

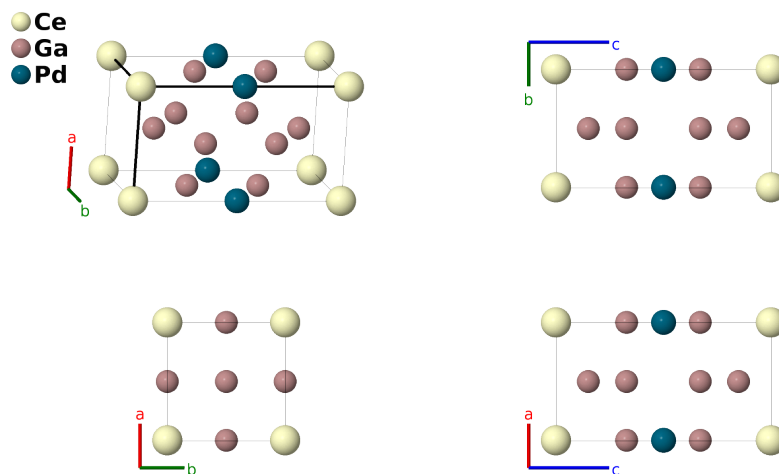
CePdGa₆ Structure:

AB6C_tP8_123_a_hi_b-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/1ALT>

https://aflow.org/p/AB6C_tP8_123_a_hi_b-001



Prototype	CeGa ₆ Pd
AFLOW prototype label	AB6C_tP8_123_a_hi_b-001
ICSD	240161
Pearson symbol	tP8
Space group number	123
Space group symbol	<i>P4/mmm</i>
AFLOW prototype command	<code>aflow --proto=AB6C_tP8_123_a_hi_b-001 --params=a, c/a, z₃, z₄</code>

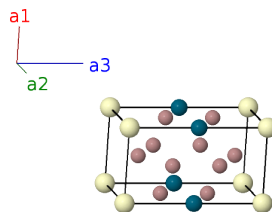
Other compounds with this structure

LaPdGa₆, SrAu(Au_{0.5}Ga_{0.5})₂Ga₄

- The Springer Materials website gives SrAu(Au_{0.5}Ga_{0.5})₂Ga₄ as the prototype, but we have chosen to use the stoichiometric CeGa₆Pd version.

Simple Tetragonal primitive vectors

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



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, CePdGa₆*, J. Solid State Chem. **174**, 296–301 (2003), doi:10.1016/S0022-4596(03)00223-8.