

LaFe₄P₁₂ Structure:

A4BC12_cI34_204_c_a_g-001

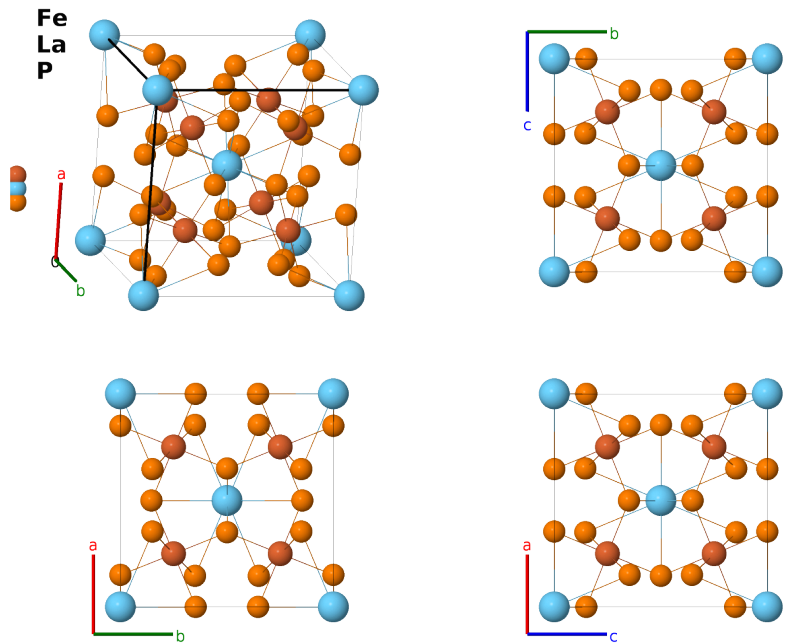
This structure previously used the label(s) **A4BC12_cI34_204_c_a_g**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A4BC12_cI34_204_c_a_g-001



Prototype	LaFe ₄ P ₁₂
AFLOW prototype label	A4BC12_cI34_204_c_a_g-001
ICSD	1286
CCDC	1591437
Pearson symbol	cI34
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	<code>aflow --proto=A4BC12_cI34_204_c_a_g-001 --params=a, y₃, z₃</code>

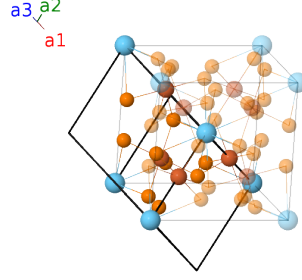
Other compounds with this structure

CeFe₄P₁₂, EuFe₄P₁₂, NdFe₄P₁₂, PrFe₄P₁₂, SmFe₄P₁₂, CeRu₄P₁₂, EuRu₄P₁₂, LaRu₄P₁₂, NdRu₄P₁₂, PrRu₄P₁₂, SmRu₄P₁₂, CeOs₄P₁₂, LaOs₄P₁₂, NdOs₄P₁₂, PrOs₄P₁₂, SmOs₄P₁₂, CeFe₄Sb₁₂, LaFe₄Sb₁₂, PrFe₄Sb₁₂, SmFe₄Sb₁₂, CeRu₄Sb₁₂, EuRu₄Sb₁₂, LaRu₄Sb₁₂, NdRu₄Sb₁₂, PrRu₄Sb₁₂, SmRu₄Sb₁₂, CeOs₄Sb₁₂, EuOs₄Sb₁₂, LaOs₄Sb₁₂, NdOs₄Sb₁₂, PrOs₄Sb₁₂, SmOs₄Sb₁₂

- 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

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



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, *LaFe₄P₁₂ with filled CoAs₃-type structure and isotypic lanthanoid-transition metal polyphosphides*, Acta Crystallogr. Sect. B **33**, 3401–3406 (1977), doi:10.1107/S056774087701108X.

Found in

- [1] C. R. Rotundu, *Novel Heavy Fermion Behavior in Praseodymium-based Materials: Experimental Study of PrOs₄Sb₁₂* (2007). Ph. D. Thesis, University of Florida.
- [2] D. J. Braun and W. Jeitschko, *Preparation and structural investigations of antimonides with the LaFe₄P₁₂ structure*, J. Less-Common Met. **72**, 147–156 (1980), doi:10.1016/0022-5088(80)90260-X.

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