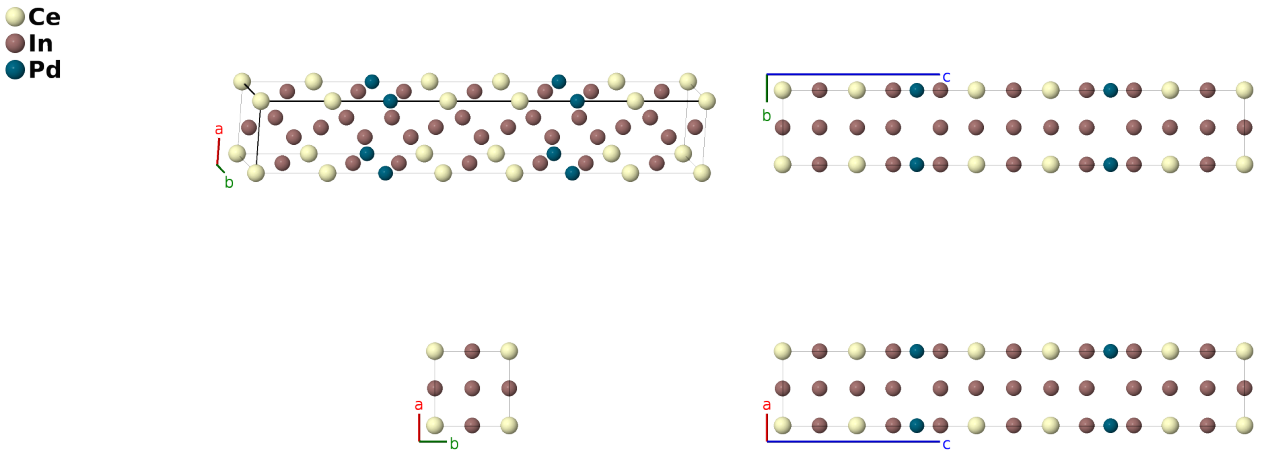
# $Ce_5Pd_2In_{19}$ Structure: A5B19C2_tP26_123_a2g_ce2h3i_g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/RR9W

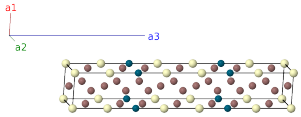
https://aflow.org/p/A5B19C2_tP26_123_a2g_ce2h3i_g-001




| | |
|---|---|
| **Prototype** | $Ce_5In_{19}Pd_2$ |
| **AFLOW prototype label** | A5B19C2_tP26_123_a2g_ce2h3i_g-001 |
| **ICSD** | 247863 |
| **Pearson symbol** | tP26 |
| **Space group number** | 123 |
| **Space group symbol** | $P4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=A5B19C2_tP26_123_a2g_ce2h3i_g-001 --params=`$a, c/a, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}$ |

**Simple Tetragonal primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Ce I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$ | (1c) | In I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2e) | In II |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2e) | In II |
| $\mathbf{B_5}$ | = | $z_4\,\mathbf{a}_3$ | = | $cz_4\,\hat{\mathbf{z}}$ | (2g) | Ce II |
| $\mathbf{B_6}$ | = | $-z_4\,\mathbf{a}_3$ | = | $-cz_4\,\hat{\mathbf{z}}$ | (2g) | Ce II |
| $\mathbf{B_7}$ | = | $z_5\,\mathbf{a}_3$ | = | $cz_5\,\hat{\mathbf{z}}$ | (2g) | Ce III |
| $\mathbf{B_8}$ | = | $-z_5\,\mathbf{a}_3$ | = | $-cz_5\,\hat{\mathbf{z}}$ | (2g) | Ce III |
| $\mathbf{B_9}$ | = | $z_6\,\mathbf{a}_3$ | = | $cz_6\,\hat{\mathbf{z}}$ | (2g) | Pd I |
| $\mathbf{B_{10}}$ | = | $-z_6\,\mathbf{a}_3$ | = | $-cz_6\,\hat{\mathbf{z}}$ | (2g) | Pd I |
| $\mathbf{B_{11}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (2h) | In III |
| $\mathbf{B_{12}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$ | (2h) | In III |
| $\mathbf{B_{13}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (2h) | In IV |
| $\mathbf{B_{14}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (2h) | In IV |
| $\mathbf{B_{15}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (4i) | In V |
| $\mathbf{B_{16}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$ | (4i) | In V |
| $\mathbf{B_{17}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (4i) | In V |
| $\mathbf{B_{18}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_9\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$ | (4i) | In V |
| $\mathbf{B_{19}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$ | (4i) | In VI |
| $\mathbf{B_{20}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$ | (4i) | In VI |
| $\mathbf{B_{21}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$ | (4i) | In VI |
| $\mathbf{B_{22}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$ | (4i) | In VI |
| $\mathbf{B_{23}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$ | (4i) | In VII |
| $\mathbf{B_{24}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{11}\,\hat{\mathbf{z}}$ | (4i) | In VII |
| $\mathbf{B_{25}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$ | (4i) | In VII |
| $\mathbf{B_{26}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{11}\,\hat{\mathbf{z}}$ | (4i) | In VII |

## References


[1] A. Tursina, S. Nesterenko, Y. Seropegin, H. Noël, and D. Kaczorowski, *$Ce_2PdIn_8$, $Ce_3PdIn_{11}$ and $Ce_5Pd_2In_{19}$–members of homological series based on $AuCu_{3-}$ and $PtHg_{2-}$ type structural units*, J. Solid State Chem. **200**, 7–12 (2013), doi:10.1016/j.jssc.2012.12.037.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[1] M. Kratochvilova, M. Dusek, K. Uhlirova, A. Rudajevova, J. Prokleska, B. Vondrackova, J. Custers, and V. Sechovsky, *Single crystal study of the layered heavy fermion compounds $Ce_2PdIn_8$, $Ce_3PdIn_{11}$, $Ce_2PtIn_8$ and $Ce_3PtIn_{11}$*, J. Cryst. Growth **397**, 47–52 (2014), doi:10.1016/j.jcrysgro.2014.04.008.