Pyrochlore Iridate ($Eu_2Ir_2O_7$, $E8_1$) Structure: A2B2C7_cF88_227_c_d_af-001

This structure originally had the label `A2B2C7_cF88_227_c_d_af`. Calls to that address will be redirected here.

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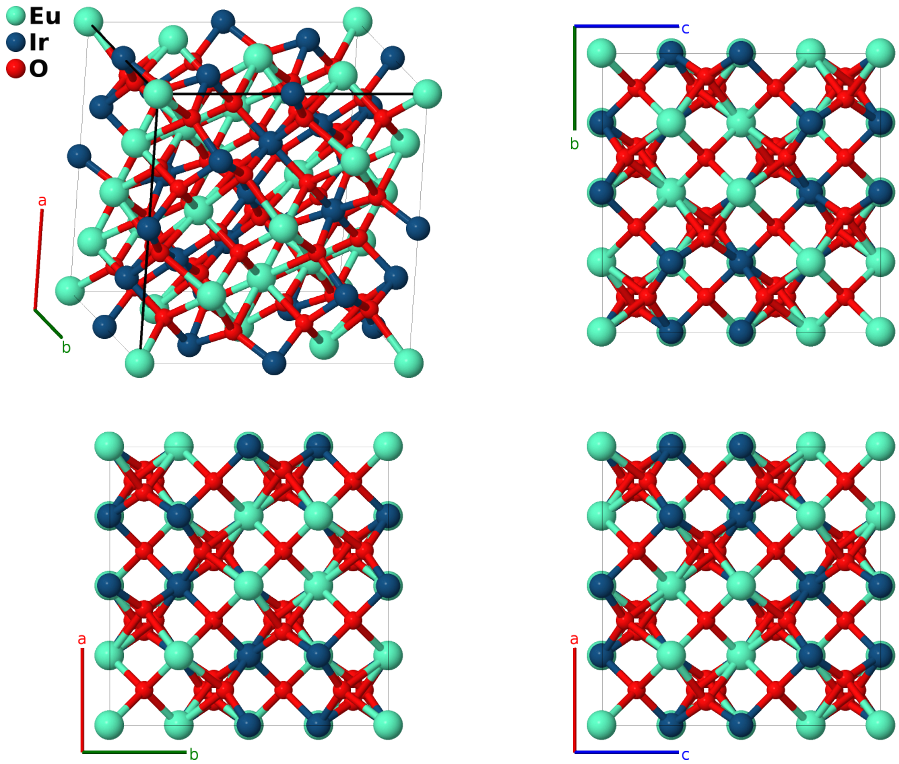
https://aflow.org/p/0R9R

https://aflow.org/p/A2B2C7_cF88_227_c_d_af-001



Prototype	$Eu_2Ir_2O_7$
AFLOW prototype label	A2B2C7_cF88_227_c_d_af-001
***Strukturbericht* designation**	$E8_1$
Mineral name	pyrochlore iridate
ICSD	135031
Pearson symbol	cF88
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B2C7_cF88_227_c_d_af-001` `--params=`a, x_4

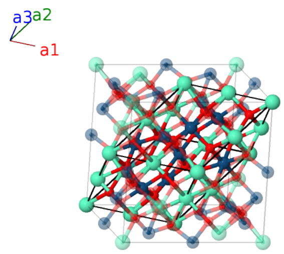
Other compounds with this structure

$FNb_2(Nb, Ca)_2O_6$ ("synthetic" pyrochlore), $(Nb, Ta, Ti)_2(Ca, Ce, Na, K)_2(F, O)_7$ ("natural" pyrhochlore), $(F, O, OH)(Nb, Fe)_2(Ca, Ce, Na, K)_2O_6$ (Koppit), $(F, OH)Sb_2(Ca, Mn, Na)_2O_6$ (Roméite), $(OH)Sb_2(Ca, Fe, Na)_2O_6$ (Scheebergite), $(Sb, Ti)_2(Ca, Fe, Mn, Na)_2(O, OH)_6$ (Lewisite), $(OH, F)(Nb, Ta, Ti)_2(Ca, Fe, Na)_2O_6$ (Pyrrhite), $(OH, F)(Nb, Ta)_2(Ca, Fe, Na)_2O_6$ (Mikrolith), $Sb_2Pb_2O_7$ (Bindheimite), $(H_2O)_{0.875}(Al_{0.8125}Mg_{0.1875})_2Na_{0.375}[F_{0.65}(OH)_{0.35}]_6$ (Ralstonite), Sb_3O_6OH, $BiTa_2O_6F$, $Sn_2Nb_2O_7$, $Sn_2Nd_2O_7$, $Sn_2Ta_2O_7$, $Ca_2Nb_2O_7$, $Ca_2Ru_2O_7$, Dy_2GaSbO_7, $In_2Ge_2O_7$, Pr_3IrO_7, $Y_2Mn_2O_7$, $Yb_2Ir_2O_7$

- (Herrmann, 1943) uses *Strukturbericht* $E8_1$ to describe the cubic pyrochlore structures. These have the general formula $R_2Q_2X_7$, where the X atoms or radicals occupy the (4a) and (48f) sites, and the R and Q atoms occupy the (16c) and(16d) sites. In many cases the sites are only partially filled and/or have mixed chemistry. We use $Eu_2Ir_2O_7$ as our prototype because it represents a fully filled system.
- We take our data from (Sagayama, 2013), but the ICSD entry is from the later work of (Nenoff, 2021).

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_2}$	=	$\frac{7}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	O I
$\mathbf{B_3}$	=	0	=	0	(16c)	Eu I
$\mathbf{B_4}$	=	$\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Eu I
$\mathbf{B_5}$	=	$\frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Eu I
$\mathbf{B_6}$	=	$\frac{1}{2}\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Eu I
$\mathbf{B_7}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Ir I
$\mathbf{B_8}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Ir I
$\mathbf{B_9}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Ir I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Ir I
$\mathbf{B_{11}}$	=	$-\left(x_4 - \frac{1}{4}\right)\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{4}\right)\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	O II
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(48f)	O II
$\mathbf{B_{16}}$	=	$-\left(x_4 - \frac{1}{4}\right)\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(48f)	O II

$\mathbf{B_{17}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + a\left(x_4+\frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	O II
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} - a x_4\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	O II
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	O II
$\mathbf{B_{20}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-a x_4\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	O II
$\mathbf{B_{21}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} - a x_4\,\mathbf{\hat{z}}$	(48f)	O II
$\mathbf{B_{22}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + a\left(x_4+\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(48f)	O II

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