# $CePdGa_6$ Structure: AB6C_tP8_123_a_hi_b-001

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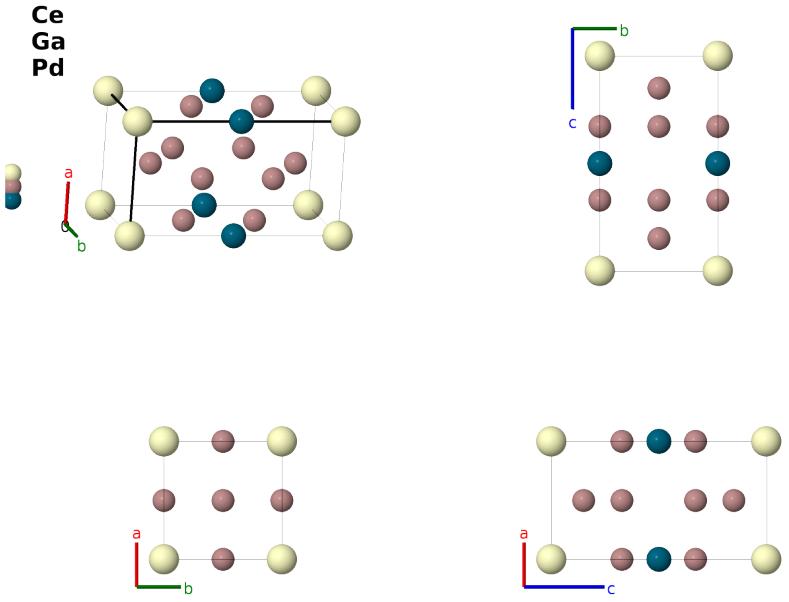
https://aflow.org/prototype-encyclopedia/1ALT

https://aflow.org/prototype-encyclopedia/AB6C_tP8_123_a_hi_b-001




| | |
|---|---|
| **Prototype** | $CeGa_6Pd$ |
| **AFLOW prototype label** | AB6C_tP8_123_a_hi_b-001 |
| **ICSD** | 240161 |
| **CCDC** | 1710910 |
| **Pearson symbol** | tP8 |
| **Space group number** | 123 |
| **Space group symbol** | $P4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=AB6C_tP8_123_a_hi_b-001 --params=`$a, c/a, z_3, z_4$ |

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**Other compounds with this structure**
$LaPdGa_6$, $SrAu(Au_{0.5}Ga_{0.5})_2Ga_4$

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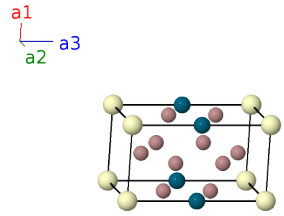
- The Springer Materials website gives $SrAu(Au_{0.5}Ga_{0.5})_2Ga_4$ as the prototype, but we have chosen to use the stoichiometric $CeGa_6Pd$ version.

### 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 |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (1b) | Pd I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2h) | Ga I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2h) | Ga I |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4i) | Ga II |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$ | (4i) | Ga II |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4i) | Ga II |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$ | (4i) | Ga II |

### References


[1] R. T. Macaluso, S. Nakatsuji, H. Lee, Z. Fisk, M. Moldovan, D. P. Young, and J. Y. Chan, *Synthesis, structure, and magnetism of a new heavy-fermion antiferromagnet, $CePdGa_6$*, J. Solid State Chem. **174**, 296–301 (2003), doi:10.1016/S0022-4596(03)00223-8.


### First cited in

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