

Sm₁₁Cd₄₅ Structure:

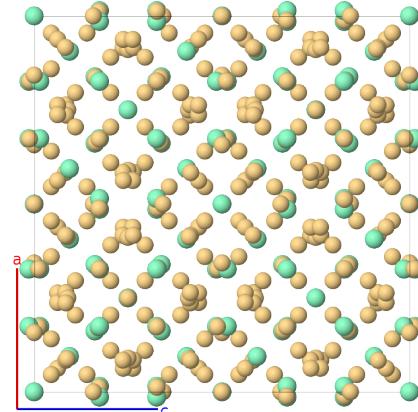
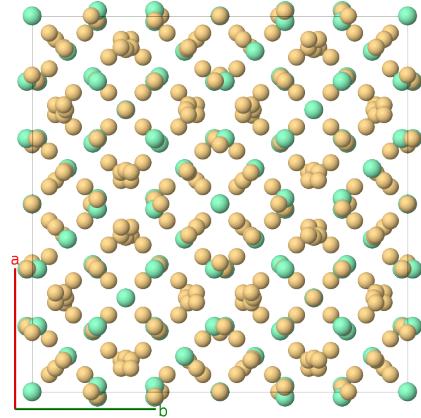
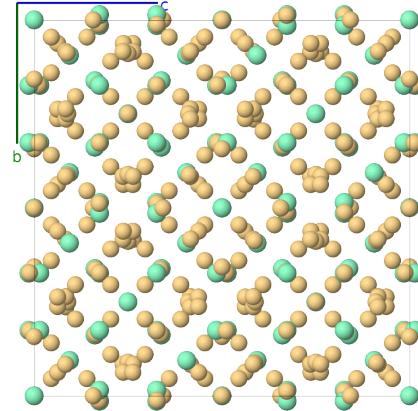
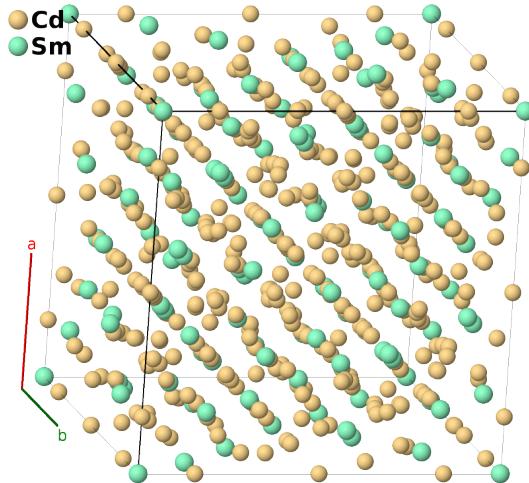
A45B11_cF448_216_ac4efg5h_bd2eh-001

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

Cite this page as: 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.

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

https://aflow.org/p/A45B11_cF448_216_ac4efg5h_bd2eh-001



Prototype Cd₄₅Sm₁₁

AFLOW prototype label A45B11_cF448_216_ac4efg5h_bd2eh-001

ICSD 2246

Pearson symbol cF448

Space group number 216

Space group symbol $F\bar{4}3m$

AFLOW prototype command

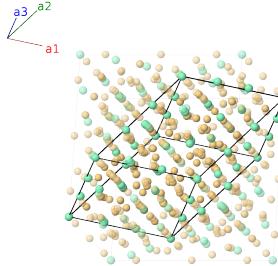
```
aflow --proto=A45B11_cF448_216_ac4efg5h_bd2eh-001  
--params=a,x5,x6,x7,x8,x9,x10,x11,x12,x13,z13,x14,z14,x15,z15,x16,z16,x17,z17,  
x18,z18
```

Other compounds with this structure

Dy₁₁Cd₄₅, Er₁₁Cd₄₅, Gd₁₁Cd₄₅, Ho₁₁Cd₄₅, Lu₁₁Cd₄₅, Nd₁₁Cd₄₅, Tb₁₁Cd₄₅, Tm₁₁Cd₄₅, Pr₁₁Cd₄₅, Y₁₁Cd₄₅, Ce₁₁Hg₄₅, Nd₁₁Hg₄₅, Pr₁₁Hg₄₅, Sm₁₁Hg₄₅

