

# Ti<sub>3</sub>P Structure:

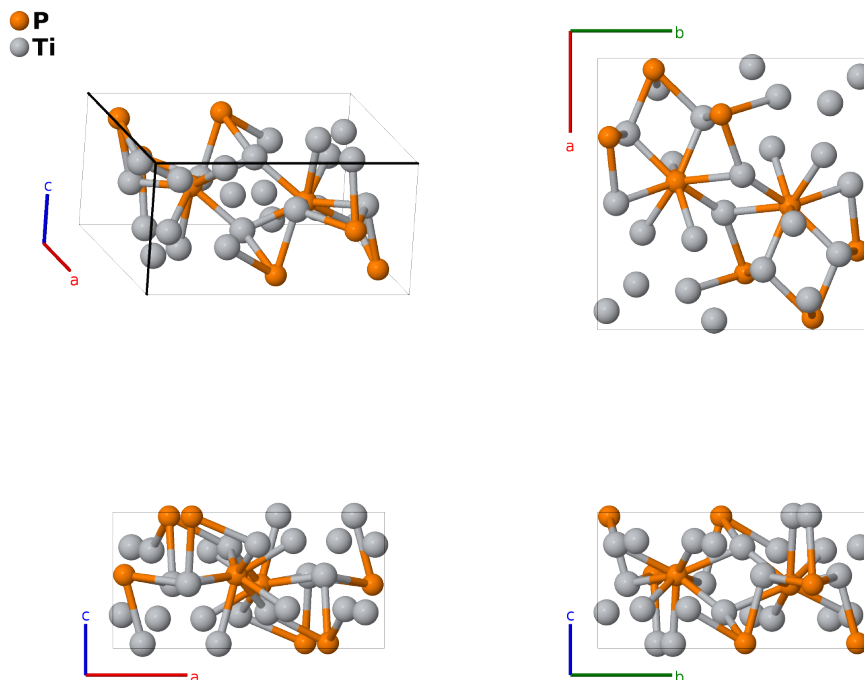
## AB3\_tP32\_86\_g\_3g-001

This structure originally had the label AB3\_tP32\_86\_g\_3g. Calls to that address will be redirected here.

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<https://aflow.org/p/ENA6>

[https://aflow.org/p/AB3\\_tP32\\_86\\_g\\_3g-001](https://aflow.org/p/AB3_tP32_86_g_3g-001)



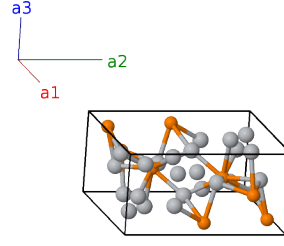
Prototype	PTi <sub>3</sub>
AFLOW prototype label	AB3_tP32_86_g_3g-001
ICSD	648227
Pearson symbol	tP32
Space group number	86
Space group symbol	$P4_2/n$
AFLOW prototype command	<code>aflow --proto=AB3_tP32_86_g_3g-001 --params=a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></code>

### Other compounds with this structure

$\alpha$ -Ta<sub>3</sub>P, Ti<sub>3</sub>Si, Zr<sub>3</sub>P

### Simple Tetragonal primitive vectors

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




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## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_4$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - a y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_7$	$= y_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_8$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{11}$	$= -y_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{12}$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{15}$	$= y_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_2 \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{16}$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{19}$	$= -y_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{20}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{22}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8g)	Ti II
$\mathbf{B}_{23}$	$= y_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Ti II

$$\begin{aligned}
\mathbf{B}_{24} &= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\quad \text{Ti II} \\
\mathbf{B}_{25} &= 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}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{26} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{27} &= -y_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{28} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{29} &= -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}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{30} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{31} &= y_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= ay_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\quad \text{Ti III} \\
\mathbf{B}_{32} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\quad \text{Ti III}
\end{aligned}$$

## References

- [1] V. N. Eremenko and V. E. Listovnichii, *State diagram of the Ti-P system*, Dopov. Akad. Nauk Ukr. RSR pp. 1176–1179 (1965).

## Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.