$BaCd_{11}$ Structure: AB11_tI48_141_b_aci-001

This structure previously used the label(s) `AB11_tI48_141_a_bdi`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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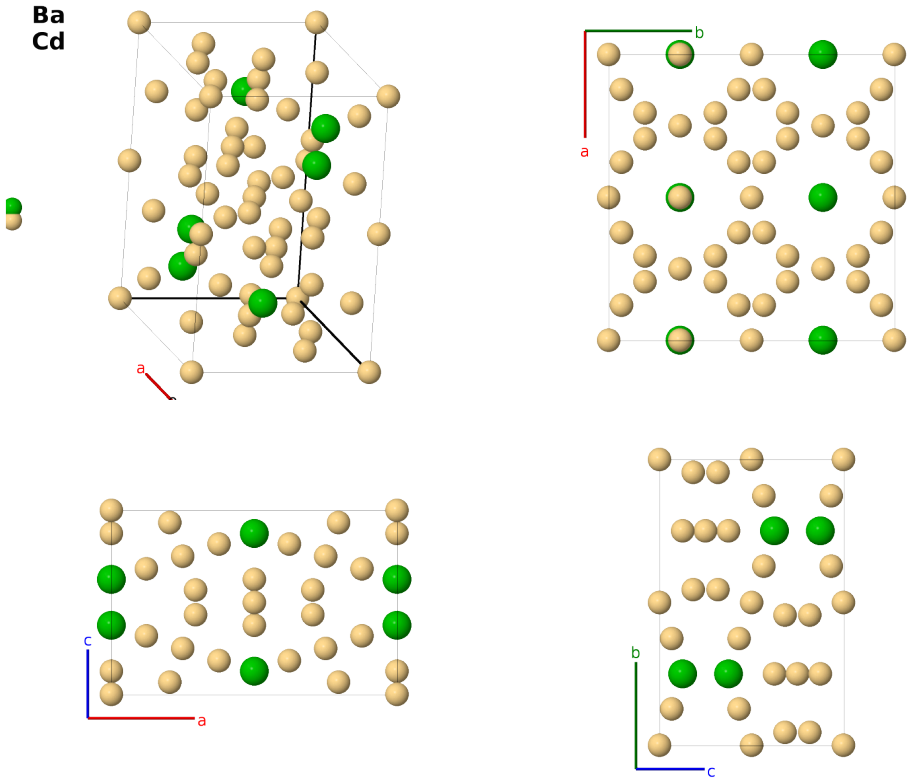
https://aflow.org/prototype-encyclopedia/EV03

https://aflow.org/prototype-encyclopedia/AB11_tI48_141_b_aci-001



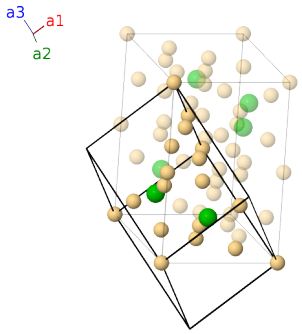
Prototype	$BaCd_{11}$
AFLOW prototype label	AB11_tI48_141_b_aci-001
ICSD	150492
CCDC	1667659
Pearson symbol	tI48
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=AB11_tI48_141_b_aci-001 --params=`$a, c/a, x_4, y_4, z_4$

Other compounds with this structure
$CaZn_{11}$, $CeZn_{11}$, $EuCd_{11}$, $EuZn_{11}$, $LaZn_{11}$, $NdZn_{11}$, $PrZn_{11}$, $SrCd_{11}$

- (Sanderson, 1953) gave the atomic positions in setting 1 of space group $I4_1/amd$ #141. We used FINDSYM to transform this to the standard setting 2.
- The ICSD entry is for $SrCd_{11}$, as $BaCd_{11}$ is not in the ICSD database, despite being the lead structure in (Sanderson, 1953). The lattice constants of the two structures are very similar, and the atomic positions are identical.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B_3}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4b)	Ba I
$\mathbf{B_4}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4b)	Ba I
$\mathbf{B_5}$	=	0	=	0	(8c)	Cd II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(8c)	Cd II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	Cd II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	Cd II
$\mathbf{B_9}$	=	$(y_4+z_4)\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{10}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - \left(x_4+y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{11}}$	=	$(x_4+z_4)\,\mathbf{a}_1 + \left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{12}}$	=	$-(x_4-z_4)\,\mathbf{a}_1 + (y_4+z_4)\,\mathbf{a}_2 + \left(-x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{13}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1 - (x_4+z_4)\,\mathbf{a}_2 + \left(-x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{14}}$	=	$-(y_4+z_4)\,\mathbf{a}_1 + (x_4-z_4)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{15}}$	=	$(x_4-z_4)\,\mathbf{a}_1 + \left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III

$\mathbf{B_{16}}$	=	$-\left(x_4+z_4\right)\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2-\left(x_4+y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{17}}$	=	$-\left(y_4+z_4\right)\,\mathbf{a}_1-\left(x_4+z_4\right)\,\mathbf{a}_2-\left(x_4+y_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{18}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4-z_4\right)\,\mathbf{a}_2+\left(x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{19}}$	=	$-\left(x_4+z_4\right)\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_4-y_4\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{20}}$	=	$\left(x_4-z_4\right)\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2+\left(x_4-y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{21}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+z_4\right)\,\mathbf{a}_2+\left(x_4-y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{22}}$	=	$\left(y_4+z_4\right)\,\mathbf{a}_1-\left(x_4-z_4\right)\,\mathbf{a}_2-\left(x_4-y_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{23}}$	=	$-\left(x_4-z_4\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_4+y_4\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III
$\mathbf{B_{24}}$	=	$\left(x_4+z_4\right)\,\mathbf{a}_1+\left(y_4+z_4\right)\,\mathbf{a}_2+\left(x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\,\hat{\mathbf{y}}+c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32i)	Cd III

References

[1] M. J. Sanderson and N. C. Baenziger, *The Crystal Structure of $BaCd_{11}$*, Acta Cryst. **6**, 627–631 (1953), doi:10.1107/S0365110X53001745.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.