

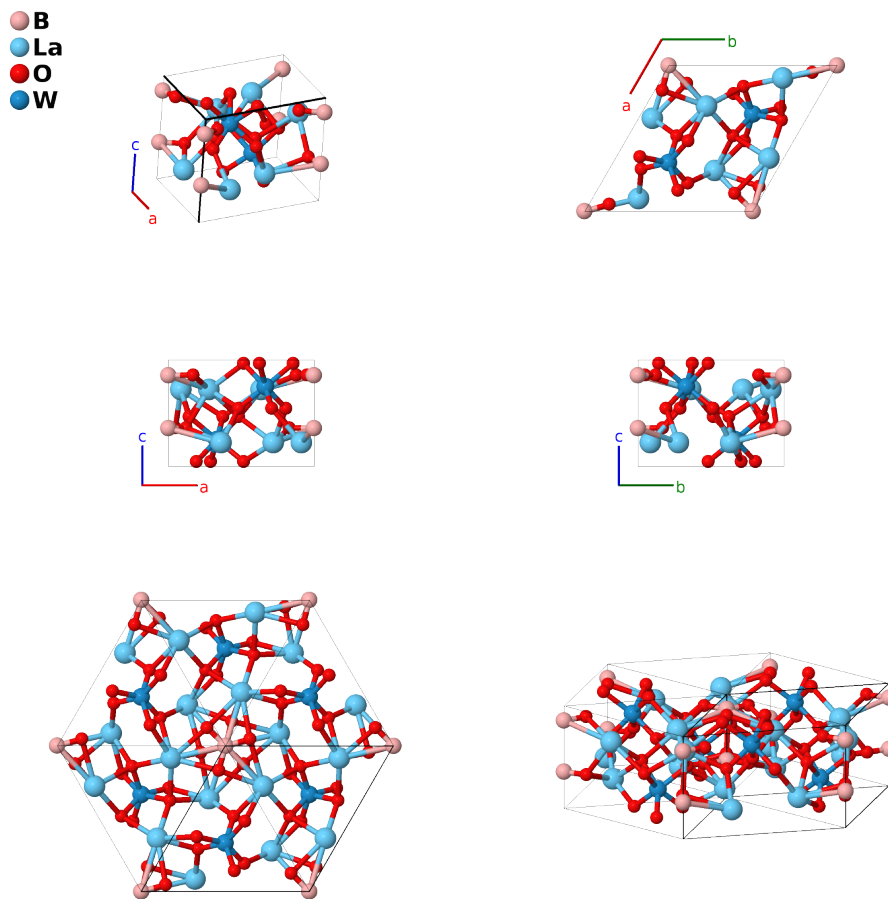
$P6_3$ La_3BWO_9 Structure: AB3C9D_hP28_173_a_c_3c_b-001

This structure originally had the label AB3C9D_hP28_173_a_c_3c_b. Calls to that address will be redirected here.

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<https://aflow.org/p/DVKH>

https://aflow.org/p/AB3C9D_hP28_173_a_c_3c_b-001



Prototype	$\text{BLa}_3\text{O}_9\text{W}$
AFLOW prototype label	AB3C9D_hP28_173_a_c_3c_b-001
ICSD	8359
Pearson symbol	hP28
Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	<code>aflow --proto=AB3C9D_hP28_173_a_c_3c_b-001 --params=a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6</code>

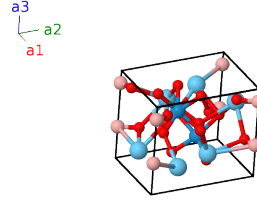
Other compounds with this structure

La₃BWO₉, Ce₃BWO₉, Nd₃BWO₉, Pr₃BWO₉, Sm₃BWO₉, Gd₃BWO₉, Tb₃BWO₉, Dy₃BWO₉, Ho₃BWO₉

- Most refinements of the BLi₃O₉W 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 lanthanum site in the (Han, 2018) sample, which contains 3% boron, while (Ashtar, 2020) claim to have very pure samples. Given this, we withhold judgment on which structure is correct and present both.
- Space group $P6_3$ does not specify the origin of the z -axis. Here it is set so that the coordinate of the tungsten atom is $z_2 = 1/4$.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	B I
\mathbf{B}_2	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	B I
\mathbf{B}_3	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	W I
\mathbf{B}_4	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	W I
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_6	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_7	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_8	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_9	$y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{10}	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{11}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{12}	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{13}	$-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{14}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{15}	$y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{16}	$(x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{17}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{18}	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{19}	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	O II

$$\begin{aligned}
\mathbf{B}_{20} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \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}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{21} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{22} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O II} \\
\mathbf{B}_{23} &= 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}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{24} &= -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}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{25} &= -(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}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{26} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \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}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{27} &= y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O III} \\
\mathbf{B}_{28} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (6c) & \quad \text{O III}
\end{aligned}$$

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].