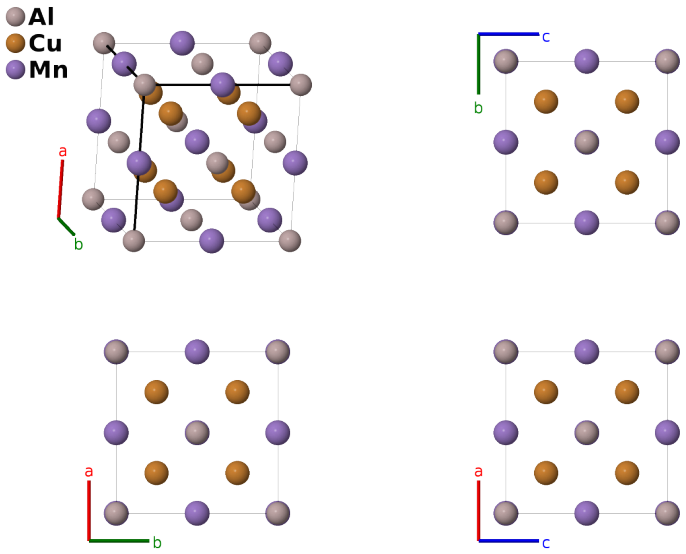
Heusler (Cu_2AlMn, $L2_1$) Structure: AB2C_cF16_225_a_c_b-001

This structure originally had the label `AB2C_cF16_225_a_c_b`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/02WQ

https://aflow.org/p/AB2C_cF16_225_a_c_b-001



Prototype	$AlCu_2Mn$
AFLOW prototype label	AB2C_cF16_225_a_c_b-001
***Strukturbericht* designation**	$L2_1$
Mineral name	heusler
ICSD	607008
Pearson symbol	cF16
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB2C_cF16_225_a_c_b-001 --params=`a

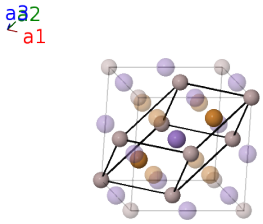
Other compounds with this structure

Ag_2AlMn, Cd_2AgAu, Co_2AlHf, Co_2AlMn, Co_2AlNb, Co_2AlTa, Co_2AlZr, Co_2FeGe, Co_2GaMn, Co_2GaMn, Co_2GaNb, Co_2GaTa, Co_2GaTi, Co_2MnSi, Co_2MnSn, Co_2SiV, Co_2SnTi, Co_2SnV, Cu_2AlMn, Cu_2AlZr, Cu_2CoSn, Cu_2FeSn, Cu_2GaMn, Cu_2InMn, Cu_2InTi, Cu_2MnSb, Cu_2MnSn, Cu_2NiSn, Fe_2AlV, Fe_2AlCo, Fe_2GaTi, Fe_2GaV, Fe_2SnTi, K_2CsSb, Li_2AuSn, Li_2NaSb, Mg_2LiTl, Na_2KSb, Ni_2AlHf, Ni_2AlNb, Ni_2AlTa, Ni_2AlTi, Ni_2AlZr, Ni_2GaHf, Ni_2GaMn, Ni_2GaNb, Ni_2GaTa, Ni_2GaV, Ni_2GeMn, Ni_2InMg, Ni_2InMn, Ni_2InTi, Ni_2MgSb, Ni_2MgSn, Ni_2MnGa, Ni_2MnSb, Ni_2MnSn, Ni_2SnTi, Ni_2SnV, Pd_2AlMn, Pd_2InMn, Pd_2MnSb, Pd_2MnSn, Zn_2AgAu, β-Zn_2AuCu

- All of the atoms are located on the sites of a body-centered cubic lattice. If we replace the Mn atom by another copper atom, the structure reduces to the crystallographically equivalent $D0_3$ (BiF_3) structure.
- If we replace one of the copper atoms by an fourth species we get the the "quaternary-Heusler," LiMgAuSn.
- Also see the $C1_b$ (AsAgMg) "half–Heusler" structure.
- The ICSD entry is from (Heusler, 1934). It is identical to the structure describe by (Bradley, 1934) except for a small change in the lattice constant.

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)	Al 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)	Mn I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	Cu I

References

[1] A. J. Bradley and J. W. Rodgers, *The Crystal Structure of Heusler Alloys*, Proc. R. Soc. A Math. Phys. Eng. Sci. **144**, 340–359 (1934), doi:10.1098/rspa.1934.0053.

[2] O. Heusler, *Kristallstruktur und Ferromagnetismus der Mangan-Aluminium-Kupferlegierungen*, Ann. Phys. **411**, 155–201 (1934). Originally referenced as "5.Folge. Band 19.".