

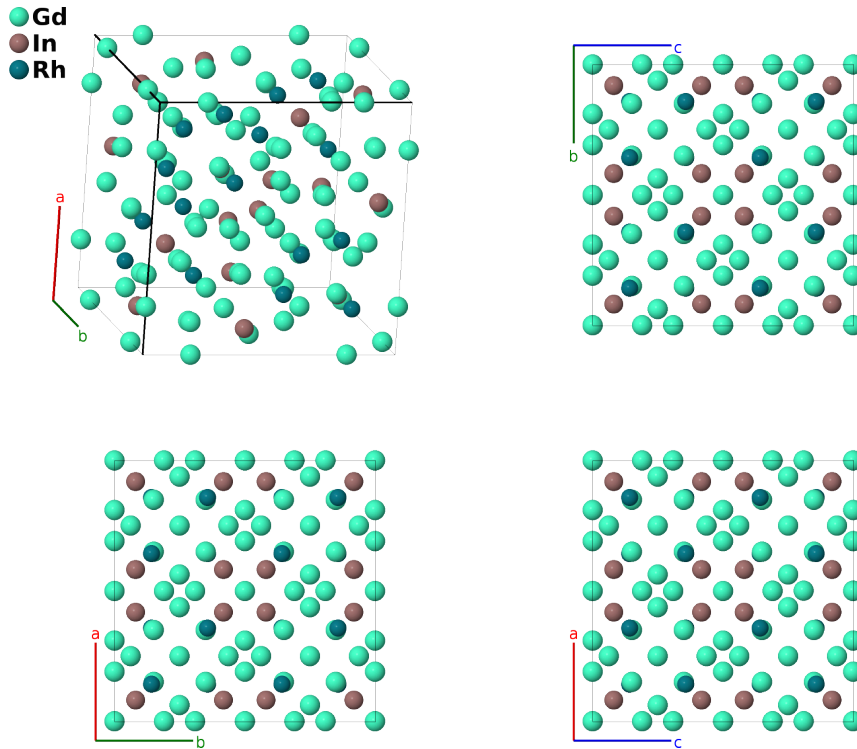
Gd₄RhIn Structure:

A4BC_cF96_216_efg_e_e-001

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<https://aflow.org/p/39CF>

https://aflow.org/p/A4BC_cF96_216_efg_e_e-001



Prototype	Gd ₄ InRh
AFLOW prototype label	A4BC_cF96_216_efg_e_e-001
ICSD	417515
Pearson symbol	cF96
Space group number	216
Space group symbol	$F\bar{4}3m$
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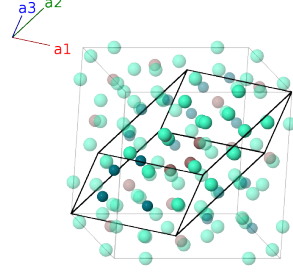
Other compounds with this structure

Ca₄AgMg, Ca₄AuMg, Ca₄PdMg, Ce₄RuMg, Dy₄CoCd, Dy₄CoMg, Dy₄PdAl, Dy₄PdMg, Dy₄PtAl, Dy₄PtMg, Dy₄RhCd, Dy₄RhIn, Er₄CoMg, Er₄PdAl, Er₄PdMg, Er₄PtAl, Er₄PtMg, Er₄RhAl, Er₄RhIn, Eu₄AuMg, Eu₄PdMg, Eu₄PtMg, Gd₄CoMg, Gd₄PdAl, Gd₄PtAl, Gd₄RhAl, Gd₄RhIn, Ho₄CoCd, Ho₄CoMg, Ho₄PdAl, Ho₄PdMg, Ho₄PtAl, Ho₄PtMg, Ho₄RhAl, Ho₄RhCd, Ho₄RhIn, La₄CoMg, Lu₄PdAl, Lu₄PdMg, Lu₄PtAl, Lu₄PtMg, Lu₄RhIn, Nd₄CdIr, Nd₄CoMg, Pr₄CoMg, Sm₄CoMg, Sm₄PdAl, Sm₄PdMg, Sm₄PtAl, Tb₄CoCd, Tb₄CoMg, Tb₄PdAl, Tb₄PtAl, Tb₄PtMg, Tb₄RhAl, Tb₄RhCd, Tb₄RhIn, Tm₄CoMg, Tm₄PdAl, Tm₄PdMg, Tm₄PtAl, Tm₄PtMg, Tm₄RhIn, Y₄CoMg, Y₄PdAl, Y₄PtAl, Yb₄AgMg, Yb₄AuMg, Yb₄PdMg, Yb₄PtMg

