Er_2Co_7 Structure: A7B2_hR18_166_a2cdh_2c-001

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https://aflow.org/p/VGKE

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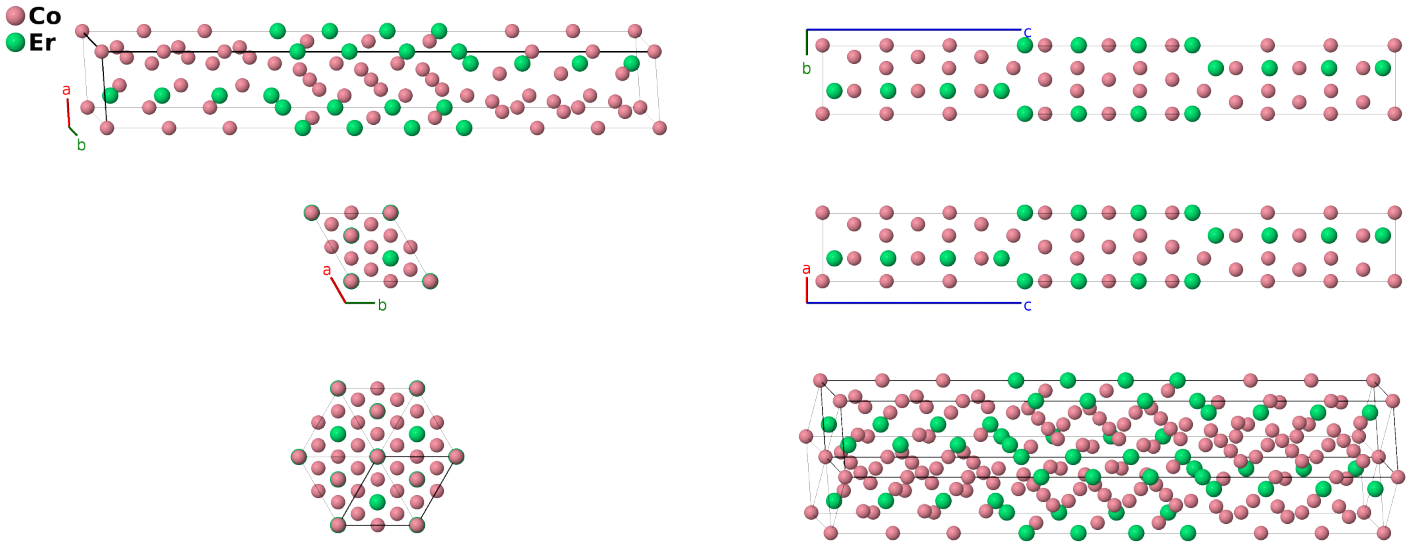


Prototype	Co_7Er_2
AFLOW prototype label	A7B2_hR18_166_a2cdh_2c-001
ICSD	102366
Pearson symbol	hR18
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A7B2_hR18_166_a2cdh_2c-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, x_7, z_7$

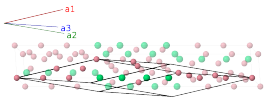
Other compounds with this structure

Dy_2Co_7, Er_2Ni_7, Gd_2Co_7, Gd_2Ni_7, Ho_2Co_7, La_2Ni_7, Lu_2Co_7, Tb_2Co_7, Th_2Fe_7, Th_2Ni_7, Tm_2Co_7, Y_2Co_7, Y_2Ni_7

- The ICSD lists Gd_2Co_7 as the prototype, but (Ostertag, 1967) only gives atomic coordinates for Er_2Co_7, so we will use that instead.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Co I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Co II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Co II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Co III
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Co III
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Er I
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Er I
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	Er II
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	Er II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Co IV
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Co IV
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Co IV
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V
$\mathbf{B_{14}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V
$\mathbf{B_{16}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V
$\mathbf{B_{17}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	Co V

References

[1] W. Ostertag, *The crystal structure of Er_2Co_7 and other rare earth-cobalt compounds R_2Co_7 (R = Gd, Tb, Dy, Ho, Tm, Lu, Y)*, J. Less-Common Met. **13**, 385–390 (1967), doi:10.1016/0022-5088(67)90032-X.