Face-centered Cubic primitive vectors

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



Basis vectors

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

| | | | | | |
|---------------------|---|-----|--|-------|---------|
| $\mathbf{B}_{26} =$ | $x_{10}\mathbf{a}_1 + x_{10}\mathbf{a}_2 - 3x_{10}\mathbf{a}_3$ | $=$ | $-ax_{10}\hat{\mathbf{x}} - ax_{10}\hat{\mathbf{y}} + ax_{10}\hat{\mathbf{z}}$ | (16e) | Sm IV |
| $\mathbf{B}_{27} =$ | $x_{10}\mathbf{a}_1 - 3x_{10}\mathbf{a}_2 + x_{10}\mathbf{a}_3$ | $=$ | $-ax_{10}\hat{\mathbf{x}} + ax_{10}\hat{\mathbf{y}} - ax_{10}\hat{\mathbf{z}}$ | (16e) | Sm IV |
| $\mathbf{B}_{28} =$ | $-3x_{10}\mathbf{a}_1 + x_{10}\mathbf{a}_2 + x_{10}\mathbf{a}_3$ | $=$ | $ax_{10}\hat{\mathbf{x}} - ax_{10}\hat{\mathbf{y}} - ax_{10}\hat{\mathbf{z}}$ | (16e) | Sm IV |
| $\mathbf{B}_{29} =$ | $-x_{11}\mathbf{a}_1 + x_{11}\mathbf{a}_2 + x_{11}\mathbf{a}_3$ | $=$ | $ax_{11}\hat{\mathbf{x}}$ | (24f) | Cd VII |
| $\mathbf{B}_{30} =$ | $x_{11}\mathbf{a}_1 - x_{11}\mathbf{a}_2 - x_{11}\mathbf{a}_3$ | $=$ | $-ax_{11}\hat{\mathbf{x}}$ | (24f) | Cd VII |
| $\mathbf{B}_{31} =$ | $x_{11}\mathbf{a}_1 - x_{11}\mathbf{a}_2 + x_{11}\mathbf{a}_3$ | $=$ | $ax_{11}\hat{\mathbf{y}}$ | (24f) | Cd VII |
| $\mathbf{B}_{32} =$ | $-x_{11}\mathbf{a}_1 + x_{11}\mathbf{a}_2 - x_{11}\mathbf{a}_3$ | $=$ | $-ax_{11}\hat{\mathbf{y}}$ | (24f) | Cd VII |
| $\mathbf{B}_{33} =$ | $x_{11}\mathbf{a}_1 + x_{11}\mathbf{a}_2 - x_{11}\mathbf{a}_3$ | $=$ | $ax_{11}\hat{\mathbf{z}}$ | (24f) | Cd VII |
| $\mathbf{B}_{34} =$ | $-x_{11}\mathbf{a}_1 - x_{11}\mathbf{a}_2 + x_{11}\mathbf{a}_3$ | $=$ | $-ax_{11}\hat{\mathbf{z}}$ | (24f) | Cd VII |
| $\mathbf{B}_{35} =$ | $-(x_{12} - \frac{1}{2})\mathbf{a}_1 + x_{12}\mathbf{a}_2 + x_{12}\mathbf{a}_3$ | $=$ | $ax_{12}\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{36} =$ | $x_{12}\mathbf{a}_1 - (x_{12} - \frac{1}{2})\mathbf{a}_2 - (x_{12} - \frac{1}{2})\mathbf{a}_3$ | $=$ | $-a(x_{12} - \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{37} =$ | $x_{12}\mathbf{a}_1 - (x_{12} - \frac{1}{2})\mathbf{a}_2 + x_{12}\mathbf{a}_3$ | $=$ | $\frac{1}{4}a\hat{\mathbf{x}} + ax_{12}\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{38} =$ | $-(x_{12} - \frac{1}{2})\mathbf{a}_1 + x_{12}\mathbf{a}_2 - (x_{12} - \frac{1}{2})\mathbf{a}_3$ | $=$ | $\frac{1}{4}a\hat{\mathbf{x}} - a(x_{12} - \frac{1}{2})\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{39} =$ | $x_{12}\mathbf{a}_1 + x_{12}\mathbf{a}_2 - (x_{12} - \frac{1}{2})\mathbf{a}_3$ | $=$ | $\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + ax_{12}\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{40} =$ | $-(x_{12} - \frac{1}{2})\mathbf{a}_1 - (x_{12} - \frac{1}{2})\mathbf{a}_2 + x_{12}\mathbf{a}_3$ | $=$ | $\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - a(x_{12} - \frac{1}{2})\hat{\mathbf{z}}$ | (24g) | Cd VIII |
