Hg_2TiCu Inverse Heusler Structure: AB2C_cF16_216_a_bc_d-001

This structure previously used the label(s) `AB2C_cF16_216_b_ad_c`. Calls to these addresses will be redirected here.

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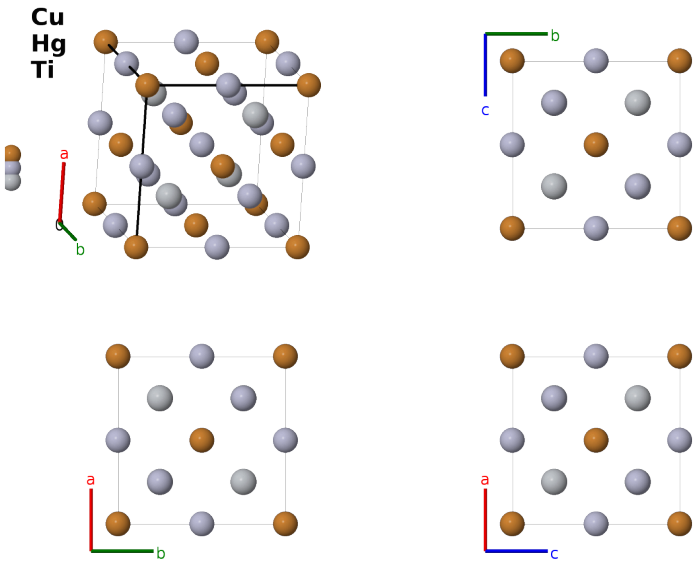
https://aflow.org/prototype-encyclopedia/4M8A

https://aflow.org/prototype-encyclopedia/AB2C_cF16_216_a_bc_d-001



Prototype	$CuHg_2Ti$
AFLOW prototype label	AB2C_cF16_216_a_bc_d-001
Mineral name	Inverse Heusler
ICSD	102972
CCDC	1660933
Pearson symbol	cF16
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB2C_cF16_216_a_bc_d-001 --params=`a

Other compounds with this structure

Mn_2CoAl, Mn_2CoGa, Mn_2CoIn, Li_2AgSb, Li_2CuSn, Li_2CuSb, Li_2AgAl, Li_2AgIn, Li_2AgSb, Li_2AgSn, Li_2AgPb, Li_2AgBi, Li_2AuGa, Li_2AuIn, Li_2AuSb, Li_2AuSn, Li_2AuPb, Li_2AuTl

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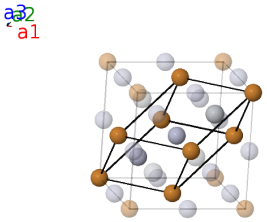
- Most of the literature on inverse Heusler compounds identifies Hg_2TiCu as the prototype structure, however (Villars, 2016) and (Villars, 2016a) use the Li_2AgSb structure found in (Pauly, 1968) as the prototype.
- Although it is tempting to use the older paper, we follow the majority and use Hg_2TiCu as the prototype.
- The inverse Heusler structure is a variation of the quaternary Heusler structure, where the mercury atoms are on adjacent face-centered cubic sublattices, forming a diamond structure.
- Contrast this with the standard Heusler ($L1_2$) structure, where the like atoms are at second-neighbor positions in the fcc lattice.
- This structure is also referred to as the XA or X_a structure.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Hg I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	Hg II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(4d)	Ti I

References

[1] M. Pušelj and Z. Ban, *The Crystal Structure of $TiCuHg_2$*, Croatica Chemica Acta **41**, 79–83 (1969).

[2] H. Pauly, A. Weiss, and H. Witte, *The Crystal Structure of the Ternary Intermetallic Phases Li_2EX (E=Cu,Ag,Au; X=Al,Ga,In,Tl,Si,Ge,Sn,Pb,Sb,Bi)*, Z. Metallkd. **59**, 47–58 (1968).

[3] P. Villars, *Li_2AgSb Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.).

Found in

[1] P. Villars, *$TiCuHg_2$ ($CuHg_2Ti$) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.