

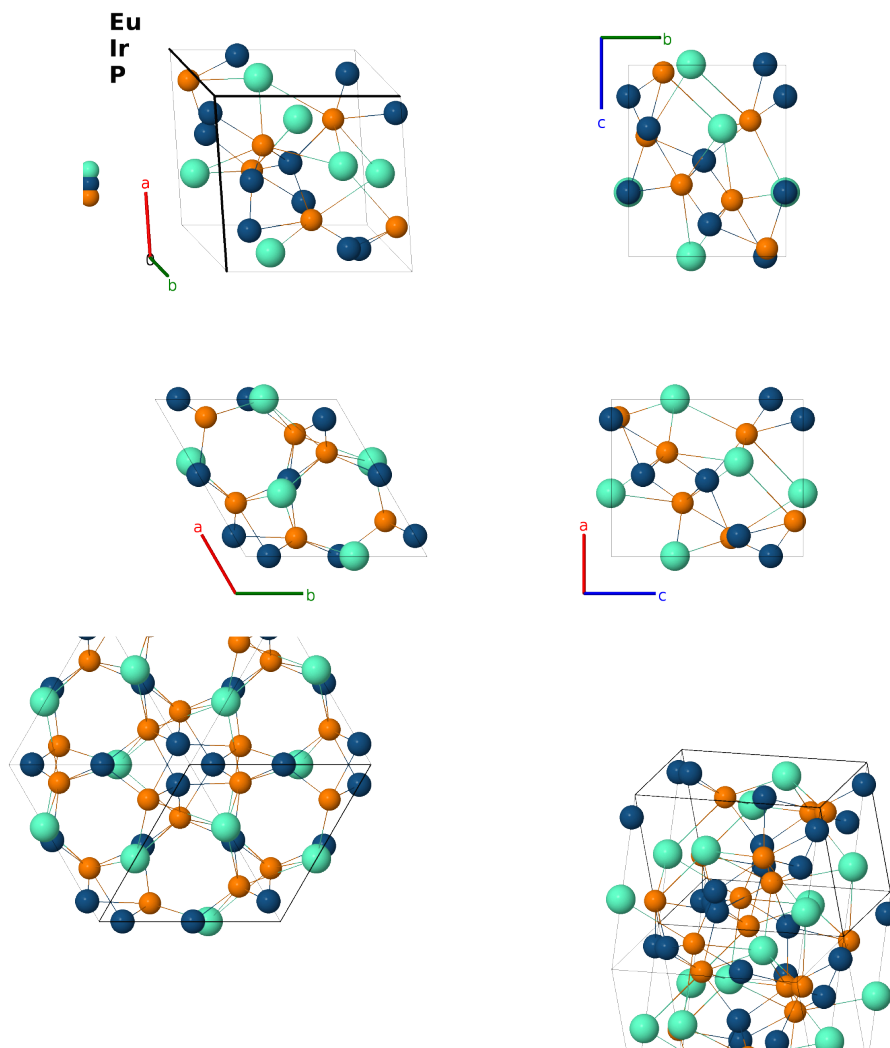
EuIr₂P₂ Structure: AB2C2_hP15_154_a_ab_c-001

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<https://aflow.org/prototype-encyclopedia/3CT8>

https://aflow.org/prototype-encyclopedia/AB2C2_hP15_154_a_ab_c-001



Prototype	EuIr ₂ P ₂
AFLOW prototype label	AB2C2_hP15_154_a_ab_c-001
ICSD	73530
CCDC	1634316
Pearson symbol	hP15

Space group number 154
Space group symbol $P3_221$
AFLOW prototype command `aflow --proto=AB2C2_hP15_154_a_ab_c-001`
--params= $a, c/a, x_1, x_2, x_3, x_4, y_4, z_4$

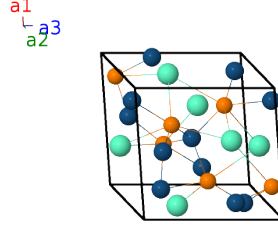
Other compounds with this structure

CaIr₂P₂, SrIr₂P₂

- We shifted the origin used by (Lux, 1993) so that the europium atoms are on a (3a) Wyckoff position.

Trigonal (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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Eu I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Eu I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}}$	(3a)	Eu I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Ir I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Ir I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(3a)	Ir I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3b)	Ir II
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3b)	Ir II
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3b)	Ir II
$\mathbf{B}_{10}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B}_{12}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B}_{13}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B}_{14}$	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}}$	(6c)	P I

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- [1] C. Lux, A. Mewis, S. Junk, A. Gruetz, and G. Michels, *Kristallstrukturen und Eigenschaften neuer ternärer iridiumphosphide*, J. Alloys Compd. **200**, 135–139 (1993), doi:10.1016/0925-8388(93)90483-4.

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