

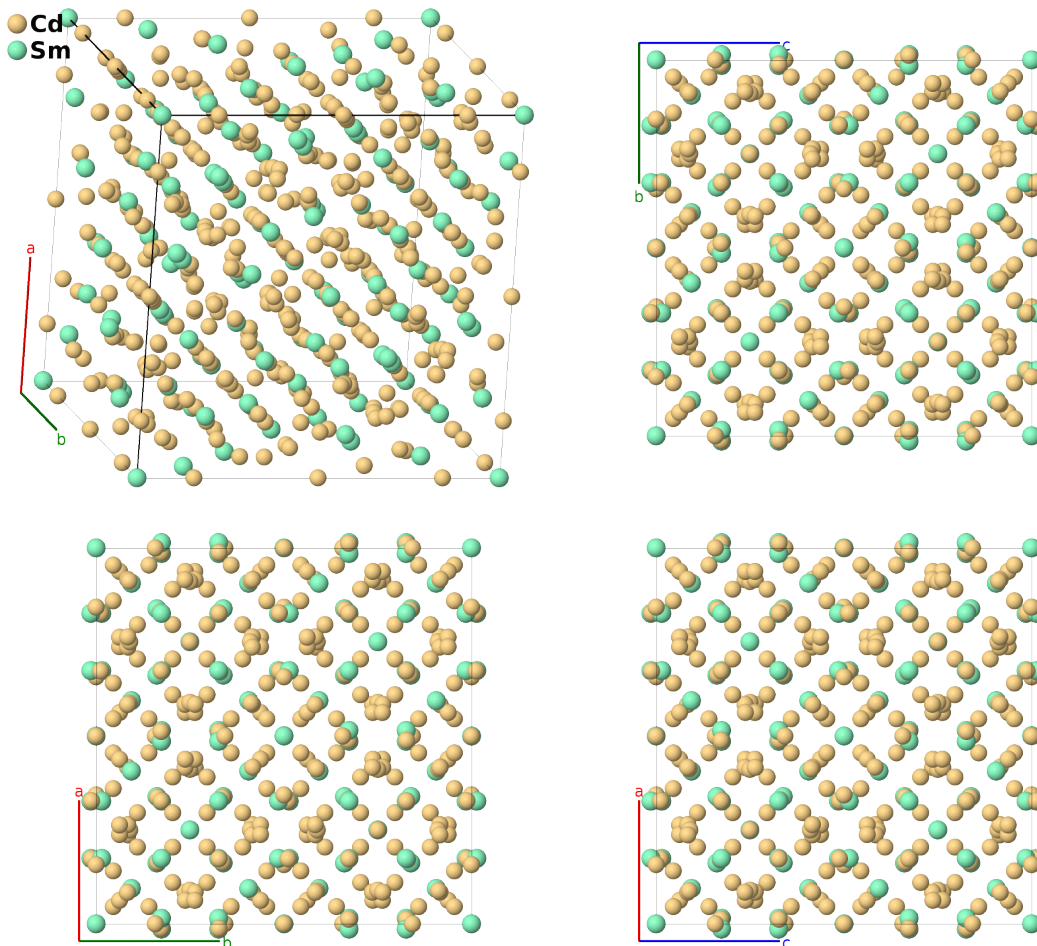
# Sm<sub>11</sub>Cd<sub>45</sub> Structure: A45B11\_cF448\_216\_ac4efg5h\_bd2eh-001

This structure originally had the label `A45B11_cF448_216_bd4efg5h_ac2eh`. Calls to that address will be redirected here.

