

Fe₃PO₇ Structure: A3B7C_hR11_160_b_a2b_a-001

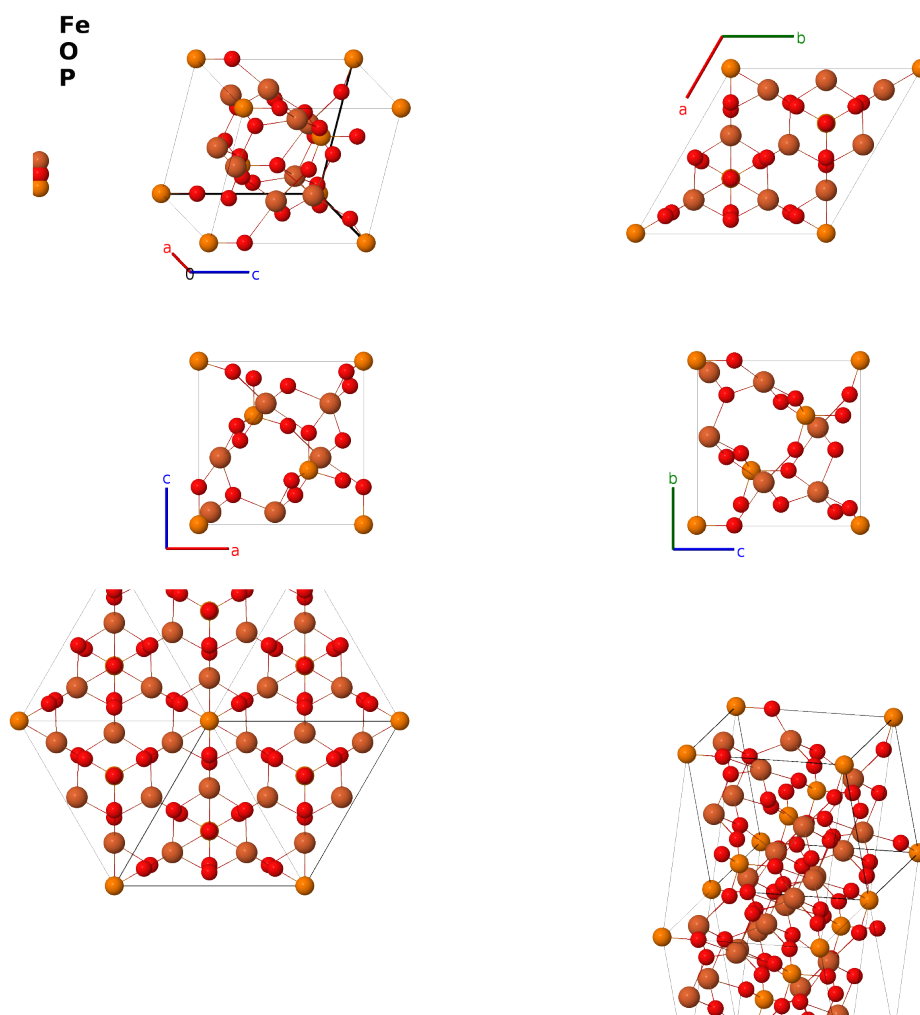
This structure previously used the label(s) **A3B7C_hR11_160_b_a2b_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/JN4A>

https://aflow.org/prototype-encyclopedia/A3B7C_hR11_160_b_a2b_a-001



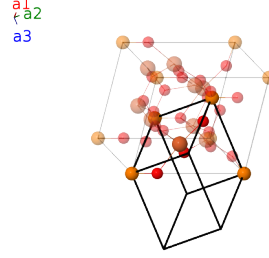
Prototype	Fe ₃ O ₇ P
AFLOW prototype label	A3B7C_hR11_160_b_a2b_a-001
ICSD	36207
CCDC	1607977
Pearson symbol	hR11

Space group number	160
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B7C_hR11_160_b_a2b_a-001</code> <code>--params=a, c/a, x₁, x₂, x₃, z₃, x₄, z₄, x₅, z₅</code>

- Space group $R\bar{3}m$ #160 allows an arbitrary definition of the zero of the z -axis. Here we select $z_1 = 0$, putting the phosphorous atom at the origin.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$c x_1 \hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$c x_2 \hat{\mathbf{z}}$	(1a)	P I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Fe I
$\mathbf{B}_4$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Fe I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(3b)	Fe I
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	O II
$\mathbf{B}_7$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	O II
$\mathbf{B}_8$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(3b)	O II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	O III
$\mathbf{B}_{10}$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	O III
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(3b)	O III

References

- [1] A. Modaressi, A. Courtois, R. Gerardin, B. Malaman, and C. Gleitzer, *Fe₃PO₇, Un cas de coordinence 5 du fer trivalent, etude structurale et magnetique*, J. Solid State Chem. **47**, 245–255 (1983), doi:10.1016/0022-4596(83)90016-6.

Found in

- [1] C. L. Sarkis, M. J. Tarne, J. R. Neilson, H. B. Cao, E. Coldren, M. P. Gelfand, and K. A. Ross, *Partial Antiferromagnetic Helical Order in Single Crystal Fe₃PO₄O₃*, Phys. Rev. B **101**, 184417 (2020), doi:10.1103/PhysRevB.101.184417.

First cited in

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