Li_2PrO_3 Structure: A2B3C_oC12_65_h_ah_b-001

This structure previously used the label(s) `A2B3C_oC12_65_h_bh_a`. Calls to these addresses will be redirected here.

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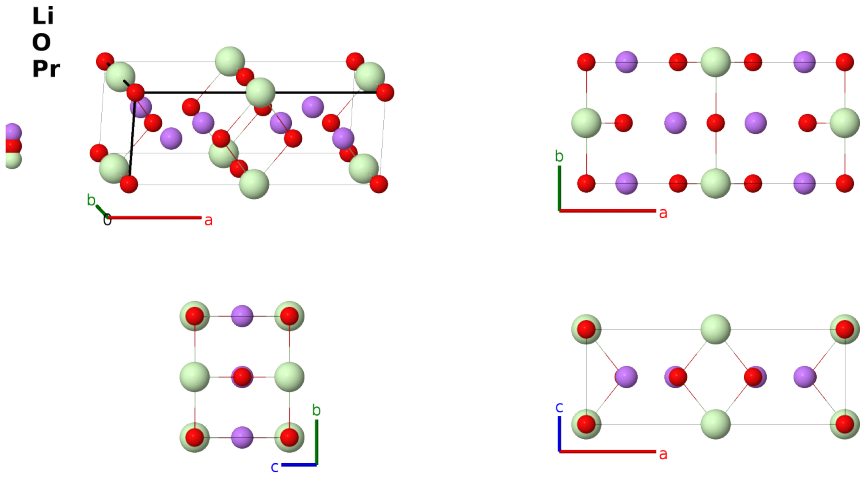
https://aflow.org/prototype-encyclopedia/2B54

https://aflow.org/prototype-encyclopedia/A2B3C_oC12_65_h_ah_b-001



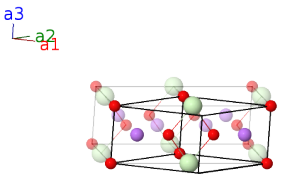
Prototype	Li_2O_3Pr
AFLOW prototype label	A2B3C_oC12_65_h_ah_b-001
ICSD	154704
CCDC	1671327
Pearson symbol	oC12
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A2B3C_oC12_65_h_ah_b-001 --params=`$a, b/a, c/a, x_3, x_4$

Other compounds with this structure
Na_2PrO_3

- Data was taken at 20K.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Pr I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Li I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Li I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O II

References

[1] Y. Hinatsu and Y. Doi, *Crystal structures and magnetic properties of alkali-metal lanthanide oxides A_2LnO_3 (A = Li, Na; Ln = Ce, Pr, Tb)*, J. Alloys Compd. **418**, 155–160 (2006), doi:10.1016/j.jallcom.2005.08.100.

[2] R. Okuma, K. MacFarquharson, and R. Coldea, *Selective Synthesis and Crystal Chemistry of Candidate Rare-Earth Kitaev Materials: Honeycomb and Hyperhoneycomb Na_2PrO_3*, Inorganic Chemistry **63**, 15941–15950 (2024), doi:10.1021/acs.inorgchem.4c02294.

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