δ_1-$LiZnPO_4$ Structure: AB4CD_oP28_33_a_4a_a_a-001

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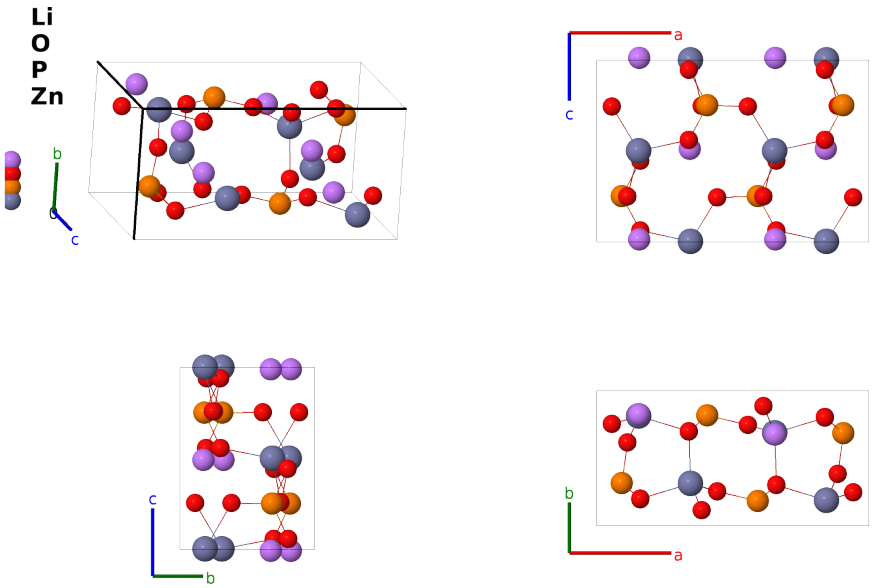
https://aflow.org/prototype-encyclopedia/FVBE

https://aflow.org/prototype-encyclopedia/AB4CD_oP28_33_a_4a_a_a-001



Prototype	LiO_4PZn
AFLOW prototype label	AB4CD_oP28_33_a_4a_a_a-001
ICSD	79537
CCDC	1639784
Pearson symbol	oP28
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	`aflow --proto=AB4CD_oP28_33_a_4a_a_a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

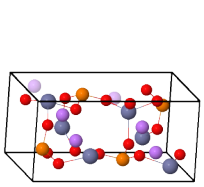
Other compounds with this structure
$LiCoPO_4$, $LiNiPO_4$

- $LiZnPO_4$ has been observed in a variety of structures. We list those which have know crystal structures:

  - α-$LiZnPO_4$
  - δ_1-$LiZnPO_4$, (this structure) and
  - rhombohedral $LiZnPO_4$.
- (Jensen, 1995) find that the lithium site is 8

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_3}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_4}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_7}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_8}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{11}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{12}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{15}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{16}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{19}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{20}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	P I

$\mathbf{B_{22}}$	$=$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_{23}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_{24}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_{25}}$	$=$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{26}}$	$=$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{27}}$	$=$	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B_{28}}$	$=$	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Zn I

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