$EuIr_2P_2$ Structure: AB2C2_hP15_154_a_ab_c-001

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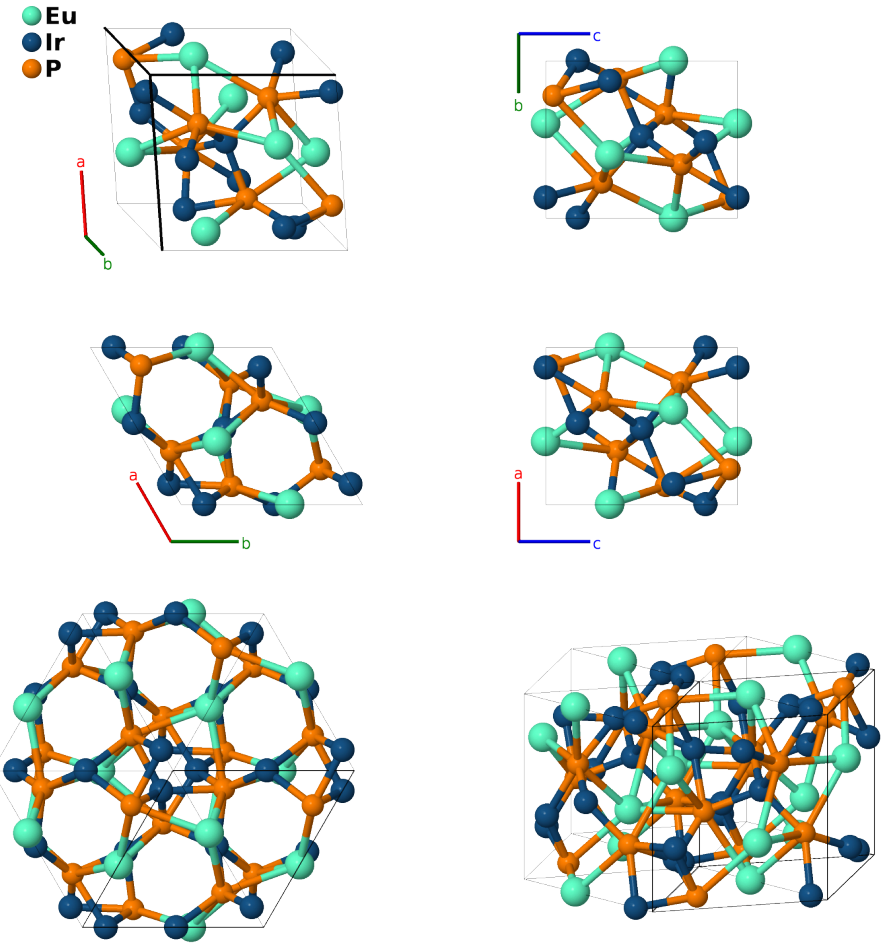
https://aflow.org/p/AB2C2_hP15_154_a_ab_c-001



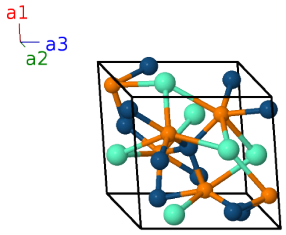
Prototype	$EuIr_2P_2$
AFLOW prototype label	AB2C2_hP15_154_a_ab_c-001
ICSD	73530
Pearson symbol	hP15
Space group number	154
Space group symbol	$P3_221$
AFLOW prototype command	`aflow --proto=AB2C2_hP15_154_a_ab_c-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, y_4, z_4$

Other compounds with this structure
$CaIr_2P_2$, $SrIr_2P_2$

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

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_4 + 2)\,\hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B_{12}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_4 - 2)\,\hat{\mathbf{z}}$	(6c)	P I

References

[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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