Ta_2P Structure: AB2_oP36_58_3g_6g-001

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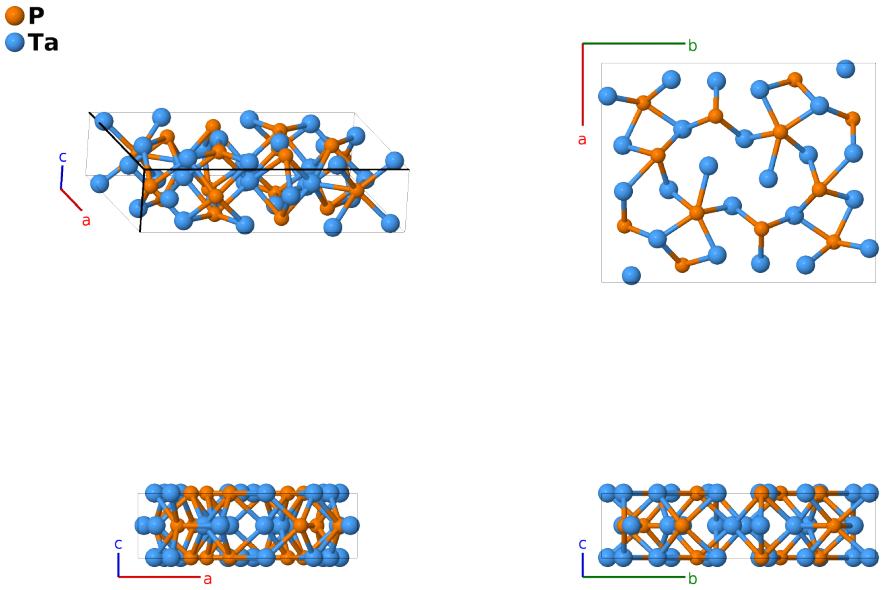
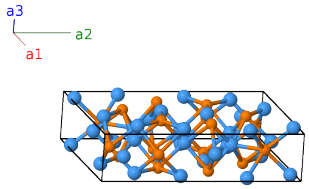


Prototype	PTa_2
AFLOW prototype label	AB2_oP36_58_3g_6g-001
ICSD	87507
Pearson symbol	oP36
Space group number	58
Space group symbol	*Pnnm*
AFLOW prototype command	`aflow --proto=AB2_oP36_58_3g_6g-001 --params=`$a, b/a, c/a, x_1, y_1, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9$

Other compounds with this structure
Ta_2As, Ta_2S, Zr_2Se

Simple Orthorhombic primitive vectors

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



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
$\mathbf{B_3}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	P I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_7}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B_8}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	P III
$\mathbf{B_{12}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{15}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Ta I
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{19}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Ta II
$\mathbf{B_{20}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{23}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Ta VI

References

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