Eu_3O_4 Structure: A3B4_oP28_62_3c_4c-003

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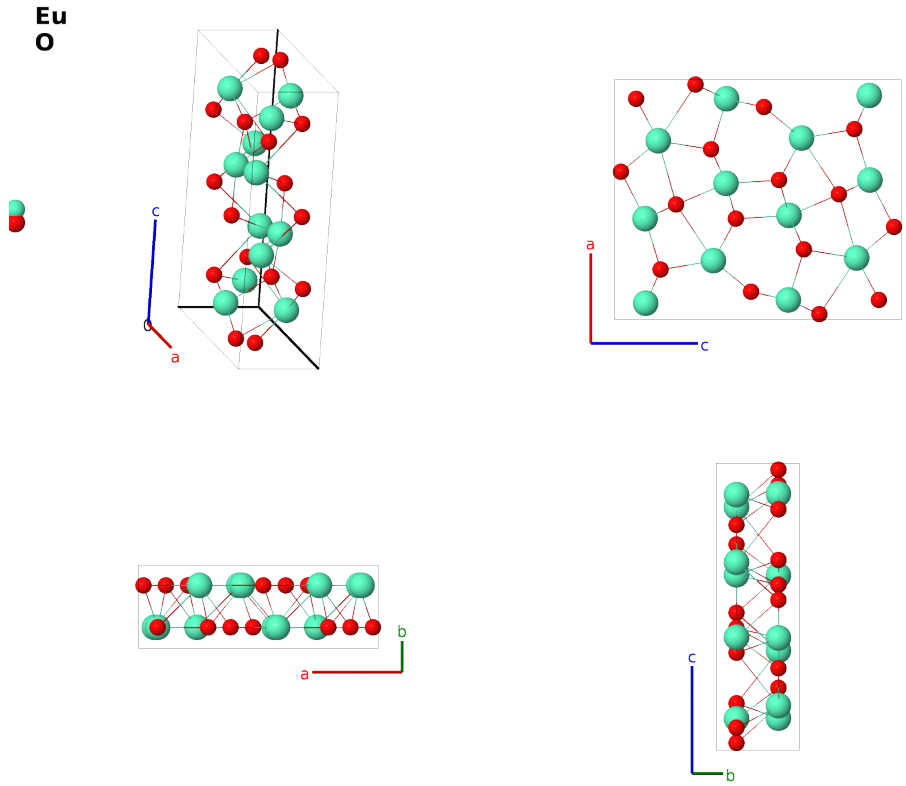
https://aflow.org/prototype-encyclopedia/6KWS

https://aflow.org/prototype-encyclopedia/A3B4_oP28_62_3c_4c-003



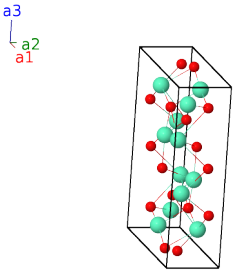
Prototype	Eu_3O_4
AFLOW prototype label	A3B4_oP28_62_3c_4c-003
ICSD	631473
CCDC	1754473
Pearson symbol	oP28
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A3B4_oP28_62_3c_4c-003 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7$

Other compounds with this structure
Mn_3O_4, Yb_3O_4, Yb_3Se_4

- This is the binary form of the ternary Bi_2PbS_4 and the quaternary $FeSbBiS_4$ structures. We chose it as the prototype as it is the earliest entry for this class in the ICSD.
- (Rau, 2007) put this structure in the *Pnam* setting of space group #62, but the ICSD gives the entry in the standard *Pnma* setting.
- Orthorhombic Ni_4B_3, Rh_4P_3, and Eu_3O_4 have the same AFLOW prototype label, A3B4_oP28_62_3c_4c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Eu I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Eu I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Eu II
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Eu II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Eu III
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	Eu III
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Eu III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	O I

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\begin{array}{rcccccc}
\mathbf{B_{16}} & = & \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O I} \\
\mathbf{B_{17}} & = & x_5\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & ax_5\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} & \text{(4c)} & \text{O II} \\
\mathbf{B_{18}} & = & -\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O II} \\
\mathbf{B_{19}} & = & -x_5\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_5\,\mathbf{a}_3 & = & -ax_5\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} & \text{(4c)} & \text{O II} \\
\mathbf{B_{20}} & = & \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O II} \\
\mathbf{B_{21}} & = & x_6\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_6\,\mathbf{a}_3 & = & ax_6\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} & \text{(4c)} & \text{O III} \\
\mathbf{B_{22}} & = & -\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O III} \\
\mathbf{B_{23}} & = & -x_6\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_6\,\mathbf{a}_3 & = & -ax_6\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}} & \text{(4c)} & \text{O III} \\
\mathbf{B_{24}} & = & \left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O III} \\
\mathbf{B_{25}} & = & x_7\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & ax_7\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(4c)} & \text{O IV} \\
\mathbf{B_{26}} & = & -\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O IV} \\
\mathbf{B_{27}} & = & -x_7\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_7\,\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} & \text{(4c)} & \text{O IV} \\
\mathbf{B_{28}} & = & \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4c)} & \text{O IV}
\end{array}
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References

[1] K. S. Vorres, ed., *R. C. Rau, X-ray crystallographic studies of europium oxides and hydroxides*, vol. II (Gordon and Breach, New York, London, 1964).

Found in

[1] ICSD, *Eu_3O_4, Inorganic Crystal Structure Database*. ID 631473.

First cited in

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