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<https://aflow.org/p/LZ4J>

[https://aflow.org/p/A45B11\\_cF448\\_216\\_ac4efg5h\\_bd2eh-001](https://aflow.org/p/A45B11_cF448_216_ac4efg5h_bd2eh-001)



<b>Prototype</b>	Cd <sub>45</sub> Sm <sub>11</sub>
<b>AFLOW prototype label</b>	A45B11_cF448_216_ac4efg5h_bd2eh-001
<b>ICSD</b>	2246
<b>Pearson symbol</b>	cF448
<b>Space group number</b>	216
<b>Space group symbol</b>	$F\bar{4}3m$
<b>AFLOW prototype command</b>	<code>aflow --proto=A45B11_cF448_216_ac4efg5h_bd2eh-001</code> <code>--params=<math>a, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}, x_{16}, z_{16}, x_{17}, z_{17}, x_{18}, z_{18}</math></code>

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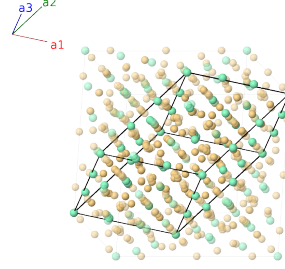
### Other compounds with this structure

Dy<sub>11</sub>Cd<sub>45</sub>, Er<sub>11</sub>Cd<sub>45</sub>, Gd<sub>11</sub>Cd<sub>45</sub>, Ho<sub>11</sub>Cd<sub>45</sub>, Lu<sub>11</sub>Cd<sub>45</sub>, Nd<sub>11</sub>Cd<sub>45</sub>, Tb<sub>11</sub>Cd<sub>45</sub>, Tm<sub>11</sub>Cd<sub>45</sub>, Pr<sub>11</sub>Cd<sub>45</sub>, Y<sub>11</sub>Cd<sub>45</sub>, Ce<sub>11</sub>Hg<sub>45</sub>, Nd<sub>11</sub>Hg<sub>45</sub>, Pr<sub>11</sub>Hg<sub>45</sub>, Sm<sub>11</sub>Hg<sub>45</sub>

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### Face-centered Cubic primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$0$	$=$	$0$	(4a) Cd I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$	(4b) Sm I
$\mathbf{B}_3$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(4c) Cd II
$\mathbf{B}_4$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{x} + \frac{3}{4}a\hat{y} + \frac{3}{4}a\hat{z}$	(4d) Sm II
$\mathbf{B}_5$	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} + ax_5\hat{y} + ax_5\hat{z}$	(16e) Cd III
$\mathbf{B}_6$	$=$	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} - ax_5\hat{y} + ax_5\hat{z}$	(16e) Cd III
$\mathbf{B}_7$	$=$	$x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} + ax_5\hat{y} - ax_5\hat{z}$	(16e) Cd III
$\mathbf{B}_8$	$=$	$-3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} - ax_5\hat{y} - ax_5\hat{z}$	(16e) Cd III
$\mathbf{B}_9$	$=$	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} + ax_6\hat{y} + ax_6\hat{z}$	(16e) Cd IV
$\mathbf{B}_{10}$	$=$	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 - 3x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} - ax_6\hat{y} + ax_6\hat{z}$	(16e) Cd IV
$\mathbf{B}_{11}$	$=$	$x_6\mathbf{a}_1 - 3x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} + ax_6\hat{y} - ax_6\hat{z}$	(16e) Cd IV
$\mathbf{B}_{12}$	$=$	$-3x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} - ax_6\hat{y} - ax_6\hat{z}$	(16e) Cd IV
$\mathbf{B}_{13}$	$=$	$x_7\mathbf{a}_1 + x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$ax_7\hat{x} + ax_7\hat{y} + ax_7\hat{z}$	(16e) Cd V
$\mathbf{B}_{14}$	$=$	$x_7\mathbf{a}_1 + x_7\mathbf{a}_2 - 3x_7\mathbf{a}_3$	$=$	$-ax_7\hat{x} - ax_7\hat{y} + ax_7\hat{z}$	(16e) Cd V
$\mathbf{B}_{15}$	$=$	$x_7\mathbf{a}_1 - 3x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$-ax_7\hat{x} + ax_7\hat{y} - ax_7\hat{z}$	(16e) Cd V
$\mathbf{B}_{16}$	$=$	$-3x_7\mathbf{a}_1 + x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$ax_7\hat{x} - ax_7\hat{y} - ax_7\hat{z}$	(16e) Cd V
$\mathbf{B}_{17}$	$=$	$x_8\mathbf{a}_1 + x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$ax_8\hat{x} + ax_8\hat{y} + ax_8\hat{z}$	(16e) Cd VI
$\mathbf{B}_{18}$	$=$	$x_8\mathbf{a}_1 + x_8\mathbf{a}_2 - 3x_8\mathbf{a}_3$	$=$	$-ax_8\hat{x} - ax_8\hat{y} + ax_8\hat{z}$	(16e) Cd VI
$\mathbf{B}_{19}$	$=$	$x_8\mathbf{a}_1 - 3x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$-ax_8\hat{x} + ax_8\hat{y} - ax_8\hat{z}$	(16e) Cd VI
$\mathbf{B}_{20}$	$=$	$-3x_8\mathbf{a}_1 + x_8\mathbf{a}_2 + x_8\mathbf{a}_3$	$=$	$ax_8\hat{x} - ax_8\hat{y} - ax_8\hat{z}$	(16e) Cd VI
$\mathbf{B}_{21}$	$=$	$x_9\mathbf{a}_1 + x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{x} + ax_9\hat{y} + ax_9\hat{z}$	(16e) Sm III
$\mathbf{B}_{22}$	$=$	$x_9\mathbf{a}_1 + x_9\mathbf{a}_2 - 3x_9\mathbf{a}_3$	$=$	$-ax_9\hat{x} - ax_9\hat{y} + ax_9\hat{z}$	(16e) Sm III
$\mathbf{B}_{23}$	$=$	$x_9\mathbf{a}_1 - 3x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$-ax_9\hat{x} + ax_9\hat{y} - ax_9\hat{z}$	(16e) Sm III
$\mathbf{B}_{24}$	$=$	$-3x_9\mathbf{a}_1 + x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{x} - ax_9\hat{y} - ax_9\hat{z}$	(16e) Sm III
$\mathbf{B}_{25}$	$=$	$x_{10}\mathbf{a}_1 + x_{10}\mathbf{a}_2 + x_{10}\mathbf{a}_3$	$=$	$ax_{10}\hat{x} + ax_{10}\hat{y} + ax_{10}\hat{z}$	(16e) Sm IV





