

# BPS<sub>4</sub> Structure:

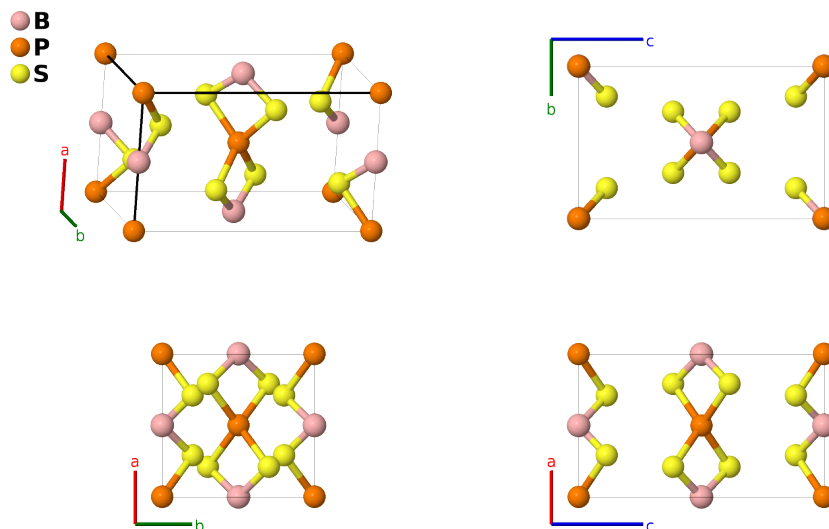
## ABC4\_oI12\_23\_a\_b\_k-001

This structure originally had the label ABC4\_oI12\_23\_a\_b\_k. Calls to that address will be redirected here.

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<https://aflow.org/p/ZCCT>

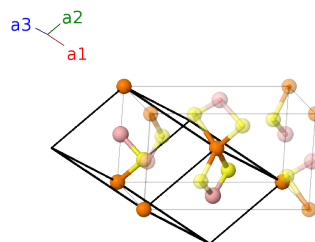
[https://aflow.org/p/ABC4\\_oI12\\_23\\_a\\_b\\_k-001](https://aflow.org/p/ABC4_oI12_23_a_b_k-001)



Prototype	BPS <sub>4</sub>
AFLOW prototype label	ABC4_oI12_23_a_b_k-001
ICSD	24618
Pearson symbol	oI12
Space group number	23
Space group symbol	<i>I</i> 222
AFLOW prototype command	<code>aflow --proto=ABC4_oI12_23_a_b_k-001 --params=a, b/a, c/a, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub></code>

### Body-centered Orthorhombic primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) B I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}}$	(2b) 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 BPS<sub>4</sub>*, Z. Naturforsch. B **18**, 81–82 (1963), doi:10.1515/znb-1963-0117.