$LaFe_4P_{12}$ Structure: A4BC12_cI34_204_c_a_g-001

This structure originally had the label `A4BC12_cI34_204_c_a_g`. Calls to that address will be redirected here.

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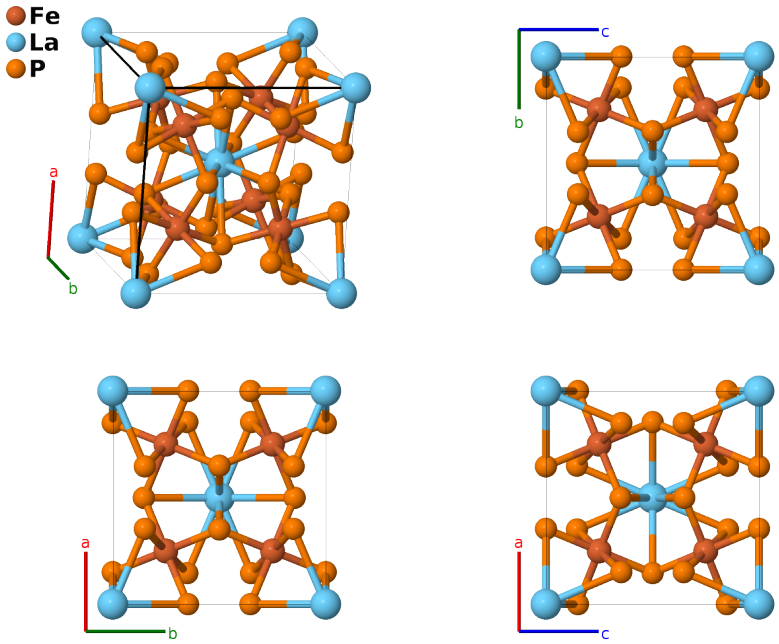
https://aflow.org/p/GXVQ

https://aflow.org/p/A4BC12_cI34_204_c_a_g-001



Prototype	$LaFe_4P_{12}$
AFLOW prototype label	A4BC12_cI34_204_c_a_g-001
ICSD	1286
Pearson symbol	cI34
Space group number	204
Space group symbol	$Im\overline{3}$
AFLOW prototype command	`aflow --proto=A4BC12_cI34_204_c_a_g-001 --params=`a, y_3, z_3

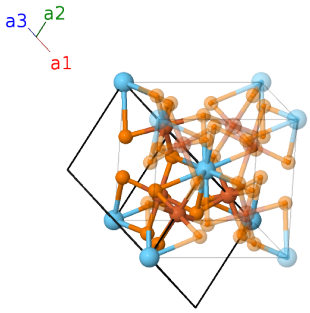
Other compounds with this structure

$CeFe_4P_{12}$, $EuFe_4P_{12}$, $NdFe_4P_{12}$, $PrFe_4P_{12}$, $SmFe_4P_{12}$, $CeRu_4P_{12}$, $EuRu_4P_{12}$, $LaRu_4P_{12}$, $NdRu_4P_{12}$, $PrRu_4P_{12}$, $SmRu_4P_{12}$, $CeOs_4P_{12}$, $LaOs_4P_{12}$, $NdOs_4P_{12}$, $PrOs_4P_{12}$, $SmOs_4P_{12}$, $CeFe_4Sb_{12}$, $LaFe_4Sb_{12}$, $PrFe_4Sb_{12}$, $SmFe_4Sb_{12}$, $CeRu_4Sb_{12}$, $EuRu_4Sb_{12}$, $LaRu_4Sb_{12}$, $NdRu_4Sb_{12}$, $PrRu_4Sb_{12}$, $SmRu_4Sb_{12}$, $CeOs_4Sb_{12}$, $EuOs_4Sb_{12}$, $LaOs_4Sb_{12}$, $NdOs_4Sb_{12}$, $PrOs_4Sb_{12}$, $SmOs_4Sb_{12}$

- This is a filled skutterudite ($CoAs_3$, $D0_2$) structure. Removing the rare-earth atom from the (2a) position leaves the skutterudite structure.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	La I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_6}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_7}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_8}$	=	$(y_3 - z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_9}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_{10}}$	=	$y_3\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_{13}}$	=	$-y_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24g)	P I
$\mathbf{B_{14}}$	=	$z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(24g)	P I
$\mathbf{B_{15}}$	=	$z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}}$	(24g)	P I
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + (y_3 - z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(24g)	P I
$\mathbf{B_{17}}$	=	$-z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - (y_3 + z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}}$	(24g)	P I

References

[1] W. Jeitschko and D. Braun, *$LaFe_4P_{12}$ with filled $CoAs_3$-type structure and isotypic lanthanoid-transition metal polyphosphides*, Acta Crystallogr. Sect. B **33**, 3401–3406 (1977), doi:10.1107/S056774087701108X.

Found in

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[2] D. J. Braun and W. Jeitschko, *Preparation and structural investigations of antimonides with the $LaFe_4P_{12}$ structure*, J. Less-Common Met. **72**, 147–156 (1980), doi:10.1016/0022-5088(80)90260-X.