Rhombohedral $LiZnPO_4$ Structure: AB4CD_hR42_146_2b_8b_2b_2b-001

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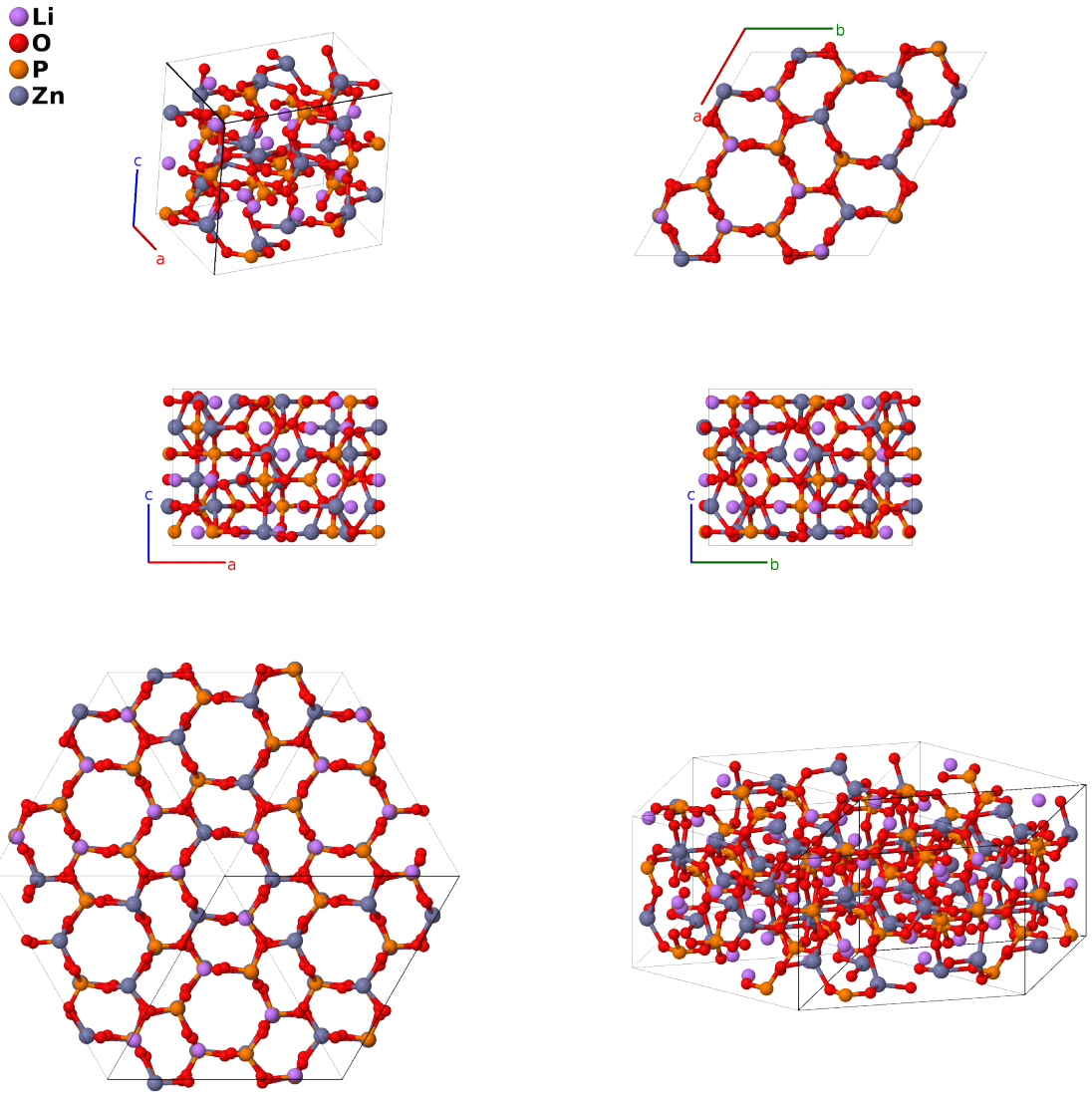
https://aflow.org/p/BGS4

https://aflow.org/p/AB4CD_hR42_146_2b_8b_2b_2b-001



Prototype	LiO_4PZn
AFLOW prototype label	AB4CD_hR42_146_2b_8b_2b_2b-001
ICSD	83652
Pearson symbol	hR42
Space group number	146
Space group symbol	$R3$

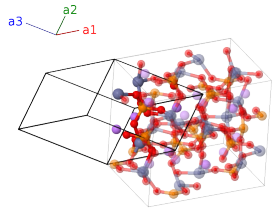
AFLOW prototype command `aflow --proto=AB4CD_hR42_146_2b_8b_2b_2b-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

Other compounds with this structure
$LiAlSiO_4$ (α-eucryptite)

