Fe_3PO_7 Structure: A3B7C_hR11_160_b_a2b_a-001

This structure originally had the label `A3B7C_hR11_160_b_a2b_a`. Calls to that address will be redirected here.

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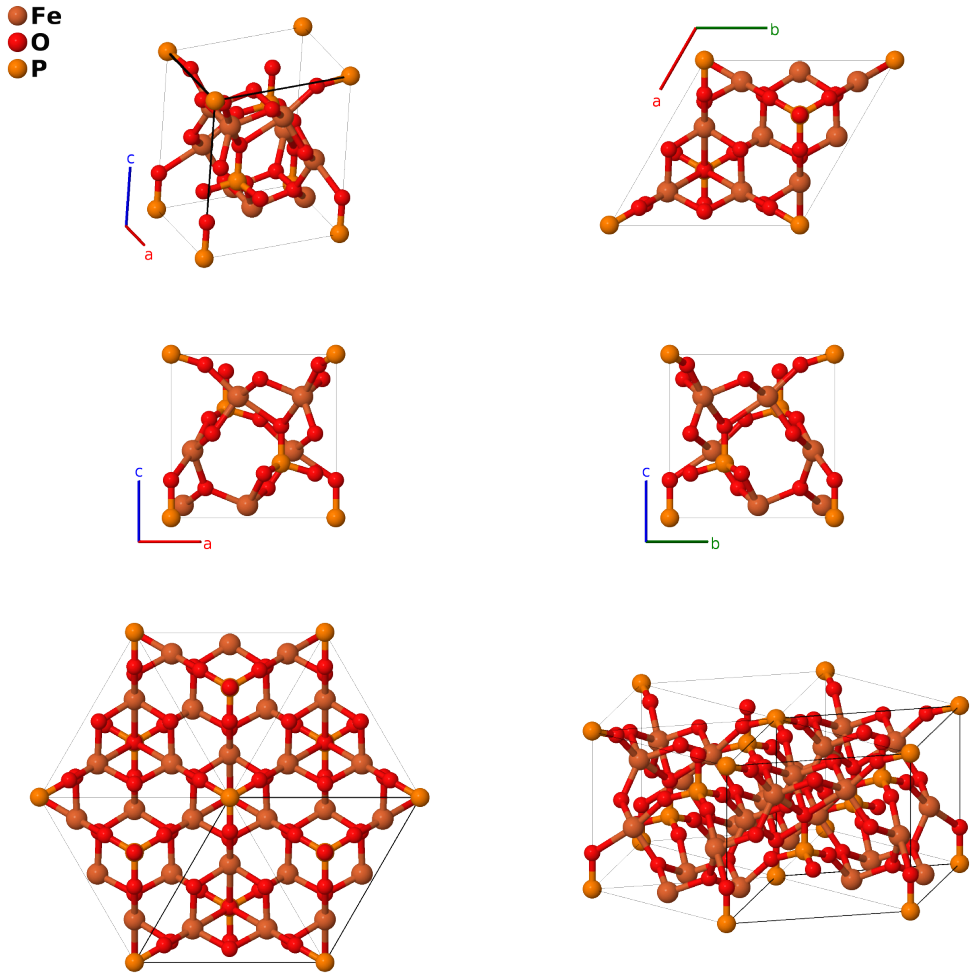
https://aflow.org/p/JN4A

https://aflow.org/p/A3B7C_hR11_160_b_a2b_a-001

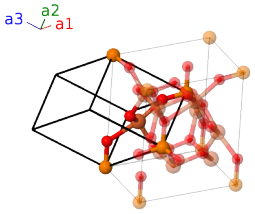


Prototype	Fe_3O_7P
AFLOW prototype label	A3B7C_hR11_160_b_a2b_a-001
ICSD	36207
Pearson symbol	hR11
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A3B7C_hR11_160_b_a2b_a-001 --params=`$a, c/a, x_1, x_2, x_3, z_3, x_4, z_4, x_5, z_5$

- Space group $R3m$ #160 allows an arbitary definition of the zero of the z-axis. Here we select $z_1 = 0$, putting the phosphorous atom at the origin.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	P I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_4 + z_4)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(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, *Fe_3PO_7, 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 $Fe_3PO_4O_3$*, Phys. Rev. B **101**, 184417 (2020), doi:10.1103/PhysRevB.101.184417.