# $CePt_2In_7$ Structure: AB7C2_tI20_139_a_bdg_e-001

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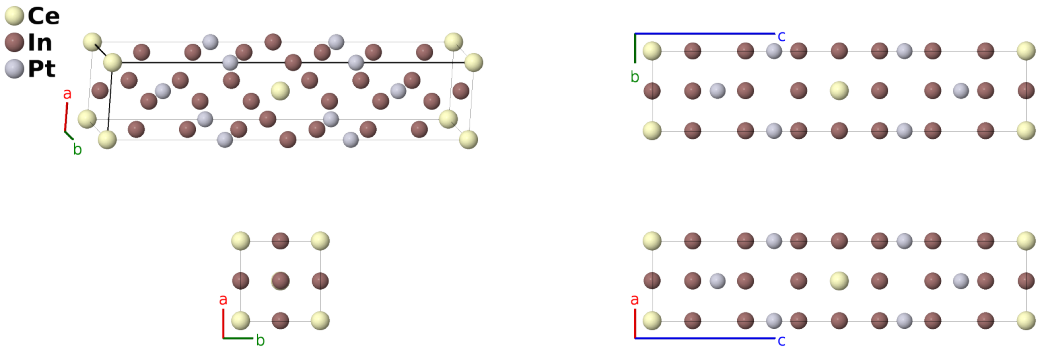
https://aflow.org/p/P6JF

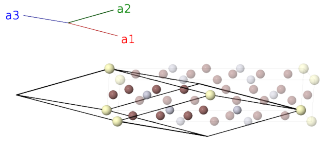
https://aflow.org/p/AB7C2_tI20_139_a_bdg_e-001




| | |
|---|---|
| **Prototype** | $CeIn_7Pt_2$ |
| **AFLOW prototype label** | AB7C2_tI20_139_a_bdg_e-001 |
| **ICSD** | 161312 |
| **Pearson symbol** | tI20 |
| **Space group number** | 139 |
| **Space group symbol** | $I4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=AB7C2_tI20_139_a_bdg_e-001 --params=`$a, c/a, z_4, z_5$ |

## Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Ce I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | In I |
| $\mathbf{B_3}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | In II |
| $\mathbf{B_4}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | In II |
| $\mathbf{B_5}$ | = | $z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$ | = | $cz_4\,\hat{\mathbf{z}}$ | (4e) | Pt I |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_6}$ | = | $-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$ | = | $-cz_4\,\hat{\mathbf{z}}$ | (4e) | Pt I |
| $\mathbf{B_7}$ | = | $\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (8g) | In III |
| $\mathbf{B_8}$ | = | $z_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$ | (8g) | In III |
| $\mathbf{B_9}$ | = | $-\left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (8g) | In III |
| $\mathbf{B_{10}}$ | = | $-z_5\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$ | (8g) | In III |

## References


[1] Z. M. Kurenbaeva, E. V. Murashova, Y. D. Seropegin, H. Noël, and A. I. Tursina, *The crystal structure of the new indide $CePt_2In_7$ from powder data*, Intermetallics **16**, 979–981 (2008), doi:10.1016/j.intermet.2008.04.018.


## Found in


[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.