$YCrB_4$ Structure: A4BC_oP24_55_4g_h_h-001

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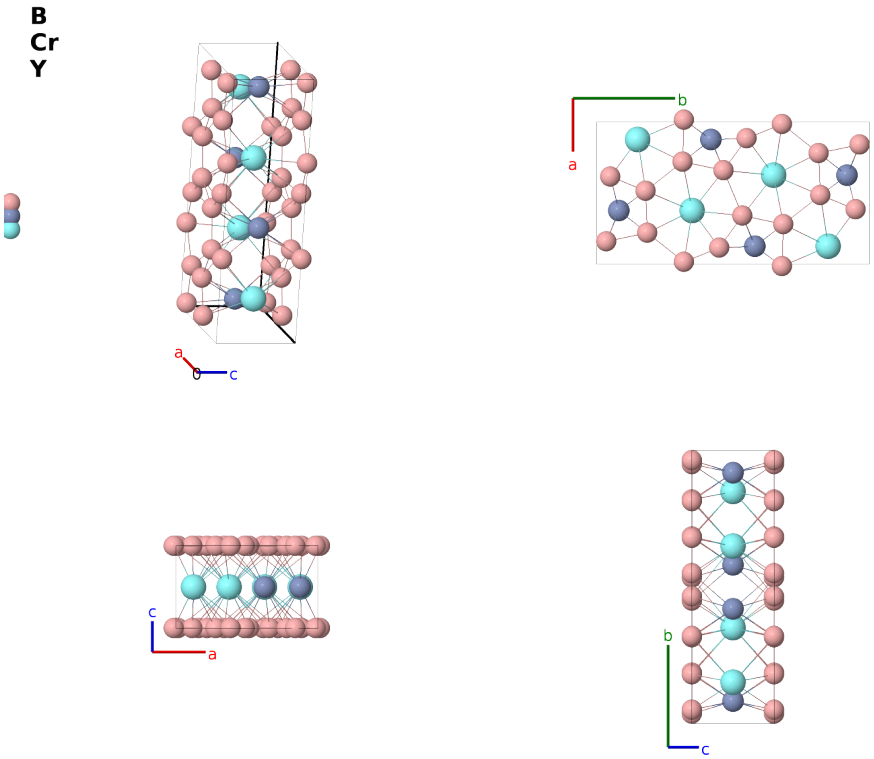
https://aflow.org/prototype-encyclopedia/67TW

https://aflow.org/prototype-encyclopedia/A4BC_oP24_55_4g_h_h-001



Prototype	B_4CrY
AFLOW prototype label	A4BC_oP24_55_4g_h_h-001
ICSD	101057
CCDC	2134769
Pearson symbol	oP24
Space group number	55
Space group symbol	*Pbam*
AFLOW prototype command	`aflow --proto=A4BC_oP24_55_4g_h_h-001 --params=`$a, b/a, c/a, x_1, y_1, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6$

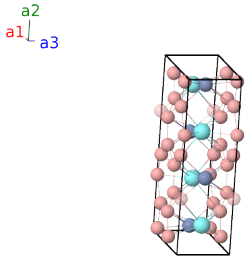
Other compounds with this structure

$AlLuB_4$, $CeCrB_4$, $CeReB_4$, $CoYbB_4$, $DyCrB_4$, $DyFeB_4$, $DyMnB_4$, $DyMoB_4$, $DyOsB_4$, $DyReB_4$, $DyRuB_4$, $DyVB_4$, $DyWB_4$, $ErCrB_4$, $ErFeB_4$, $ErMnB_4$, $ErMoB_4$, $ErNiB_4$, $ErOsB_4$, $ErReB_4$, $ErRhB_4$, $ErRuB_4$, $ErVB_4$, $ErWB_4$, $EuRuB_4$, $GdCoB_4$, $GdCrB_4$, $GdFeB_4$, $GdMnB_4$, $GdMoB_4$, $GdOsB_4$, $GdReB_4$, $GdRuB_4$, $GdVB_4$, $GdWB_4$, $HoCrB_4$, $HoMnB_4$, $HoMoB_4$, $HoOsB_4$, $HoReB_4$, $HoRuB_4$, $HoVB_4$, $HoWB_4$, $LuAlB_4$, $LuCrB_4$, $LuFeB_4$, $LuNiB_4$, $LuOsB_4$, $LuRuB_4$, $NdCrB_4$, $NdMnB_4$, $PrCrB_4$, $PrMnB_4$, $PuMoB_4$, $PuOsB_4$, $RePuB_4$, $RuPuB_4$, $ScCoB_4$, $ScFeB_4$, $ScNiB_4$, $SmCrB_4$, $SmFeB_4$, $SmMnB_4$, $TbCrB_4$, $TbMnB_4$, $TbMoB_4$, $TbOsB_4$, $TbReB_4$, $TbRuB_4$, $TbVB_4$, $TbWB_4$, $TcPuB_4$, $ThCrB_4$, $TmAlB_4$, $TmCrB_4$, $TmNiB_4$, $TmOsB_4$, $TmRhB_4$, $TmRuB_4$, $UCoB_4$, $UCrB_4$, $UFeB_4$, $UMnB_4$, UVB_4, $WPuB_4$, $YCoB_4$, $YCrB_4$, $YFeB_4$, $YMnB_4$, $YMoB_4$, $YOsB_4$, $YReB_4$, $YRhB_4$, $YRuB_4$, YVB_4, YWB_4, $YbAlB_4$, $YbCoB_4$, $YbFeB_4$, $YbNiB_4$, $YbOsB_4$, $YbRhB_4$

- The AFLOW prototype label protocol shifts the origin so that the boron atoms are in the $z = 0$ plane.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(4g)	B II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(4g)	B II
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4g)	B III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(4g)	B III
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B III
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4g)	B IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(4g)	B IV
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B IV
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	B IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cr I
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cr I

$\mathbf{B_{19}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cr I
$\mathbf{B_{20}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cr I
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Y I
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Y I
$\mathbf{B_{23}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Y I
$\mathbf{B_{24}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Y I

References

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Found in

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First cited in

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