$Ce_8Pd_{24}Sb$ Structure: A8B24C_cP33_221_g_efh_a-001

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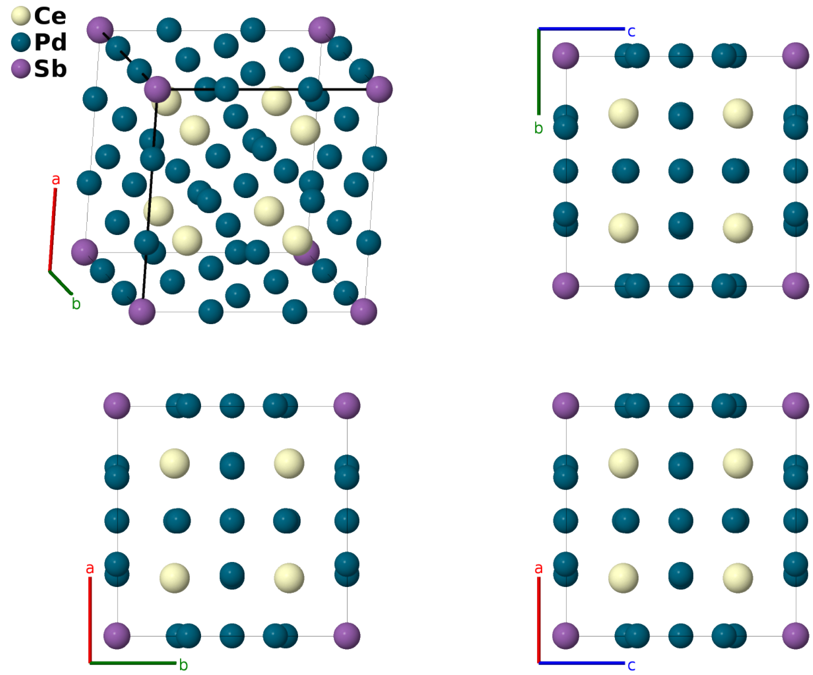
https://aflow.org/p/CLMU

https://aflow.org/p/A8B24C_cP33_221_g_efh_a-001

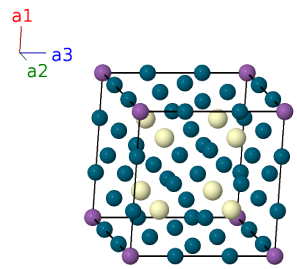


Prototype	$Ce_8Pd_{24}Sb$
AFLOW prototype label	A8B24C_cP33_221_g_efh_a-001
ICSD	83378
Pearson symbol	cP33
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A8B24C_cP33_221_g_efh_a-001` `--params=`a, x_2, x_3, x_4, x_5

- $CePd_3$ forms in the $L1_2$ Cu_3Au Structure. Adding antimony at some octahedral sites gives this structure. Alternatively, this can be viewed as a cubic perovskite ($E2_1$) structure with 7/8 of the B atoms removed in an ordered manner.

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Sb I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}}$	(6e)	Pd I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1$	=	$-ax_2\,\hat{\mathbf{x}}$	(6e)	Pd I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{y}}$	(6e)	Pd I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{y}}$	(6e)	Pd I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{z}}$	(6e)	Pd I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{z}}$	(6e)	Pd I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(6f)	Pd II
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{20}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{21}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8g)	Ce I
$\mathbf{B_{22}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	Pd III
$\mathbf{B_{23}}$	=	$-x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12h)	Pd III
$\mathbf{B_{24}}$	=	$x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{25}}$	=	$-x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(12h)	Pd III
$\mathbf{B_{29}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(12h)	Pd III
$\mathbf{B_{30}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	Pd III

$\mathbf{B_{31}}$	=	$-x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{32}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12h)	Pd III
$\mathbf{B_{33}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12h)	Pd III

References

[1] R. A. Gordon and F. J. DiSalvo, *Crystal Structure and Magnetic Susceptibility of $Ce_8Pd_{24}Sb$*, Z. Naturforsch. B **51**, 52–56 (1996), doi:10.1515/znb-1996-0112.