

Zn₃P₂ (*D*5₉) Structure: A2B3_tP40_137_cdf_3g-001

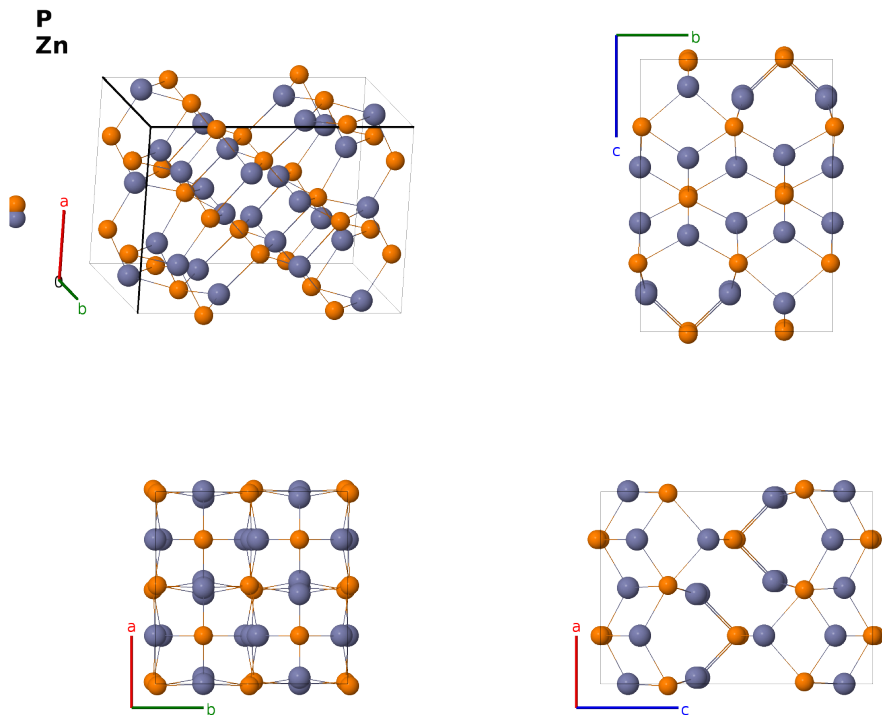
This structure previously used the label(s) **A2B3_tP40_137_cdf_3g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/68SX>

https://aflow.org/prototype-encyclopedia/A2B3_tP40_137_cdf_3g-001



Prototype	P ₂ Zn ₃
AFLOW prototype label	A2B3_tP40_137_cdf_3g-001
<i>Strukturbericht</i> designation	<i>D</i> 5 ₉
ICSD	26876
CCDC	1602248
Pearson symbol	tP40
Space group number	137
Space group symbol	<i>P</i> 4 ₂ / <i>nmc</i>
AFLOW prototype command	<code>aflow --proto=A2B3_tP40_137_cdf_3g-001</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>z</i>₁, <i>z</i>₂, <i>x</i>₃, <i>y</i>₄, <i>z</i>₄, <i>y</i>₅, <i>z</i>₅, <i>y</i>₆, <i>z</i>₆</code>

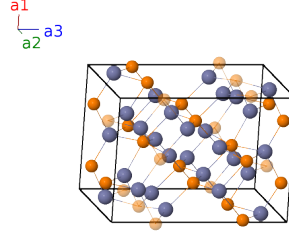
Other compounds with this structure

α -As₂Cd₃, α -As₂Zn₃, Cd₃P₂

- (Stackelberg, 1935) gives the atomic positions in the first setting of space group $P4_2/nmc$ #137. We have changed this to the second setting, placing the origin of the system at the inversion site.
- (Pearson, 1958, p. 803) gives the space group as $P4_2/mmc$ #131, but it is correctly given as $P4_2/nmc$ on page 111.

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
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4d)	P II
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	P II
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4d)	P II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	P II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{14}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{15}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{16}$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	P III
$\mathbf{B}_{17}$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{18}$	$= \frac{1}{4} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{19}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{20}$	$= y_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn I

$\mathbf{B}_{21} =$	$\frac{3}{4} \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{22} =$	$\frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{23} =$	$(y_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{24} =$	$-y_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn I
$\mathbf{B}_{25} =$	$\frac{1}{4} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{26} =$	$\frac{1}{4} \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{27} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 +$ $(z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{28} =$	$y_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{29} =$	$\frac{3}{4} \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{30} =$	$\frac{3}{4} \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{31} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{32} =$	$-y_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn II
$\mathbf{B}_{33} =$	$\frac{1}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{34} =$	$\frac{1}{4} \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{35} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 +$ $(z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{36} =$	$y_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{37} =$	$\frac{3}{4} \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{38} =$	$\frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{39} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{40} =$	$-y_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	Zn III

References

- [1] M. v. Stackelberg and R. Paulu, *Untersuchungen an den Phosphiden und Arseniden des Zinks und Cadmiums. Das Zn_3P_2 -Gitter*, Z. phys. Chem. B **28**, 427–460 (1935), doi:10.1515/zpch-1935-2841.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).
- [2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

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