Quaternary Heusler (LiMgAuSn) Structure: ABCD_cF16_216_a_b_c_d-001

This structure originally had the label `ABCD_cF16_216_c_d_b_a`. Calls to that address will be redirected here.

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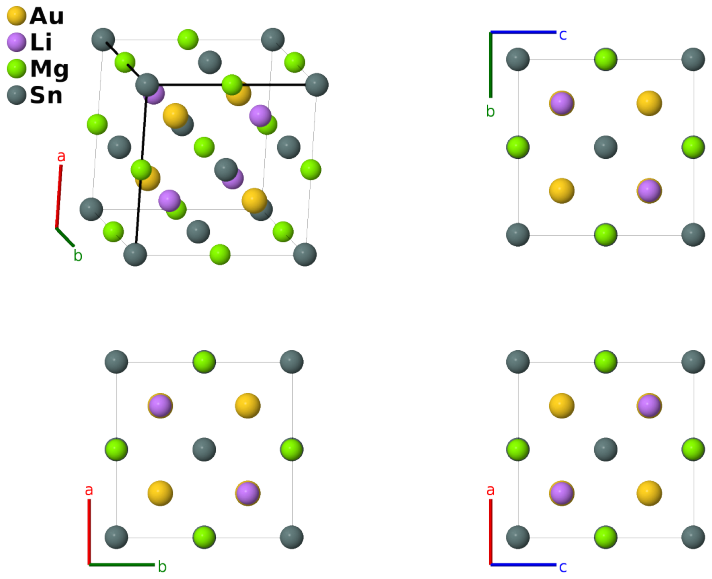
https://aflow.org/p/4CEX

https://aflow.org/p/ABCD_cF16_216_a_b_c_d-001



Prototype	AuLiMgSn
AFLOW prototype label	ABCD_cF16_216_a_b_c_d-001
ICSD	16477
Pearson symbol	cF16
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=ABCD_cF16_216_a_b_c_d-001 --params=`a

Other compounds with this structure
AuLiMgSn, LiMgPdSn, LiMgPtSn, $CuMg_2Ti$, $AuBiLi_2$, $AgLi_2Sn$, $AuLi_2Sn$, $CuHfHg_2$, $MnPd_2Sn$

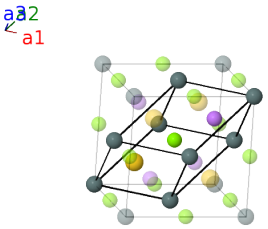
- This "quaternary-Heusler" structure can be considered as the parent of a wide variety of structures, depending on the occupancy of the (4a), (4b), (4c), and (4d) Wyckoff positions. Consider atoms of type A, B, C, D, distributed in this structure. We can get:

Structure	*Strukturbericht*	AFLOW Label	(4a)	(4b)	(4c)	(4d)
simple cubic	A_h	A_cP1_221_a	A	A	-	-
fcc	A1	A_cF4_225_a	A	-	-	-
bcc	A2	A_cI2_229_a	A	A	-	-
bcc	A2	A_cI2_229_a	A	A	A	A
diamond	A4	A_cF8_227_a	A	-	A	-
NaCl	B1	AB_cF8_225_a_b	A	B	-	-
CsCl	B2	AB_cP2_221_a_b	A	A	B	B
ZnS (zincblende)	B3	AB_cF8_216_c_a	A	-	B	-
BiF_3	$D0_3$	AB3_cF16_225_a_bc	A	B	B	B
NaTl	B32	AB_cF16_227_a_b	A	B	A	B
Fluorite	C1	AB2_cF12_225_a_c	A	-	B	B
half-Heusler	$C1_b$	ABC_cF12_216_a_b_c	A	B	C	-
Heusler	$L2_1$	AB2C_cF16_225_a_c_b	A	C	B	B
Inverse-Heusler		AB2C_cF16_216_a_bc_d	A	B	B	C

- The ordering of this structure is somewhat arbitary. We will get the same structure if Sn and Mg are on either the (4a)/(4b) or (4c)/(4d) sites with Au and Li on the opposite sites.

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)	Au 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)	Li 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)	Mg I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(4d)	Sn I

References

[1] U. Eberz, W. Seelentag, and H.-U. Schuster, *Zur Kenntnis farbiger ternärer und quaternärer Zintl-Phasen Coloured Ternary and Quaternary Zintl-Phases*, Z. Naturforsch. B **35**, 1341–1343 (1980), doi:10.1515/znb-1980-1103.

Found in

[1] P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database)* (Springer Materials, Heigelberg, 2016), chap. LiMgPdSn Crystal Structure.