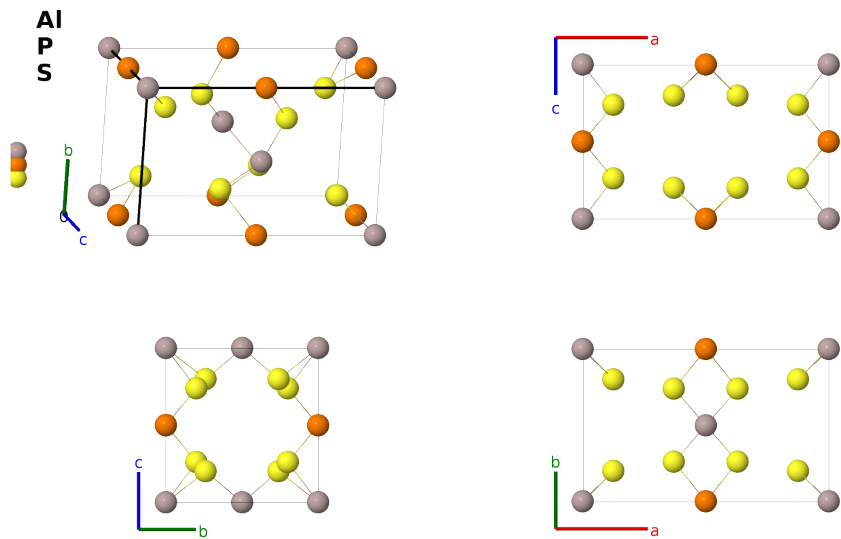
This structure previously used the label(s) **ABC4_oP12.16_ag_cd.2u**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/8PL6>

https://aflow.org/prototype-encyclopedia/ABC4_oP12.16_ae_bd_2u-001

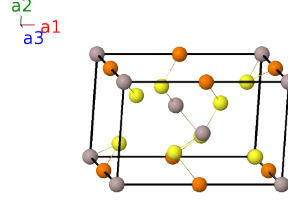


Prototype	AlPS ₄
AFLOW prototype label	ABC4_oP12.16_ae_bd_2u-001
ICSD	15910
CCDC	1596581
Pearson symbol	oP12
Space group number	16
Space group symbol	<i>P</i> 222
AFLOW prototype command	<code>aflow --proto=ABC4_oP12.16_ae_bd_2u-001 --params=a, b/a, c/a, x₅, y₅, z₅, x₆, y₆, z₆</code>

- 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

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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.

First cited in

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