Ga_2Hf Structure: A2B_tI24_141_2e_e-001

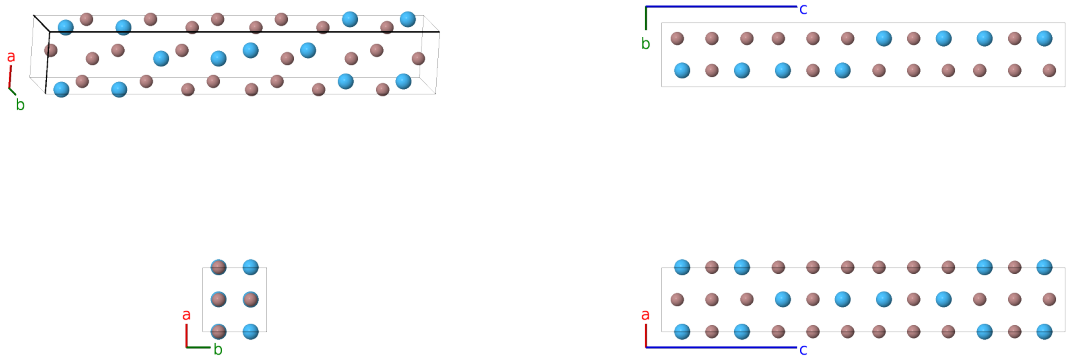
This structure originally had the label `A2B_tI24_141_2e_e`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/DBUS

https://aflow.org/p/A2B_tI24_141_2e_e-001

Ga
Hf



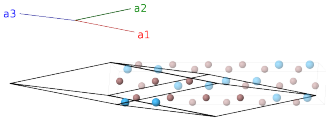
Prototype	Ga_2Hf
AFLOW prototype label	A2B_tI24_141_2e_e-001
ICSD	197276
Pearson symbol	tI24
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2B_tI24_141_2e_e-001 --params=`$a, c/a, z_1, z_2, z_3$

Other compounds with this structure
Al_2Mg, Al_2Ti, Ga_2Ti, In_2Zr, Pb_2Pr, Pb_2Pu, Sn_2Pu

- When $z_1 = 1/4$, $z_2 = 5/12$, and $z_3 = 1/12$, the atoms are on the sites of indium ($A6$) body-centered tetragonal lattice. If, in this case, $c = 6a$, the atoms are on the sites of a face-centered cubic lattice, and if $c = 3\sqrt{2}a$, the atoms are on the site of a body-centered cubic lattice. This lattice is placed with the face-centered cubic lattices because most known structures have c near $6a$.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8e)	Ga I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Ga I
$\mathbf{B_3}$	=	$-\left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8e)	Ga I
$\mathbf{B_4}$	=	$-z_1\,\mathbf{a}_1 - \left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Ga I
$\mathbf{B_5}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Ga II
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Ga II
$\mathbf{B_7}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Ga II
$\mathbf{B_8}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Ga II
$\mathbf{B_9}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8e)	Hf I
$\mathbf{B_{10}}$	=	$z_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Hf I
$\mathbf{B_{11}}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8e)	Hf I
$\mathbf{B_{12}}$	=	$-z_3\,\mathbf{a}_1 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Hf I

References

[1] K. Schubert, H. G. Meissner, M. Pötzschke, W. Rossteutscher, and E. Stolz, *Einige Strukturdaten metallischer Phasen (7)*, Naturwissenschaften **49**, 57 (1962), doi:10.1007/BF00595382.

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[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.