$$\begin{aligned}
\mathbf{B}_{89} &= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 = ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{90} &= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 = -ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{91} &= (2x_{17} - z_{17}) \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = -ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{92} &= -(2x_{17} + z_{17}) \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{93} &= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{94} &= -(2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{95} &= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 = -az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{96} &= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 = -az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{97} &= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{98} &= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = -ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{99} &= -(2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3 = ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{100} &= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3 = -ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}} & (48h) & \text{Cd XIII} \\
\mathbf{B}_{101} &= z_{18} \mathbf{a}_1 + z_{18} \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3 = ax_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} + az_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{102} &= z_{18} \mathbf{a}_1 + z_{18} \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3 = -ax_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + az_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{103} &= (2x_{18} - z_{18}) \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = -ax_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - az_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{104} &= -(2x_{18} + z_{18}) \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = ax_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - az_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{105} &= (2x_{18} - z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{106} &= -(2x_{18} + z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{107} &= z_{18} \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3 = -az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{108} &= z_{18} \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3 = -az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{109} &= z_{18} \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = ax_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{110} &= z_{18} \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = -ax_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{111} &= -(2x_{18} + z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3 = ax_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V} \\
\mathbf{B}_{112} &= (2x_{18} - z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3 = -ax_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}} & (48h) & \text{Sm V}
\end{aligned}$$

## References

- [1] M. L. Fornasini, B. Chabot, and E. Parthé, *The crystal structure of Sm<sub>11</sub>Cd<sub>45</sub> with  $\gamma$ -brass and  $\alpha$ -Mn clusters*, Acta Crystallogr. Sect. B **34**, 2093–2099 (1978), doi:10.1107/S0567740878007505.