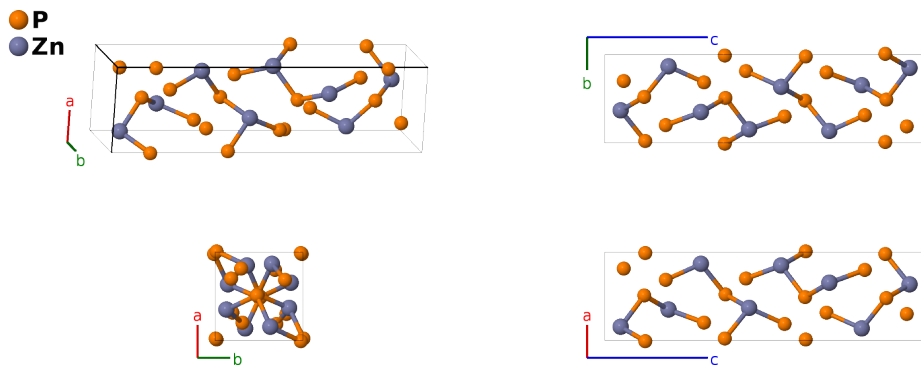


# Tetragonal (red) $\text{ZnP}_2$ Structure: A2B\_tP24\_92\_2b\_b-001

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

<https://aflow.org/p/A2B.tP24.92.2b.b-001>



Prototype	$\text{P}_2\text{Zn}$
AFLOW prototype label	A2B_tP24_92_2b_b-001
ICSD	18137
Pearson symbol	tP24
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	<code>aflow --proto=A2B_tP24_92_2b_b-001 --params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3</code>

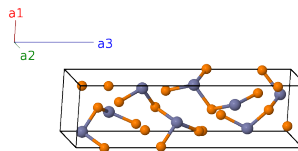
## Other compounds with this structure

$\text{CdP}_2$

- This structure can also be found in the enantiomorphic space group  $P4_32_12$  #96.
- Although (White, 1965) describes the structure as orthorhombic in the “Experimental measurements” section, it is indeed tetragonal.
- $\text{ZnP}_2$  can also be found in a monoclinic (black) form.

## Simple Tetragonal primitive vectors

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



## Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_3$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3$	=	$-a(y_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_4$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3$	=	$a(y_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_5$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{4}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_6$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{3}{4}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_7$	$= y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_8$	$= -y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	P I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{11}$	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{4}) \mathbf{a}_3$	=	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{12}$	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{3}{4}) \mathbf{a}_3$	=	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{13}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{4}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{14}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{3}{4}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{15}$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{16}$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	P II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{18}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{19}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	=	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{20}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	=	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{21}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{4}) \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{22}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{3}{4}) \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{23}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8b)	Zn I
$\mathbf{B}_{24}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Zn I

## References

- [1] J. G. White, *The crystal structure of the tetragonal modification of  $\text{ZnP}_2$* , Acta Cryst. **18**, 217–220 (1965), doi:10.1107/S0365110X6500049X.

## Found in

- [1] K. B. Aleĭnikova, A. I. Kozlov, S. G. Kozlova, and V. V. Sobolev, *Electronic and crystal structures of isomorphous  $ZnP_2$  and  $CdP_2$* , Phys. Solid State **44**, 1257–1262 (2002), doi:10.1134/1.1494619. Translated from Fizika Tverdogo Tela, Vol. 44, No. 7, 2002, pp. 1206–1210.