Gd_4RhIn Structure: A4BC_cF96_216_efg_e_e-001

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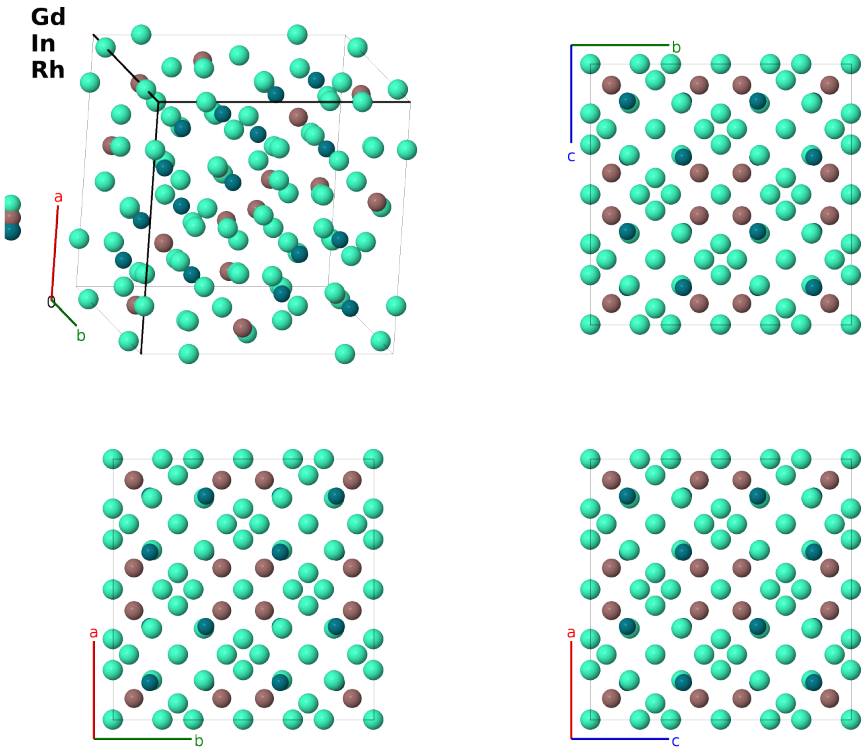
https://aflow.org/prototype-encyclopedia/39CF

https://aflow.org/prototype-encyclopedia/A4BC_cF96_216_efg_e_e-001



Prototype	Gd_4InRh
AFLOW prototype label	A4BC_cF96_216_efg_e_e-001
ICSD	417515
CCDC	1730865
Pearson symbol	cF96
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4BC_cF96_216_efg_e_e-001 --params=`$a, x_1, x_2, x_3, x_4, x_5$

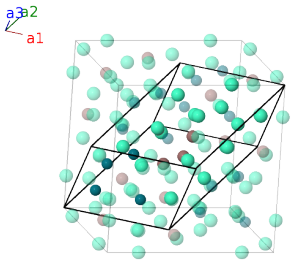
Other compounds with this structure

Ca_4AgMg, Ca_4AuMg, Ca_4PdMg, Ce_4RuMg, Dy_4CoCd, Dy_4CoMg, Dy_4PdAl, Dy_4PdMg, Dy_4PtAl, Dy_4PtMg, Dy_4RhCd, Dy_4RhIn, Er_4CoMg, Er_4PdAl, Er_4PdMg, Er_4PtAl, Er_4PtMg, Er_4RhAl, Er_4RhIn, Eu_4AuMg, Eu_4PdMg, Eu_4PtMg, Gd_4CoMg, Gd_4PdAl, Gd_4PtAl, Gd_4RhAl, Gd_4RhIn, Ho_4CoCd, Ho_4CoMg, Ho_4PdAl, Ho_4PdMg, Ho_4PtAl, Ho_4PtMg, Ho_4RhAl, Ho_4RhCd, Ho_4RhIn, La_4CoMg, Lu_4PdAl, Lu_4PdMg, Lu_4PtAl, Lu_4PtMg, Lu_4RhIn, Nd_4CdIr, Nd_4CoMg, Pr_4CoMg, Sm_4CoMg, Sm_4PdAl, Sm_4PdMg, Sm_4PtAl, Tb_4CoCd, Tb_4CoMg, Tb_4PdAl, Tb_4PtAl, Tb_4PtMg, Tb_4RhAl, Tb_4RhCd, Tb_4RhIn, Tm_4CoMg, Tm_4PdAl, Tm_4PdMg, Tm_4PtAl, Tm_4PtMg, Tm_4RhIn, Y_4CoMg, Y_4PdAl, Y_4PtAl, Yb_4AgMg, Yb_4AuMg, Yb_4PdMg, Yb_4PtMg

- The ICSD gives Dy_4CoCd as the prototype for this structure, but even (Doğan, 2007), which defines that structure, designates Gd_4RhIn as the prototype, so we use that compound.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16e)	Gd I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - 3x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16e)	Gd I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - 3x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16e)	Gd I
$\mathbf{B_4}$	=	$-3x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16e)	Gd I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	In I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - 3x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16e)	In I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - 3x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16e)	In I
$\mathbf{B_8}$	=	$-3x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16e)	In I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Rh I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Rh I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Rh I
$\mathbf{B_{12}}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Rh I
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(24f)	Gd II
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(24f)	Gd II
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}}$	(24f)	Gd II
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}}$	(24f)	Gd II
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{z}}$	(24f)	Gd II
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{z}}$	(24f)	Gd II
$\mathbf{B_{19}}$	=	$-\left(x_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	Gd III

$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	Gd III
$\mathbf{B_{21}}$	=	$x_5\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	Gd III
$\mathbf{B_{22}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+x_5\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{4}a\,\hat{\mathbf{z}}$	(24g)	Gd III
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24g)	Gd III
$\mathbf{B_{24}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	Gd III

References

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