- $LiZnPO_4$ has been observed in a variety of structures. We list those which have known crystal structures:
  - α-$LiZnPO_4$
  - δ_1-$LiZnPO_4$, and
  - rhombohedral $LiZnPO_4$ (this structure).
- (Bu, 1996) note that this structure is very close to phenakite (Be_2SiO_4, $S1_3$), the main difference being the lack of an inversion site.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - 2y_1 + z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Li I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + y_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_1 - y_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Li I
$\mathbf{B_3}$	=	$y_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 + y_1 - 2z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_1 + y_1 + z_1)\,\hat{\mathbf{z}}$	(3b)	Li I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	Li II
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	Li II
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(3b)	Li II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_8}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(3b)	O II

$$\mathbf{B_{11}} = z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_4 - z_4)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_4 + y_4 + z_4)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O II}$$

$$\mathbf{B_{12}} = y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_4 - y_4)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_4 + y_4 + z_4)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O II}$$

$$\mathbf{B_{13}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O III}$$

$$\mathbf{B_{14}} = z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_5 - z_5)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O III}$$

$$\mathbf{B_{15}} = y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_5 - y_5)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O III}$$

$$\mathbf{B_{16}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - z_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O IV}$$

$$\mathbf{B_{17}} = z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_6 - z_6)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O IV}$$

$$\mathbf{B_{18}} = y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - y_6)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O IV}$$

$$\mathbf{B_{19}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - z_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O V}$$

$$\mathbf{B_{20}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_7 - z_7)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O V}$$

$$\mathbf{B_{21}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7 - y_7)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O V}$$

$$\mathbf{B_{22}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VI}$$

$$\mathbf{B_{23}} = z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_8 - z_8)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VI}$$

$$\mathbf{B_{24}} = y_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_8 - y_8)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VI}$$

$$\mathbf{B_{25}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_9 - z_9)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_9 - 2y_9 + z_9)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VII}$$

$$\mathbf{B_{26}} = z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_9 - z_9)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2y_9 - y_9 - z_9)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VII}$$

$$\mathbf{B_{27}} = y_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_9 - y_9)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_9 + y_9 - 2z_9)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_9 + y_9 + z_9)\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VII}$$

$$\mathbf{B_{28}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} - z_{10})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{10} - 2y_{10} + z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VIII}$$

$$\mathbf{B_{29}} = z_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + y_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{10} - z_{10})\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{10} - y_{10} - z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VIII}$$

$$\mathbf{B_{30}} = y_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + x_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10} - y_{10})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{10} + y_{10} - 2z_{10})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{10} + y_{10} + z_{10})\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{O VIII}$$

$$\mathbf{B_{31}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11} - z_{11})\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11} - 2y_{11} + z_{11})\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\;\hat{\mathbf{z}} \quad \text{(3b)} \quad \text{P I}$$

$$\mathbf{B_{32}} = z_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + y_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{11} - z_{11})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{11} - y_{11} - z_{11})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}$$ (3b) P I

$$\mathbf{B_{33}} = y_{11}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + x_{11}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{11} - y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{11} + y_{11} - 2z_{11})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{11} + y_{11} + z_{11})\,\hat{\mathbf{z}}$$ (3b) P I

$$\mathbf{B_{34}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12} - z_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{12} - 2y_{12} + z_{12})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}$$ (3b) P II

$$\mathbf{B_{35}} = z_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + y_{12}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{12} - z_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{12} - y_{12} - z_{12})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}$$ (3b) P II

$$\mathbf{B_{36}} = y_{12}\,\mathbf{a}_1 + z_{12}\,\mathbf{a}_2 + x_{12}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{12} - y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{12} + y_{12} - 2z_{12})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{12} + y_{12} + z_{12})\,\hat{\mathbf{z}}$$ (3b) P II

$$\mathbf{B_{37}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{13} - z_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{13} - 2y_{13} + z_{13})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}$$ (3b) Zn I

$$\mathbf{B_{38}} = z_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + y_{13}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{13} - z_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{13} - y_{13} - z_{13})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}$$ (3b) Zn I

$$\mathbf{B_{39}} = y_{13}\,\mathbf{a}_1 + z_{13}\,\mathbf{a}_2 + x_{13}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{13} - y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{13} + y_{13} - 2z_{13})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{13} + y_{13} + z_{13})\,\hat{\mathbf{z}}$$ (3b) Zn I

$$\mathbf{B_{40}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{14} - z_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{14} - 2y_{14} + z_{14})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{14} + y_{14} + z_{14})\,\hat{\mathbf{z}}$$ (3b) Zn II

$$\mathbf{B_{41}} = z_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + y_{14}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_{14} - z_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_{14} - y_{14} - z_{14})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{14} + y_{14} + z_{14})\,\hat{\mathbf{z}}$$ (3b) Zn II

$$\mathbf{B_{42}} = y_{14}\,\mathbf{a}_1 + z_{14}\,\mathbf{a}_2 + x_{14}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{14} - y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_{14} + y_{14} - 2z_{14})\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_{14} + y_{14} + z_{14})\,\hat{\mathbf{z}}$$ (3b) Zn II

References

[1] X. Bu, T. E. Gier, and G. D. Stucky, *A New Form of Lithium Zinc Phosphate with an Ordered Phenakite Structure, $LiZnPO_4$*, Acta Crystallogr. Sect. C **52**, 1601–1603 (1996), doi:10.1107/S0108270195015940.