

BPS₄ Structure:

ABC4_oI12_23_a_b_k-001

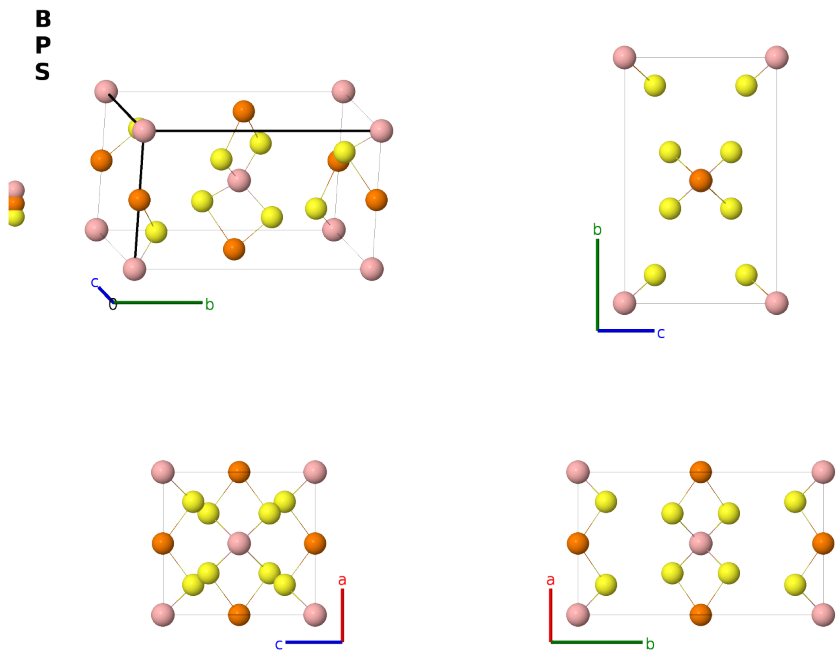
This structure previously used the label(s) **ABC4_oI12_23_a_b_k**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/ZCCT>

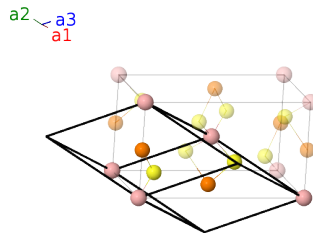
https://aflow.org/prototype-encyclopedia/ABC4_oI12_23_a_b_k-001



Prototype	BPS ₄
AFLOW prototype label	ABC4_oI12_23_a_b_k-001
ICSD	24618
CCDC	1600637
Pearson symbol	oI12
Space group number	23
Space group symbol	I222
AFLOW prototype command	<code>aflow --proto=ABC4_oI12_23_a_b_k-001 --params=a, b/a, c/a, x₃, y₃, z₃</code>

Body-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	B I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	P I
$\mathbf{B}_3$	$=$	$(y_3 + z_3)\mathbf{a}_1 + (x_3 + z_3)\mathbf{a}_2 + (x_3 + y_3)\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(8k) S I
$\mathbf{B}_4$	$=$	$-(y_3 - z_3)\mathbf{a}_1 - (x_3 - z_3)\mathbf{a}_2 - (x_3 + y_3)\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} - by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(8k) S I
$\mathbf{B}_5$	$=$	$(y_3 - z_3)\mathbf{a}_1 - (x_3 + z_3)\mathbf{a}_2 - (x_3 - y_3)\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + by_3\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(8k) S I
$\mathbf{B}_6$	$=$	$-(y_3 + z_3)\mathbf{a}_1 + (x_3 - z_3)\mathbf{a}_2 + (x_3 - y_3)\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} - by_3\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(8k) S I

References

- [1] A. Weiss and H. Schäfer, *Zur Kenntnis von Bortetrathiophosphat BPS₄*, Z. Naturforsch. B **18**, 81–82 (1963), doi:10.1515/znb-1963-0117.

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