$P3$ La_3BWO_9 Structure: AB3C9D_hP28_143_2a_2d_6d_bc-001

This structure originally had the label `AB3C9D_hP28_143_2a_2d_6d_bc`. Calls to that address will be redirected here.

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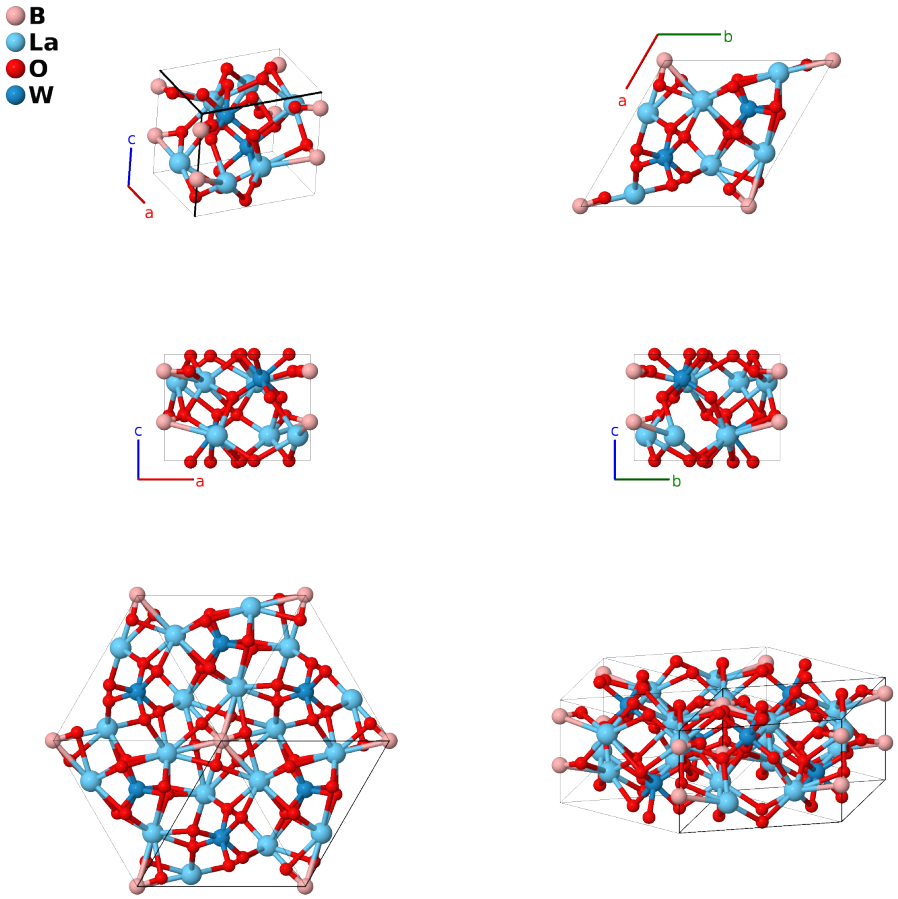
https://aflow.org/p/0XN3

https://aflow.org/p/AB3C9D_hP28_143_2a_2d_6d_bc-001

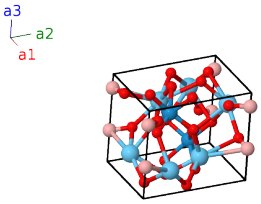


Prototype	BLi_3O_9W
AFLOW prototype label	AB3C9D_hP28_143_2a_2d_6d_bc-001
ICSD	8360
Pearson symbol	hP28
Space group number	143
Space group symbol	$P3$
AFLOW prototype command	`aflow --proto=AB3C9D_hP28_143_2a_2d_6d_bc-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- Most refinements of the BLi_3O_9W structure, including (Ashtar, 2020), place it in hexagonal space group $P6_3$ #173. (Han, 2018) find a better fit to the data by refining it in the trigonal $P3$ #143 space group, which places the lanthanum atoms on two independent crystallographic sites. This may be due to the presence of bismuth impurities on the lantanum site in the (Han, 2018) sample, and indeed the La (3d) sites are both mixed with 3% bismuth. (Ashtar, 2020) claim to have very pure samples. Given this, we withhold judgment on which structure is correct and present both.
- Space group $P3$ does not specify the origin of the z-axis. Here it is set so that the coordinate of the (1b) tungsten atom is $z_3 = 1/4$.
- (Han, 2018) mislabel the Wyckoff positions of the boron and tungsten atoms. We show the correct positions based on the coordinates in their table and the correspondence with the $P6_3$ structure.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	B I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	B II
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1b)	W I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1c)	W II
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B_6}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B_7}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	La II
$\mathbf{B_9}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	La II
$\mathbf{B_{10}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(3d)	La II
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B_{12}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B_{13}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(3d)	O II
$\mathbf{B_{15}}$	=	$-y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(3d)	O II
$\mathbf{B_{16}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(3d)	O II
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 + y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9 - y_9)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{18}}$	=	$-y_9\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_9 - 2y_9)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{19}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_9 - y_9)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{20}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV

$\mathbf{B_{21}}$	=	$-y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B_{22}}$	=	$-(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B_{23}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{11} + y_{11})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{11} - y_{11})\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B_{24}}$	=	$-y_{11}\,\mathbf{a}_1 + (x_{11} - y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{11} - 2y_{11})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B_{25}}$	=	$-(x_{11} - y_{11})\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{11} - y_{11})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(3d)	O V
$\mathbf{B_{26}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{12} + y_{12})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{12} - y_{12})\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(3d)	O VI
$\mathbf{B_{27}}$	=	$-y_{12}\,\mathbf{a}_1 + (x_{12} - y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{12} - 2y_{12})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(3d)	O VI
$\mathbf{B_{28}}$	=	$-(x_{12} - y_{12})\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{12} - y_{12})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(3d)	O VI

References

[1] J. Han, F. Pan, M. S. Molokeev, J. Dai, M. Peng, W. Zhou, and J. Wang, *Redefinition of Crystal Structure and Bi^{3+} Yellow Luminescence with Strong Near-Ultraviolet Excitation in La_3BWO_9:Bi^{3+} Phosphor for White Light-Emitting Diodes*, ACS Appl. Mater. Interfaces **10**, 13660–13668 (2018), doi:10.1021/acsami.8b00808.

[2] M. Ashtar, J. Guo, Z. Wan, Y. Wang, G. Gong, Y. Liu, Y. Su, and Z. Tian, *A new family of disorder-free Rare-Earth-based kagomé lattice magnets: structure and magnetic characterizations of RE_3BWO_9 (RE=Pr, Nd, Gd-Ho) Boratotungstates*, doi:10.48550/arXiv.2002.05420. ArXiv:2002.05420 [cond-mat.mtrl-sci].