

Ga₂Hf Structure:

A2B_tI24_141_2e_e-001

This structure previously used the label(s) **A2B_tI24_141_2e_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/DBUS>

https://aflow.org/prototype-encyclopedia/A2B_tI24_141_2e_e-001

Prototype	Ga ₂ Hf
AFLOW prototype label	A2B_tI24_141_2e_e-001
ICSD	197276
CCDC	1924176
Pearson symbol	tI24
Space group number	141
Space group symbol	<i>I</i> 4 ₁ / <i>amd</i>
AFLOW prototype command	<code>aflow --proto=A2B_tI24_141_2e_e-001</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>z</i>₁, <i>z</i>₂, <i>z</i>₃</code>

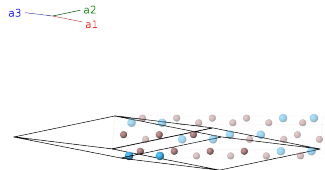
Other compounds with this structure

Al₂Mg, Al₂Ti, Ga₂Ti, In₂Zr, Pb₂Pr, Pb₂Pu, Sn₂Pu

- 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 $6a$.

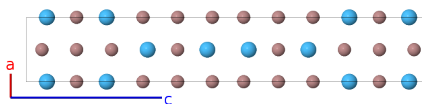
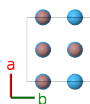
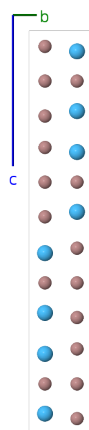
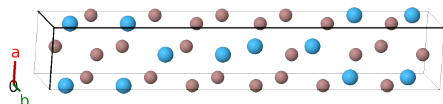
Body-centered Tetragonal primitive vectors

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



Basis vectors

Ga
Hf



	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.

Found in

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

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