

Ce₅Pd₂In₁₉ Structure:

A5B19C2_tP26_123_a2g_ce2h3i_g-001

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<https://aflow.org/prototype-encyclopedia/RR9W>

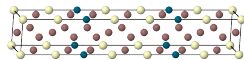
https://aflow.org/prototype-encyclopedia/A5B19C2_tP26_123_a2g_ce2h3i_g-001

Prototype	Ce ₅ In ₁₉ Pd ₂
AFLOW prototype label	A5B19C2_tP26_123_a2g_ce2h3i_g-001
ICSD	247863
CCDC	1714465
Pearson symbol	tP26
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=A5B19C2_tP26_123_a2g_ce2h3i_g-001</code> <code>--params=a, c/a, z₄, z₅, z₆, z₇, z₈, z₉, z₁₀, z₁₁</code>

Simple Tetragonal primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	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

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Ce
In
Pd

