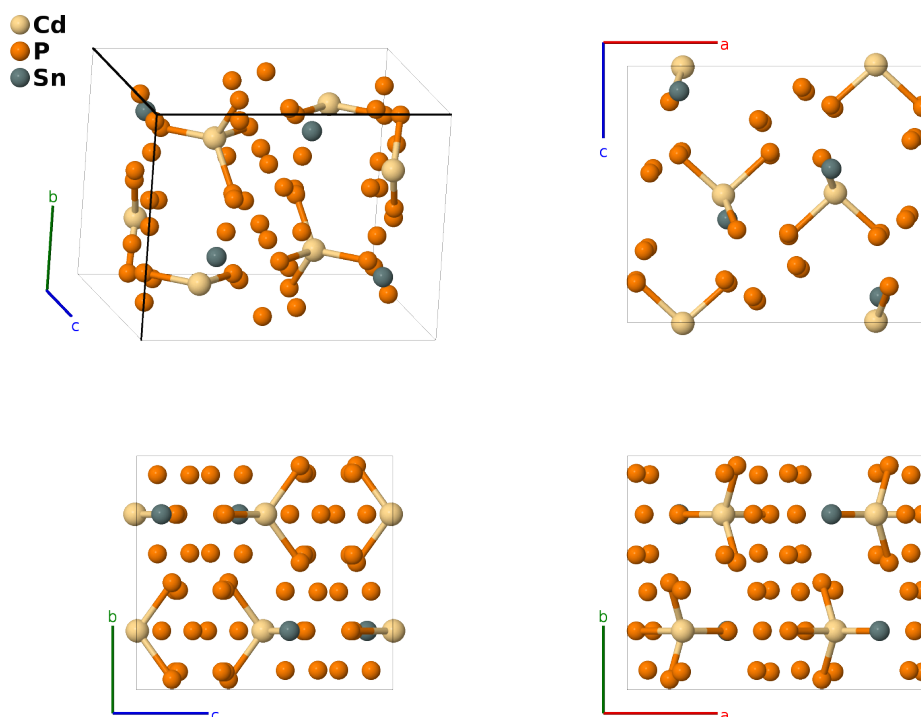


CdSnP₁₄ (HgPbP₁₄) Structure: AB14C_oP64_62_c_4c5d_c-001

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<https://afLOW.org/p/LZG8>

https://afLOW.org/p/AB14C_oP64_62_c_4c5d_c-001



| | |
|-------------------------|--|
| Prototype | CdP ₁₄ Sn |
| AFLOW prototype label | AB14C_oP64_62_c_4c5d_c-001 |
| ICSD | 42976 |
| Pearson symbol | oP64 |
| Space group number | 62 |
| Space group symbol | <i>Pnma</i> |
| AFLOW prototype command | <pre>afLOW --proto=AB14C_oP64_62_c_4c5d_c-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11</pre> |

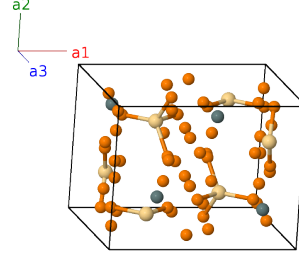
Other compounds with this structure

CdPbP₁₄, HgPbP₁₄, HgSnP₁₄, ZnPbP₁₄, ZnSnP₁₄

- Although (Krebs, 1958) first described this structure for HgPbP₁₄, but their data is very approximate, so we use the refinement made by (Scholz, 1987). They give the Wyckoff positions for CdSnP₁₄, so we use that as our prototype.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|---|-----|--|------------------|-----------|
| \mathbf{B}_1 | $= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (4c) | Cd I |
| \mathbf{B}_2 | $= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | Cd I |
| \mathbf{B}_3 | $= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$ | (4c) | Cd I |
| \mathbf{B}_4 | $= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | Cd I |
| \mathbf{B}_5 | $= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (4c) | P I |
| \mathbf{B}_6 | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P I |
| \mathbf{B}_7 | $= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$ | (4c) | P I |
| \mathbf{B}_8 | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P I |
| \mathbf{B}_9 | $= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (4c) | P II |
| \mathbf{B}_{10} | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P II |
| \mathbf{B}_{11} | $= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (4c) | P II |
| \mathbf{B}_{12} | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P II |
| \mathbf{B}_{13} | $= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (4c) | P III |
| \mathbf{B}_{14} | $= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P III |
| \mathbf{B}_{15} | $= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$ | $=$ | $-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$ | (4c) | P III |
| \mathbf{B}_{16} | $= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P III |
| \mathbf{B}_{17} | $= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$ | $=$ | $ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$ | (4c) | P IV |
| \mathbf{B}_{18} | $= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P IV |
| \mathbf{B}_{19} | $= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$ | $=$ | $-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$ | (4c) | P IV |
| \mathbf{B}_{20} | $= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | P IV |
| \mathbf{B}_{21} | $= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$ | $=$ | $ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$ | (4c) | Sn I |
| \mathbf{B}_{22} | $= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | Sn I |
| \mathbf{B}_{23} | $= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$ | $=$ | $-ax_6 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$ | (4c) | Sn I |
| \mathbf{B}_{24} | $= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4c) | Sn I |

$$\begin{aligned}
\mathbf{B}_{56} &= -\begin{pmatrix} x_{10} - \frac{1}{2} \\ z_{10} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{10} + \frac{1}{2} \\ z_{10} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= & -a \begin{pmatrix} x_{10} - \frac{1}{2} \\ z_{10} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_{10} + \frac{1}{2} \\ z_{10} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_{10} + \frac{1}{2} \\ z_{10} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{P VIII} \\
\mathbf{B}_{57} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= & ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{58} &= -\begin{pmatrix} x_{11} - \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \mathbf{a}_3 &= & -a \begin{pmatrix} x_{11} - \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c \begin{pmatrix} z_{11} + \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{59} &= -x_{11} \mathbf{a}_1 + \begin{pmatrix} y_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -ax_{11} \hat{\mathbf{x}} + b \begin{pmatrix} y_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{60} &= \begin{pmatrix} x_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= & a \begin{pmatrix} x_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} z_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{61} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{62} &= \begin{pmatrix} x_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{11} \mathbf{a}_2 - \mathbf{a}_3 &= & a \begin{pmatrix} x_{11} + \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c \begin{pmatrix} z_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{63} &= x_{11} \mathbf{a}_1 - \begin{pmatrix} y_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= & ax_{11} \hat{\mathbf{x}} - b \begin{pmatrix} y_{11} - \frac{1}{2} \\ z_{11} - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8d) & \text{P IX} \\
\mathbf{B}_{64} &= -\begin{pmatrix} x_{11} - \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{11} + \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= & -a \begin{pmatrix} x_{11} - \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_{11} + \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} z_{11} + \frac{1}{2} \\ z_{11} + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (8d) & \text{P IX}
\end{aligned}$$

References

- [1] U. D. Scholz and W. Jeitschko, *Preparation, crystal structure, and properties of HgSnP₁₄ and other polyphosphides with HgPbP₁₄-type structure*, J. Solid State Chem. **67**, 271–277 (1987), doi:10.1016/0022-4596(87)90363-X.
- [2] H. Krebs and T. Ludwig, *Über kristallisierte Metallpolyphosphide. III. Die Struktur der Metallpolyphosphide des Typs HgPbP₁₄*, Z. Anorganische und Allgemeine Chemie **294**, 257–268 (1958), doi:10.1002/zaac.19582940502.