| $\mathbf{B}_{41} =$ | $z_{13}\mathbf{a}_1 + z_{13}\mathbf{a}_2 + (2x_{13} - z_{13})\mathbf{a}_3$ | $=$ | $ax_{13}\hat{\mathbf{x}} + ax_{13}\hat{\mathbf{y}} + az_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{42} =$ | $z_{13}\mathbf{a}_1 + z_{13}\mathbf{a}_2 - (2x_{13} + z_{13})\mathbf{a}_3$ | $=$ | $-ax_{13}\hat{\mathbf{x}} - ax_{13}\hat{\mathbf{y}} + az_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{43} =$ | $(2x_{13} - z_{13})\mathbf{a}_1 - (2x_{13} + z_{13})\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $-ax_{13}\hat{\mathbf{x}} + ax_{13}\hat{\mathbf{y}} - az_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{44} =$ | $-(2x_{13} + z_{13})\mathbf{a}_1 + (2x_{13} - z_{13})\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $ax_{13}\hat{\mathbf{x}} - ax_{13}\hat{\mathbf{y}} - az_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{45} =$ | $(2x_{13} - z_{13})\mathbf{a}_1 + z_{13}\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $az_{13}\hat{\mathbf{x}} + ax_{13}\hat{\mathbf{y}} + ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{46} =$ | $-(2x_{13} + z_{13})\mathbf{a}_1 + z_{13}\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $az_{13}\hat{\mathbf{x}} - ax_{13}\hat{\mathbf{y}} - ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{47} =$ | $z_{13}\mathbf{a}_1 + (2x_{13} - z_{13})\mathbf{a}_2 - (2x_{13} + z_{13})\mathbf{a}_3$ | $=$ | $-az_{13}\hat{\mathbf{x}} - ax_{13}\hat{\mathbf{y}} + ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{48} =$ | $z_{13}\mathbf{a}_1 - (2x_{13} + z_{13})\mathbf{a}_2 + (2x_{13} - z_{13})\mathbf{a}_3$ | $=$ | $-az_{13}\hat{\mathbf{x}} + ax_{13}\hat{\mathbf{y}} - ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{49} =$ | $z_{13}\mathbf{a}_1 + (2x_{13} - z_{13})\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $ax_{13}\hat{\mathbf{x}} + az_{13}\hat{\mathbf{y}} + ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{50} =$ | $z_{13}\mathbf{a}_1 - (2x_{13} + z_{13})\mathbf{a}_2 + z_{13}\mathbf{a}_3$ | $=$ | $-ax_{13}\hat{\mathbf{x}} + az_{13}\hat{\mathbf{y}} - ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{51} =$ | $-(2x_{13} + z_{13})\mathbf{a}_1 + z_{13}\mathbf{a}_2 + (2x_{13} - z_{13})\mathbf{a}_3$ | $=$ | $ax_{13}\hat{\mathbf{x}} - az_{13}\hat{\mathbf{y}} - ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{52} =$ | $(2x_{13} - z_{13})\mathbf{a}_1 + z_{13}\mathbf{a}_2 - (2x_{13} + z_{13})\mathbf{a}_3$ | $=$ | $-ax_{13}\hat{\mathbf{x}} - az_{13}\hat{\mathbf{y}} + ax_{13}\hat{\mathbf{z}}$ | (48h) | Cd IX |
| $\mathbf{B}_{53} =$ | $z_{14}\mathbf{a}_1 + z_{14}\mathbf{a}_2 + (2x_{14} - z_{14})\mathbf{a}_3$ | $=$ | $ax_{14}\hat{\mathbf{x}} + ax_{14}\hat{\mathbf{y}} + az_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |
| $\mathbf{B}_{54} =$ | $z_{14}\mathbf{a}_1 + z_{14}\mathbf{a}_2 - (2x_{14} + z_{14})\mathbf{a}_3$ | $=$ | $-ax_{14}\hat{\mathbf{x}} - ax_{14}\hat{\mathbf{y}} + az_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |
| $\mathbf{B}_{55} =$ | $(2x_{14} - z_{14})\mathbf{a}_1 - (2x_{14} + z_{14})\mathbf{a}_2 + z_{14}\mathbf{a}_3$ | $=$ | $-ax_{14}\hat{\mathbf{x}} + ax_{14}\hat{\mathbf{y}} - az_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |
| $\mathbf{B}_{56} =$ | $-(2x_{14} + z_{14})\mathbf{a}_1 + (2x_{14} - z_{14})\mathbf{a}_2 + z_{14}\mathbf{a}_3$ | $=$ | $ax_{14}\hat{\mathbf{x}} - ax_{14}\hat{\mathbf{y}} - az_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |
| $\mathbf{B}_{57} =$ | $(2x_{14} - z_{14})\mathbf{a}_1 + z_{14}\mathbf{a}_2 + z_{14}\mathbf{a}_3$ | $=$ | $az_{14}\hat{\mathbf{x}} + ax_{14}\hat{\mathbf{y}} + ax_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |
| $\mathbf{B}_{58} =$ | $-(2x_{14} + z_{14})\mathbf{a}_1 + z_{14}\mathbf{a}_2 + z_{14}\mathbf{a}_3$ | $=$ | $az_{14}\hat{\mathbf{x}} - ax_{14}\hat{\mathbf{y}} - ax_{14}\hat{\mathbf{z}}$ | (48h) | Cd X |