- The ICSD gives Dy₄CoCd as the prototype for this structure, but even (Doğan, 2007), which defines that structure, designates Gd₄RhIn as the prototype, so we use that compound.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{x} + ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Gd I
\mathbf{B}_2	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - 3x_1 \mathbf{a}_3$	=	$-ax_1 \hat{x} - ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Gd I
\mathbf{B}_3	$x_1 \mathbf{a}_1 - 3x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$-ax_1 \hat{x} + ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Gd I
\mathbf{B}_4	$-3x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ax_1 \hat{x} - ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Gd I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{x} + ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	In I
\mathbf{B}_6	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - 3x_2 \mathbf{a}_3$	=	$-ax_2 \hat{x} - ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	In I
\mathbf{B}_7	$x_2 \mathbf{a}_1 - 3x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$-ax_2 \hat{x} + ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	In I
\mathbf{B}_8	$-3x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$ax_2 \hat{x} - ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	In I
\mathbf{B}_9	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Rh I
\mathbf{B}_{10}	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	=	$-ax_3 \hat{x} - ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Rh I
\mathbf{B}_{11}	$x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-ax_3 \hat{x} + ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Rh I
\mathbf{B}_{12}	$-3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Rh I
\mathbf{B}_{13}	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{x}$	(24f)	Gd II
\mathbf{B}_{14}	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-ax_4 \hat{x}$	(24f)	Gd II
\mathbf{B}_{15}	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{y}$	(24f)	Gd II
\mathbf{B}_{16}	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-ax_4 \hat{y}$	(24f)	Gd II
\mathbf{B}_{17}	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$ax_4 \hat{z}$	(24f)	Gd II
\mathbf{B}_{18}	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$-ax_4 \hat{z}$	(24f)	Gd II
\mathbf{B}_{19}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{x} + \frac{1}{4}a \hat{y} + \frac{1}{4}a \hat{z}$	(24g)	Gd III
\mathbf{B}_{20}	$x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{x} + \frac{1}{4}a \hat{y} + \frac{1}{4}a \hat{z}$	(24g)	Gd III
\mathbf{B}_{21}	$x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$\frac{1}{4}a \hat{x} + ax_5 \hat{y} + \frac{1}{4}a \hat{z}$	(24g)	Gd III
\mathbf{B}_{22}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{x} - a(x_5 - \frac{1}{2}) \hat{y} + \frac{1}{4}a \hat{z}$	(24g)	Gd III
\mathbf{B}_{23}	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{x} + \frac{1}{4}a \hat{y} + ax_5 \hat{z}$	(24g)	Gd III
\mathbf{B}_{24}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$\frac{1}{4}a \hat{x} + \frac{1}{4}a \hat{y} - a(x_5 - \frac{1}{2}) \hat{z}$	(24g)	Gd III

References

- [1] R. Zaremba, U. C. Rodewald, R.-D. Hoffmann, and R. Pöttgen, *The Rare Earth Metal-Rich Intermetallics RE_4RhIn ($RE = Gd-Tm, Lu$)*, *Monatsh. Chem.* **138**, 523–528 (2007), doi:10.1007/s00706-007-0663-9.
- [2] A. Doğan, S. Rayaprol, and R. Pöttgen, *Structure and magnetic properties of RE_4CoCd and RE_4RhCd ($RE = Tb, Dy, Ho$)*, *J. Phys.: Condens. Matter* **19**, 076213 (2007), doi:10.1088/0953-8984/19/7/076213.