Hg_2TiCu Inverse Heusler Structure: AB2C_cF16_216_a_bc_d-001

This structure originally had the label `AB2C_cF16_216_b_ad_c`. Calls to that address will be redirected here.

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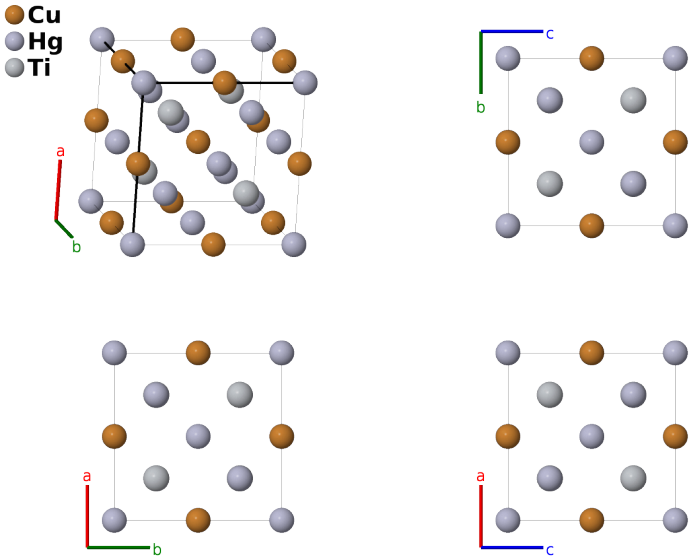
https://aflow.org/p/4M8A

https://aflow.org/p/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
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

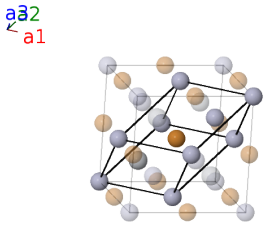
Mn_2CoAl, Mn_2CoGa, Mn_2CoIn, Li_2AgSb, Li_2CuSn, Li_2CuSb, Li_2AgAl, Li_2AgIn, Li_2AgSb, Li_2AgSn, Li_2AgPb, Li_2AgBi, Li_2AuGa, Li_2AuIn, Li_2AuSb, Li_2AuSn, Li_2AuPb, Li_2AuTl

- 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.).