| | | | | | |
|------------------------|--|-----|---|-------|---------|
| B₈₉ | $= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3$ | $=$ | $ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₀ | $= z_{17} \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3$ | $=$ | $-ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + az_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₁ | $= (2x_{17} - z_{17}) \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $-ax_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₂ | $= -(2x_{17} + z_{17}) \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $ax_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - az_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₃ | $= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₄ | $= -(2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₅ | $= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3$ | $=$ | $-az_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₆ | $= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3$ | $=$ | $-az_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₇ | $= z_{17} \mathbf{a}_1 + (2x_{17} - z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₈ | $= z_{17} \mathbf{a}_1 - (2x_{17} + z_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $-ax_{17} \hat{\mathbf{x}} + az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₉₉ | $= -(2x_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + (2x_{17} - z_{17}) \mathbf{a}_3$ | $=$ | $ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} - ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₁₀₀ | $= (2x_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 - (2x_{17} + z_{17}) \mathbf{a}_3$ | $=$ | $-ax_{17} \hat{\mathbf{x}} - az_{17} \hat{\mathbf{y}} + ax_{17} \hat{\mathbf{z}}$ | (48h) | Cd XIII |
| B₁₀₁ | $= z_{18} \mathbf{a}_1 + z_{18} \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3$ | $=$ | $ax_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} + az_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₂ | $= z_{18} \mathbf{a}_1 + z_{18} \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3$ | $=$ | $-ax_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + az_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₃ | $= (2x_{18} - z_{18}) \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $-ax_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - az_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₄ | $= -(2x_{18} + z_{18}) \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $ax_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - az_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₅ | $= (2x_{18} - z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₆ | $= -(2x_{18} + z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₇ | $= z_{18} \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3$ | $=$ | $-az_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₈ | $= z_{18} \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3$ | $=$ | $-az_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₀₉ | $= z_{18} \mathbf{a}_1 + (2x_{18} - z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $ax_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₁₀ | $= z_{18} \mathbf{a}_1 - (2x_{18} + z_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$ | $=$ | $-ax_{18} \hat{\mathbf{x}} + az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₁₁ | $= -(2x_{18} + z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 + (2x_{18} - z_{18}) \mathbf{a}_3$ | $=$ | $ax_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} - ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |
| B₁₁₂ | $= (2x_{18} - z_{18}) \mathbf{a}_1 + z_{18} \mathbf{a}_2 - (2x_{18} + z_{18}) \mathbf{a}_3$ | $=$ | $-ax_{18} \hat{\mathbf{x}} - az_{18} \hat{\mathbf{y}} + ax_{18} \hat{\mathbf{z}}$ | (48h) | Sm V |

References

- [1] M. L. Fornasini, B. Chabot, and E. Parthé, *The crystal structure of Sm₁₁Cd₄₅ with γ-brass and α-Mn clusters*, Acta Crystallogr. Sect. B **34**, 2093–2099 (1978), doi:10.1107/S0567740878007505.