

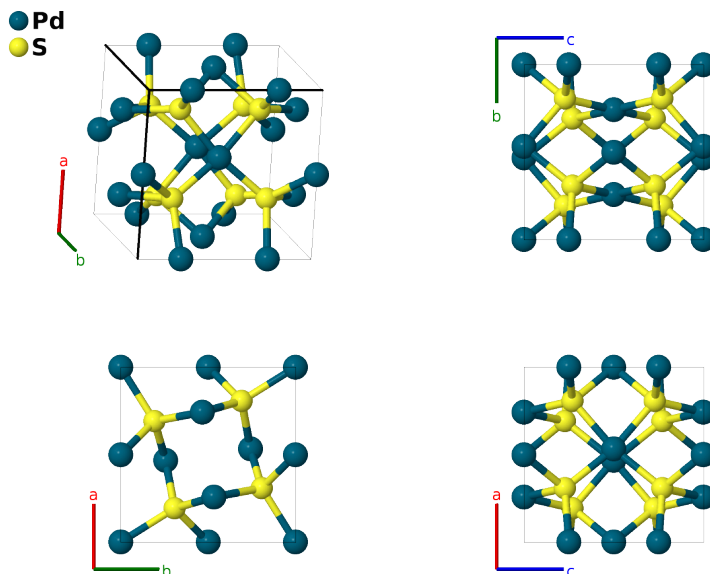
Vysotskite (PdS, *B34*) Structure: AB_tP16_84_cej_k-001

This structure originally had the label AB_tP16_84_cej_k. Calls to that address will be redirected here.

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

https://aflow.org/p/AB_tP16_84_cej_k-001



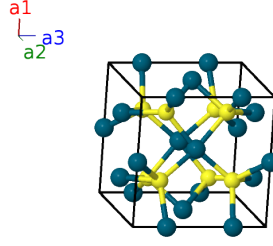
Prototype	PdS
AFLOW prototype label	AB_tP16_84_cej_k-001
<i>Strukturbericht</i> designation	<i>B34</i>
Mineral name	vysotskite
ICSD	22429
Pearson symbol	tP16
Space group number	84
Space group symbol	$P4_2/m$
AFLOW prototype command	<code>aflow --proto=AB_tP16_84_cej_k-001 --params=a, c/a, x3, y3, x4, y4, z4</code>

Other compounds with this structure

PdSe, (Pt, Pd, Ni)S (braggite)

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	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(2c)	Pd I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Pd I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2e)	Pd II
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2e)	Pd II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(4j)	Pd III
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(4j)	Pd III
\mathbf{B}_7	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4j)	Pd III
\mathbf{B}_8	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4j)	Pd III
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{11}	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{12}	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{13}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{14}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{15}	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	S I
\mathbf{B}_{16}	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	S I

References

- [1] N. E. Brese, P. J. Squattrito, and J. A. Ibers, *Reinvestigation of the structure of PdS*, Acta Crystallogr. Sect. C **41**, 1829–1830 (1985).