

Tetragonal (red) ZnP_2 Structure:

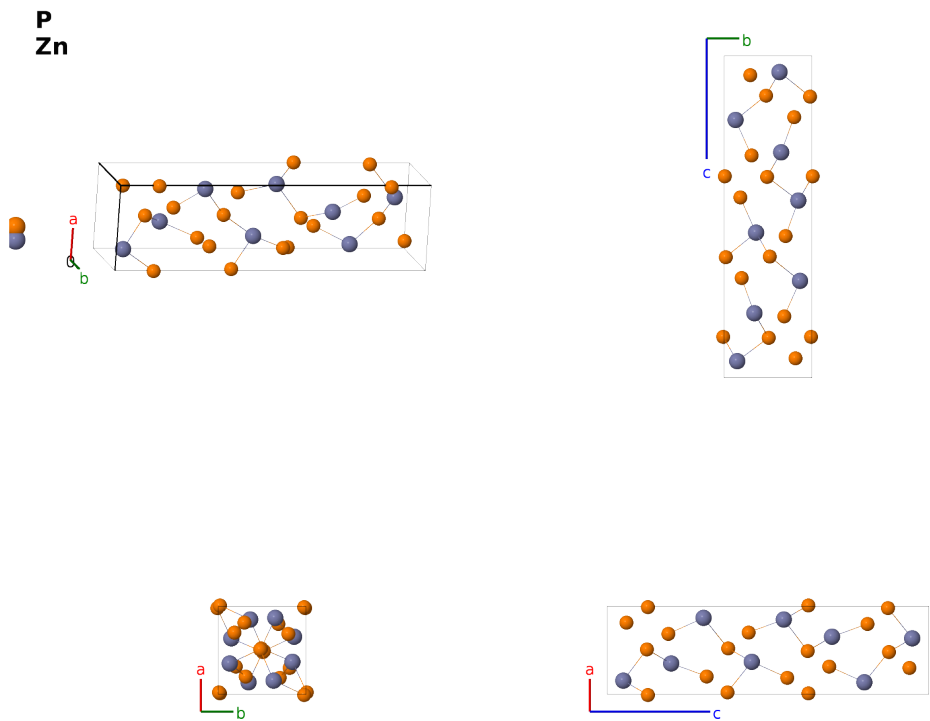
A2B_tP24_92_2b_b-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A2B_tP24_92_2b_b-001



Prototype	P_2Zn
AFLOW prototype label	A2B_tP24_92_2b_b-001
ICSD	18137
CCDC	1597694
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</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃</code>

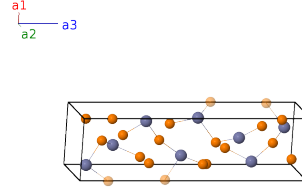
Other compounds with this structure

CdP₂

- 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.
 - ZnP₂ can also be found in a monoclinic (black) form.
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Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\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) &\text{P II} \\
\mathbf{B}_{16} &= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8b) &\text{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) &\text{Zn I} \\
\mathbf{B}_{18} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8b) &\text{Zn I} \\
\mathbf{B}_{19} &= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_3 &= -a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} &(8b) &\text{Zn I} \\
\mathbf{B}_{20} &= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right) \mathbf{a}_3 &= a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{3}{4}\right) \hat{\mathbf{z}} &(8b) &\text{Zn I} \\
\mathbf{B}_{21} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right) \mathbf{a}_3 &= -a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}} &(8b) &\text{Zn I} \\
\mathbf{B}_{22} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right) \mathbf{a}_3 &= a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{3}{4}\right) \hat{\mathbf{z}} &(8b) &\text{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) &\text{Zn I} \\
\mathbf{B}_{24} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8b) &\text{Zn I}
\end{aligned}$$

References

- [1] J. G. White, *The crystal structure of the tetragonal modification of ZnP_2* , Acta Cryst. **18**, 217–220 (1965), doi:10.1107/S0365110X6500049X.

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First cited in

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.