

NaTi₂(PS₄)₃ Structure:

A13B6C24D4_hP188_184_2a4d_2d_8d_bd-001

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<https://afLOW.org/p/7PRY>

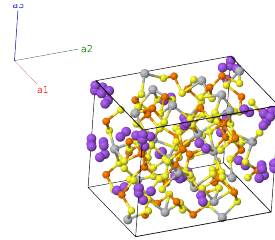
https://afLOW.org/p/A13B6C24D4_hP188_184_2a4d_2d_8d_bd-001

Prototype	NaP ₃ S ₁₂ Ti ₂
AFLOW prototype label	A13B6C24D4_hP188_184_2a4d_2d_8d_bd-001
ICSD	81997
Pearson symbol	hP188
Space group number	184
Space group symbol	<i>P6cc</i>
AFLOW prototype command	<pre>afLOW --proto=A13B6C24D4_hP188_184_2a4d_2d_8d_bd-001 --params=a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18</pre>

- None of the sodium sites is even half filled. The occupations are: Na-I 23%, Na-II 35%, Na-III 25%, Na-IV 10%, and Na-V 9%. The phosphorous, sulfur, and titanium sites are all filled.
- Space group *P6cc* #184 allows an arbitrary origin for the *z*-axis. We choose $z_3 = 0$ for the Ti-I site.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Na I
\mathbf{B}_2	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Na I
\mathbf{B}_3	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	Na II
\mathbf{B}_4	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Na II
\mathbf{B}_5	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Ti I
\mathbf{B}_6	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Ti I
\mathbf{B}_7	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Ti I

$$\mathbf{B}_{186} = y_{18} \mathbf{a}_1 + x_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Ti II}$$

$$\mathbf{B}_{187} = \begin{pmatrix} (x_{18} - y_{18}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 + \\ (z_{18} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \frac{1}{2}a(x_{18} - 2y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Ti II}$$

$$\mathbf{B}_{188} = \begin{pmatrix} -x_{18} \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 + \\ (z_{18} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -\frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Ti II}$$

References

- [1] X. Cieren, J. Angenault, J.-C. Couturier, S. Jaulmes, M. Quarton, and F. Robert, *NaTi₂(PS₄)₃: A New Thiophosphate with an Interlocked Structure*, J. Solid State Chem. **121**, 230–235 (1996), doi:10.1006/jssc.1996.0032.

- Na
- P
- S
- Ti

