Monoclinic (black) ZnP_2 Structure: A2B_mP24_14_4e_2e-001

https://aflow.org/p/BW3Z

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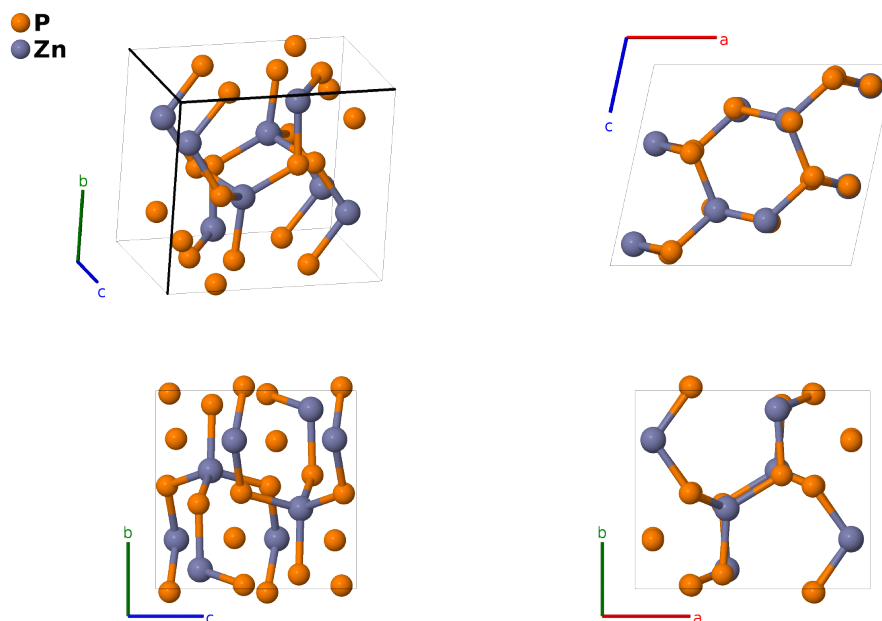
| Prototype	P_2Zn
AFLOW prototype label	A2B_mP24_14_4e_2e-001
ICSD	60011
Pearson symbol	mP24
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A2B_mP24_14_4e_2e-001
	--params=$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

$ZnAs_2$

- An earlier version of this structure by (Hegyi, 1963) had zinc-zinc bonds which are not observed in other Zn-P or Zn-As structures. We use the structure of (Fleet, 1984), which is also the one used in (Villars, 2018).

- ZnP_2 can also be found in a tetragonal (red) form.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
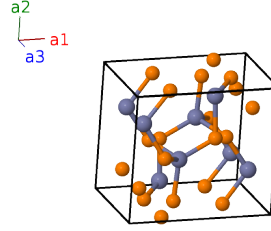
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_4}$	$=$	$x_1\,\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	P II
$\mathbf{B_6}$	$=$	$-x_2\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	P II
$\mathbf{B_8}$	$=$	$x_2\,\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	P III
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P III
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	P III
$\mathbf{B_{12}}$	$=$	$x_3\,\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	P IV
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P IV
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	P IV
$\mathbf{B_{16}}$	$=$	$x_4\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P IV
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_{20}}$	$=$	$x_5\,\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zn I
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Zn II

$$\mathbf{B_{22}} \;=\; -x_6\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 \;=\; -\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{Zn II}$$

$$\mathbf{B_{23}} \;=\; -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 \;=\; -\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{Zn II}$$

$$\mathbf{B_{24}} \;=\; x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 \;=\; \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{Zn II}$$

References

[1] M. E. Fleet and T. A. Mowles, *Structure of monoclinic black zinc diphosphide, ZnP$_2$*, Acta Crystallogr. Sect. C **40**, 1778–1779 (1984), doi:10.1107/S0108270184009513.

[2] I. J. Hegyi, E. E. Loebner, E. W. P. Jr., and J. G. White, *Two crystal forms of ZnP2, their preparation, structure, and optoelectronic properties* **24**, 333–337 (1963), doi:10.1016/0022-3697(63)90140-9.

[3] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Phosphorus-Zinc Binary Phase Diagram (2009 Tu H.). Copyright ©2006-2018 ASM International.