

Ta₂P Structure:

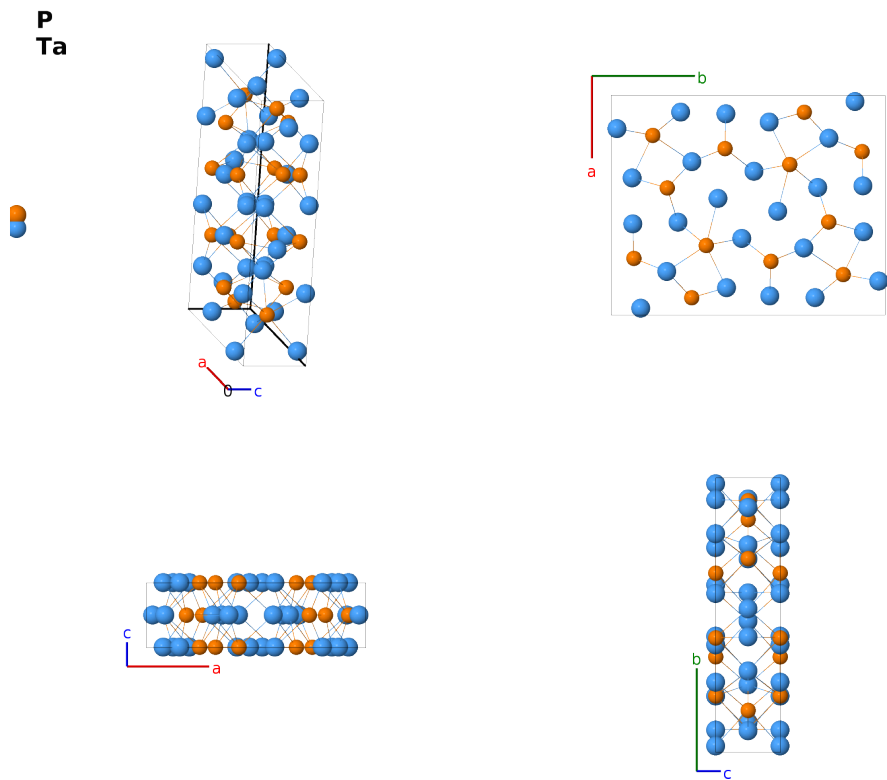
AB2_oP36_58_3g_6g-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/9JBK>

https://aflow.org/prototype-encyclopedia/AB2_oP36_58_3g_6g-001



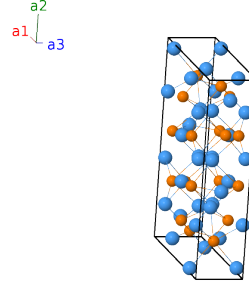
Prototype	PTa ₂
AFLOW prototype label	AB2_oP36_58_3g_6g-001
ICSD	87507
CCDC	1647291
Pearson symbol	oP36
Space group number	58
Space group symbol	<i>Pnmm</i>
AFLOW prototype command	<code>aflow --proto=AB2_oP36_58_3g_6g-001 --params=a,b/a,c/a,x₁,y₁,x₂,y₂,x₃,y₃,x₄,y₄,x₅,y₅,x₆,y₆,x₇,y₇,x₈,y₈,x₉,y₉</code>

Other compounds with this structure

Ta₂As, Ta₂S, Zr₂Se

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}}$	(4g)	P I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}}$	(4g)	P I
$\mathbf{B}_3$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g)	P II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g)	P II
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g)	P III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g)	P III
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P III
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	P III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	Ta I
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	Ta I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	Ta II
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	Ta II
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$	(4g)	Ta III
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$	(4g)	Ta III

$$\begin{aligned}
\mathbf{B}_{23} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta III} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta III} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} & (4g) & \text{Ta IV} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} & (4g) & \text{Ta IV} \\
\mathbf{B}_{27} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta IV} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta IV} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} & (4g) & \text{Ta V} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} & (4g) & \text{Ta V} \\
\mathbf{B}_{31} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta V} \\
\mathbf{B}_{32} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta V} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} & (4g) & \text{Ta VI} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} & (4g) & \text{Ta VI} \\
\mathbf{B}_{35} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta VI} \\
\mathbf{B}_{36} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4g) & \text{Ta VI}
\end{aligned}$$

References

- [1] T. E. Weirich, S. Hovmöller, H. Kalpen, R. Ramlau, and A. Simon, *Electron Diffraction Versus X-ray Diffraction – a Comparative Study of the Ta₂P Structure*, Crystallogr. Rep. **43**, 956–967 (1998). Translated from Kristallografiya, 43 1015 (1998).

Found in

- [1] T. E. Weirich, *The crystal structure of Zr₂Se reinvestigated by electron crystallography and X-ray powder diffraction*, Crystallogr. Rep. **49**, 379–389 (2004), doi:10.1134/1.1756636. Translated from Kristallografiya, 49, 455 (2004).

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