$YbBaCo_4O_7$ Structure: AB4C7D_hP26_159_b_ac_a2c_b-001

This structure originally had the label `AB4C7D_hP26_159_b_ac_a2c_b`. Calls to that address will be redirected here.

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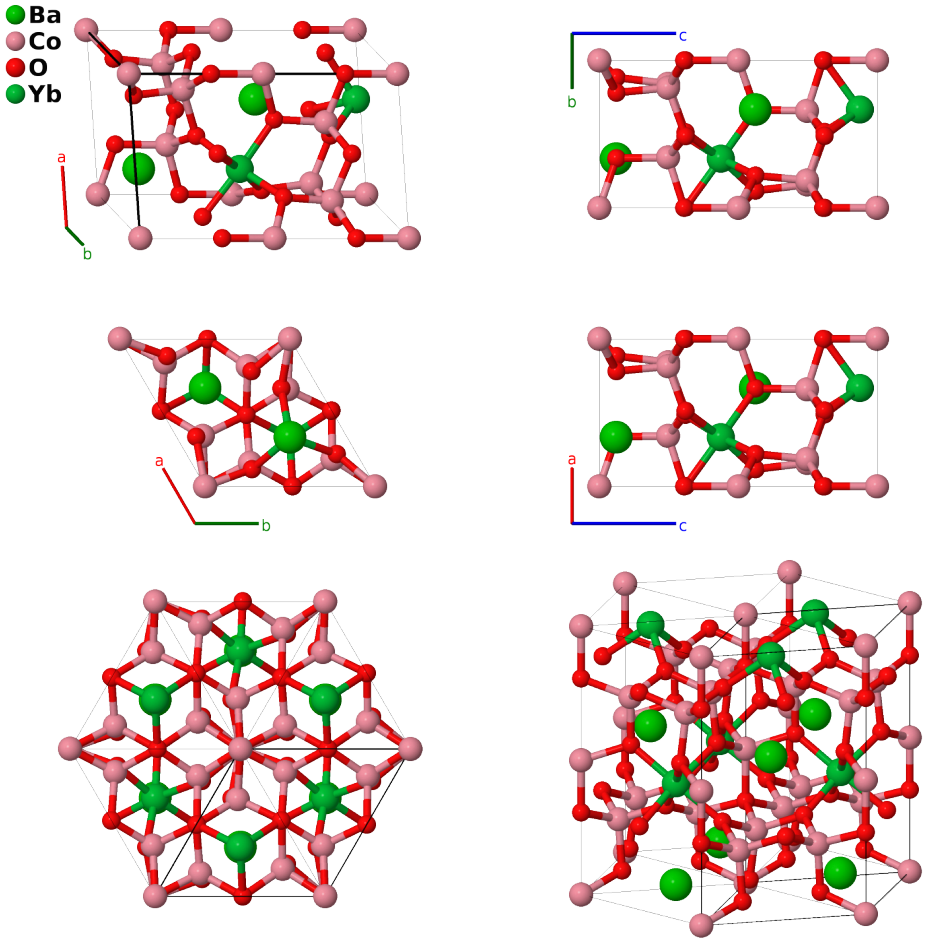
https://aflow.org/p/ZUBF

https://aflow.org/p/AB4C7D_hP26_159_b_ac_a2c_b-001

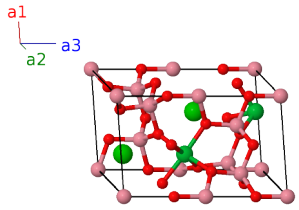


Prototype	$BaCo_4O_7Yb$
AFLOW prototype label	AB4C7D_hP26_159_b_ac_a2c_b-001
ICSD	172414
Pearson symbol	hP26
Space group number	159
Space group symbol	$P31c$
AFLOW prototype command	`aflow --proto=AB4C7D_hP26_159_b_ac_a2c_b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- We use the $YbBaCo_4O_{6.95}$ data from (Huq, 2006) at 225K.
- Space group $P31c$ #159 allows an arbitary choice of the origin of the z-axis. We chose to place one of the Co (2a) atoms at the origin, setting $z_1 = 0$.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(2b)	Yb I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Yb I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{11}}$	=	$-(x_5-y_5)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{12}}$	=	$y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{13}}$	=	$(x_5-y_5)\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Co II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{16}}$	=	$-y_6\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{17}}$	=	$-(x_6-y_6)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{18}}$	=	$y_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{19}}$	=	$(x_6-y_6)\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{22}}$	=	$-y_7\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7-2y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{23}}$	=	$-(x_7-y_7)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O III

$\mathbf{B_{24}}$	=	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{25}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III

References

[1] A. Huq, J. F. Mitchell, H. Zheng, L. C. Chapon, P. G. Radaelli, K. S. Knight, and P. W. Stephens, *Structural and magnetic properties of the Kagomé antiferromagnet $YbBaCo_4O_7$*, Solid State Commun. **179**, 1136–1145 (2006), doi:10.1016/j.jssc.2006.01.010.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.