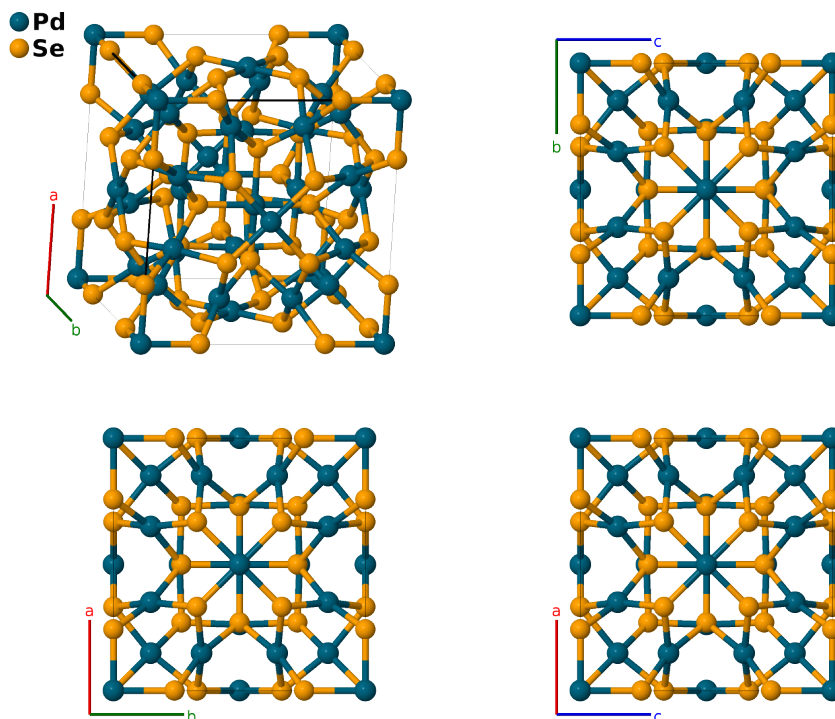


Palladseite ($\text{Pd}_{17}\text{Se}_{15}$) Structure: A17B15_cP64_221_acfm_eij-001

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<https://aflow.org/p/RWLL>

https://aflow.org/p/A17B15_cP64_221_acfm_eij-001



Prototype	$\text{Pd}_{17}\text{Se}_{15}$
AFLOW prototype label	A17B15_cP64_221_acfm_eij-001
Mineral name	palladseite
ICSD	23907
Pearson symbol	cP64
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A17B15_cP64_221_acfm_eij-001 --params=a, x3, x4, y5, y6, x7, z7</code>

Other compounds with this structure

$\text{Rh}_{17}\text{S}_{15}$

- (Geller, 1962) determined that $\text{Pd}_{17}\text{Se}_{15}$ could be in space group $Pm\bar{3}m$ #221 (this structure), $P\bar{4}3m$ #215, or $P432$ #207, and finds that $Pm\bar{3}m$ gives the best fit to single-crystal X-ray diffraction pattern, even though the fit of the parameters for the all of the Wyckoff sites could not be converged. We therefore present all three structure possibilities.

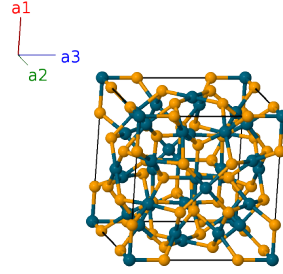
- We shifted the coordinates of (Geller, 1962) to move the Pd-I atom from the center of the cubic cell, Wyckoff position (1b), to the origin, Wyckoff position (1a).

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)	Pd I
$\mathbf{B}_2 =$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Pd II
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Pd II
$\mathbf{B}_4 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c)	Pd II
$\mathbf{B}_5 =$	$x_3 \mathbf{a}_1$	$=$	$ax_3 \hat{\mathbf{x}}$	(6e)	Se I
$\mathbf{B}_6 =$	$-x_3 \mathbf{a}_1$	$=$	$-ax_3 \hat{\mathbf{x}}$	(6e)	Se I
$\mathbf{B}_7 =$	$x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{y}}$	(6e)	Se I
$\mathbf{B}_8 =$	$-x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{y}}$	(6e)	Se I
$\mathbf{B}_9 =$	$x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{z}}$	(6e)	Se I
$\mathbf{B}_{10} =$	$-x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{z}}$	(6e)	Se I
$\mathbf{B}_{11} =$	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{12} =$	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{13} =$	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{14} =$	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{15} =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{16} =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(6f)	Pd III
$\mathbf{B}_{17} =$	$y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{18} =$	$-y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{19} =$	$y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{20} =$	$-y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{21} =$	$y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{22} =$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{23} =$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{24} =$	$-y_5 \mathbf{a}_1 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B}_{25} =$	$y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{26} =$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$-ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{27} =$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}}$	(12i)	Se II

$\mathbf{B}_{28} =$	$-y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}}$	(12i)	Se II
$\mathbf{B}_{29} =$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{30} =$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{31} =$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{32} =$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{33} =$	$y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{34} =$	$y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{35} =$	$-y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{36} =$	$-y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{37} =$	$y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{38} =$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{39} =$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{40} =$	$-y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12j)	Se III
$\mathbf{B}_{41} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{42} =$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{43} =$	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{44} =$	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{45} =$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{46} =$	$z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{47} =$	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{48} =$	$-z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{49} =$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{50} =$	$-x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{51} =$	$x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{52} =$	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{53} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{54} =$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{55} =$	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{56} =$	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{57} =$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{58} =$	$-x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{59} =$	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{60} =$	$x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{61} =$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{62} =$	$z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{63} =$	$-z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV
$\mathbf{B}_{64} =$	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24m)	Pd IV

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