Monasite ($LaPO_4$) Structure: AB4C_mP24_14_e_4e_e-002

This structure originally had the label `AB4C_mP24_14_e_4e_e`. Calls to that address will be redirected here.

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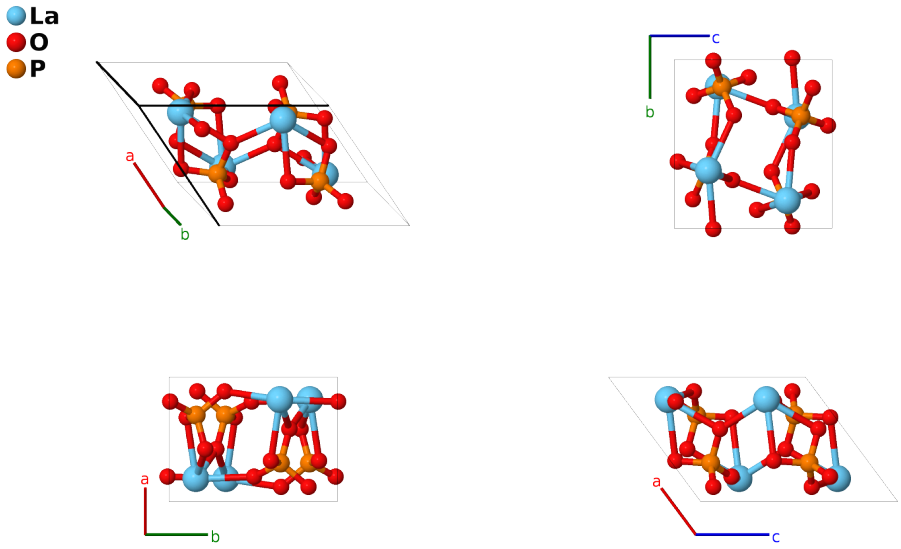
https://aflow.org/p/G325

https://aflow.org/p/AB4C_mP24_14_e_4e_e-002



Prototype	LaO_4P
AFLOW prototype label	AB4C_mP24_14_e_4e_e-002
Mineral name	monasite
ICSD	79747
Pearson symbol	mP24
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=AB4C_mP24_14_e_4e_e-002 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

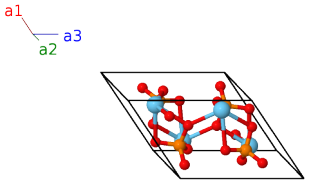
Other compounds with this structure
$CePO_4$ (monazite-Ce), $PrPO_4$ (monazite-Pr), $NdPO_4$ (monazite-Nd), $SmPO_4$ (monazite-Sm), $EuPO_4$ (monazite-Eu), $LaAsO_4$ (gasparite-La), $CeAsO_4$ (gasparite-Ce)

- Monasites (RE-PO_4) and gasparites (RE-AsO_4) can have a mixture of rare earth elements in the RE slot of the formula. Technically these minerals are called monasite-(X) and gasparite-(X), where "X" is the predominant rare earth element in the sample. All of the structures are similar. As we must pick one as the prototype, we take the first entry in (Ni, 1995) to define the class.

- (Ni, 1995) gives the structural data in the $P2_1/n$ setting of space group #14. We used FINDSYM to change this to our standard $P2_1/c$ setting. This involves a change of primitive vectors as well as a rotation of the crystal.
- This structure has the same AFLOW label as (NH_4SO_4, $K4_1$). The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Monoclinic primitive vectors

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



Basis vectors

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

$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I

References

[1] Y. Ni, J. M. Hughes, and A. N. Mariano, *Crystal chemistry of the monazite and xenotime structures*, Am. Mineral. **80**, 21–26 (1995).

Found in

[1] O. S. Vereshchagin, S. N. Britvin, E. N. Perova, A. I. Brusnitsyn, Y. S. Polekhovsky, V. V. Shilovskikh, V. N. Bocharov, A. van der Burgt, S. Cuchet, and N. Meisser, *Gasparite-(La), La(AsO_4), a new mineral from Mn ores of the Ushkatyn-III deposit, Central Kazakhstan, and metamorphic rocks of the Wanni glacier, Switzerland*, Am. Mineral. **104**, 1469–1480 (2019), doi:10.2138/am-2019-7028.