Half–Heusler (AgAsMg, $C1_b$) Structure: ABC_cF12_216_a_c_b-001

This structure originally had the label `ABC_cF12_216_b_c_a`. Calls to that address will be redirected here.

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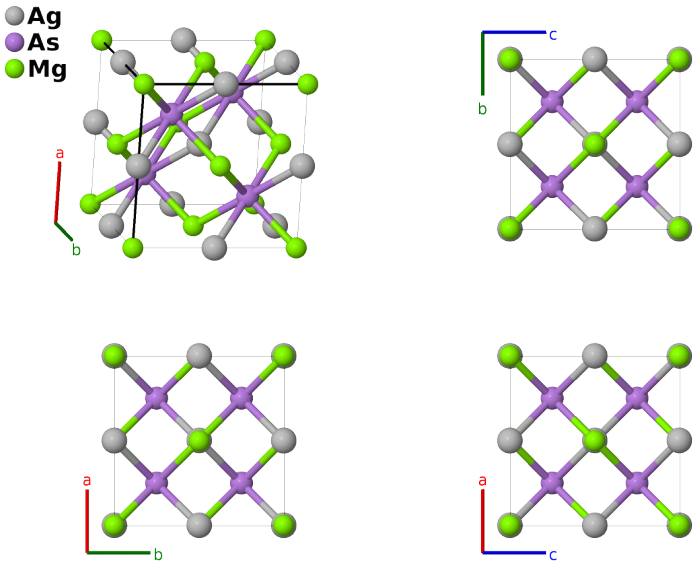
https://aflow.org/p/3BJR

https://aflow.org/p/ABC_cF12_216_a_c_b-001



Prototype	AgAsMg
AFLOW prototype label	ABC_cF12_216_a_c_b-001
***Strukturbericht* designation**	$C1_b$
Mineral name	half-heusler
ICSD	43819
Pearson symbol	cF12
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=ABC_cF12_216_a_c_b-001 --params=`a

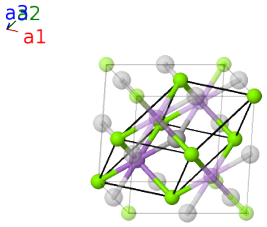
Other compounds with this structure

AlBBe, AuMgSn, AuScSn, BiCoZr, BiCuMg, BiLiMg, BiMgNi, BiPdTe, BiPtY, CdCuSb, CdLiP, CoSbTi, CoSbV, CoSbZr, CuMgSb, CuMgSn, CuMnSb, CuSbV, FeSbTi, FeSbV, LiMgSb, LiNZn, LiPZn, MgNiSb, MgPtSn, MnNiSb, NiSbTi, NiSbV, PtScSn, RhSnTi

- All of the atoms are located on the sites of a body-centered cubic lattice. This is sometimes called the "half–Heusler" structure because it is identical to the $L2_1$ (Heusler) structure, Cu_2AlMn with half of the copper atoms missing. The Mg and Ag atoms form a rock salt ($B1$) structure, while the As and either the Mg or Ag atoms form a zincblende ($B3$) structure. If the atoms on the (4a) and (4c) sites are identical, this reduces to the fluorite ($C1$) 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)	Ag 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)	Mg 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)	As I

References

[1] H. Nowotny and W. Sibert, *Ternäre Valenzverbindungen in den Systemen Kupfer(Silber)-Arsen(Antimon,Wismut)-Magnesium*, Z. Metallkd. **33**, 391–394 (1941).

Found in

[1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Tornoto, 1972).