

BaCd₁₁ Structure:

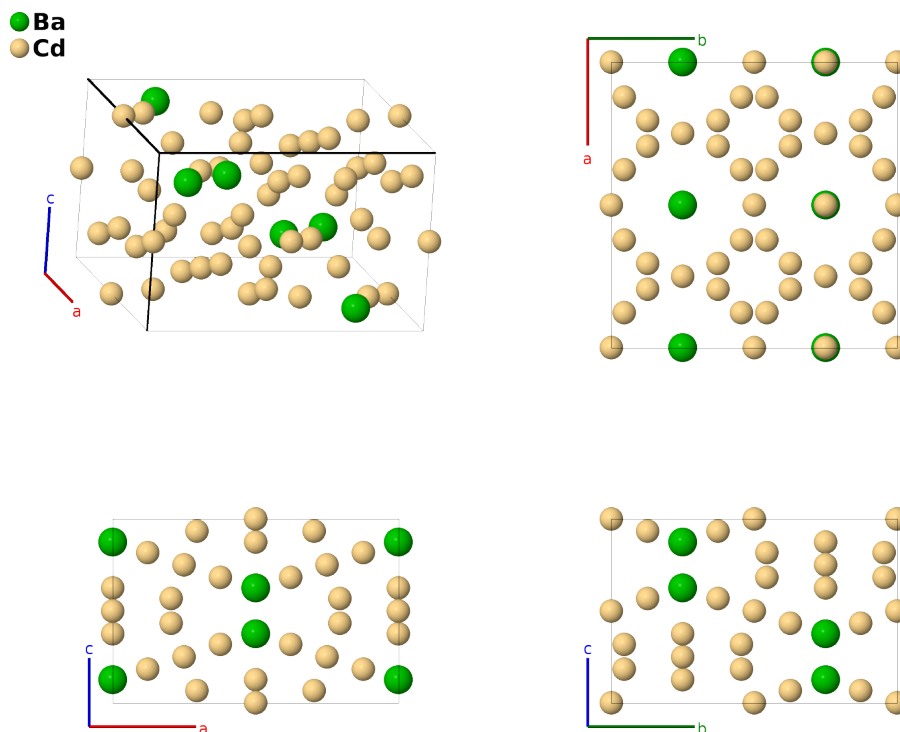
AB11_tI48_141_b_aci-001

This structure originally had the label **AB11_tI48_141_a_bdi**. Calls to that address will be redirected here.

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<https://aflow.org/p/EV03>

https://aflow.org/p/AB11_tI48_141_b_aci-001



Prototype	BaCd ₁₁
AFLOW prototype label	AB11_tI48_141_b_aci-001
ICSD	150492
Pearson symbol	tI48
Space group number	141
Space group symbol	<i>I</i> 4 ₁ / <i>amd</i>
AFLOW prototype command	<code>aflow --proto=AB11_tI48_141_b_aci-001 --params=a, c/a, x₄, y₄, z₄</code>

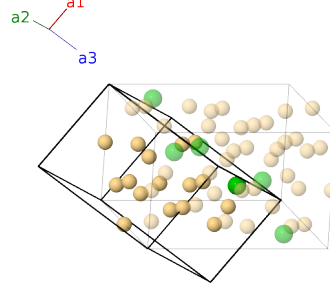
Other compounds with this structure

CaZn₁₁, CeZn₁₁, EuCd₁₁, EuZn₁₁, LaZn₁₁, NdZn₁₁, PrZn₁₁, SrCd₁₁

- (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

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



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}	$= (-y_4 + z_4 + \frac{1}{2})\mathbf{a}_1 - (x_4 - z_4)\mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - a(y_4 - \frac{1}{2})\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(32i)	Cd III
\mathbf{B}_{11}	$= (x_4 + z_4)\mathbf{a}_1 + (-y_4 + z_4 + \frac{1}{2})\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4})\hat{\mathbf{x}} + a(x_4 - \frac{1}{4})\hat{\mathbf{y}} + c(z_4 + \frac{1}{4})\hat{\mathbf{z}}$	(32i)	Cd III
\mathbf{B}_{12}	$= -(x_4 - z_4)\mathbf{a}_1 + (y_4 + z_4)\mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{4})\hat{\mathbf{x}} - a(x_4 - \frac{1}{4})\hat{\mathbf{y}} + c(z_4 - \frac{1}{4})\hat{\mathbf{z}}$	(32i)	Cd III
\mathbf{B}_{13}	$= (y_4 - z_4 + \frac{1}{2})\mathbf{a}_1 - (x_4 + z_4)\mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + a(y_4 + \frac{1}{2})\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(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}	$= (x_4 - z_4)\mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2})\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{4})\hat{\mathbf{x}} + a(x_4 - \frac{1}{4})\hat{\mathbf{y}} - c(z_4 - \frac{1}{4})\hat{\mathbf{z}}$	(32i)	Cd III
\mathbf{B}_{16}	$= -(x_4 + z_4)\mathbf{a}_1 - (y_4 + z_4)\mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4})\hat{\mathbf{x}} - a(x_4 - \frac{1}{4})\hat{\mathbf{y}} - c(z_4 + \frac{1}{4})\hat{\mathbf{z}}$	(32i)	Cd III
\mathbf{B}_{17}	$= -(y_4 + z_4)\mathbf{a}_1 - (x_4 + z_4)\mathbf{a}_2 - (x_4 + y_4)\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - ay_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(32i)	Cd III

$$\begin{aligned}
\mathbf{B}_{18} &= \begin{pmatrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{19} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{21} &= \begin{pmatrix} (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + z_4) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{22} &= \begin{pmatrix} (y_4 + z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - \\ (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(x_4 - z_4) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (32i) & \text{Cd III} \\
\mathbf{B}_{24} &= \begin{pmatrix} (x_4 + z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (32i) & \text{Cd III}
\end{aligned}$$

References

- [1] M. J. Sanderson and N. C. Baenziger, *The Crystal Structure of BaCd₁₁*, Acta Cryst. **6**, 627–631 (1953), doi:10.1107/S0365110X53001745.