Ho$_2$CoGa$_8$ Structure: AB8C2_tP11_123_a_ehi_g-003

https://aflow.org/p/G7WP

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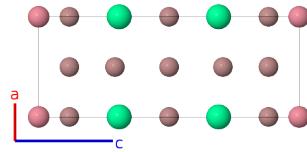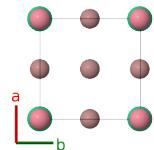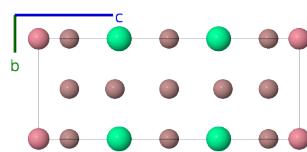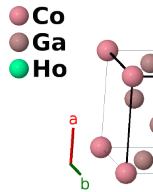
| Prototype	CoGa$_8$Ho$_2$
AFLOW prototype label	AB8C2_tP11_123_a_ehi_g-003
ICSD	198243
Pearson symbol	tP11
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	aflow --proto=AB8C2_tP11_123_a_ehi_g-003 --params=$a, c/a, z_3, z_4, z_5$

Other compounds with this structure

Ce$_2$PdIn$_8$, Ce$_2$PtIn$_8$, Ho$_2$DyGa$_8$, Ho$_2$ErGa$_8$, Ho$_2$GdGa$_8$, Ho$_2$LuGa$_8$, Ho$_2$SmGa$_8$, Ho$_2$TbGa$_8$, Ho$_2$TmGa$_8$, Ho$_2$YGa$_8$

Simple Tetragonal primitive vectors

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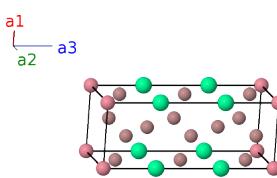
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Co I
$\mathbf{B_2}$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Ga I
$\mathbf{B_3}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Ga I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	Ho I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	Ho I
$\mathbf{B_6}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2h)	Ga II
$\mathbf{B_7}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2h)	Ga II
$\mathbf{B_8}$	=	$\frac{1}{2}\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4i)	Ga III
$\mathbf{B_9}$	=	$\frac{1}{2}\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4i)	Ga III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4i)	Ga III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(4i)	Ga III

References

[1] Y. N. Grin', Y. P. Yarmolyuk, and E. I. Gladyshevskiia, *Crystal structures of R_2CoGa_a compounds (R= Sm, Gd, Tb, Dy, Er, Tm, Lu, Y) and $RCoGa_5$ compounds (R = Gd, Tb, Dy, Ho, Er,Tm, Lu, or Y)*, Sov. Phys. Crystallogr. **24**, 137–139 (1976). Translated from Kristallografiya 24, 242 (1979).

Found in

[1] M. Kratochvilova, M. Dusek, K. Uhlirova, A. Rudajevova, J. Prokleska, B. Vondrackova, J. Custers, and V. Sechovsky, *Single crystal study of the layered heavy fermion compounds Ce_2PdIn_8, Ce_3PdIn_{11}, Ce_2PtIn_8 and Ce_3PtIn_{11}*, J. Cryst. Growth **397**, 47–52 (2014), doi:10.1016/j.jcrysgro.2014.04.008.