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

This structure previously used the label(s) `AB2C_cF16_225_a_c_b`. Calls to these addresses will be redirected here.

Cite this page as:

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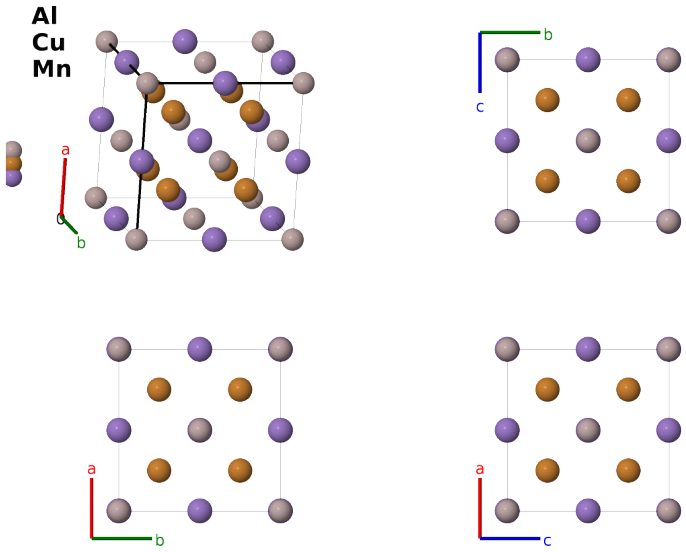
https://aflow.org/prototype-encyclopedia/02WQ

https://aflow.org/prototype-encyclopedia/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
CCDC	1742311
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

Ac_2HgSn, Ag_2AlMn, Ag_2AlSc, Ag_2CdMg, Ag_2CeAl, Ag_2CeIn, Ag_2DyIn, Ag_2ErIn, Ag_2GdIn, Ag_2HoIn, Ag_2InLa, Ag_2InMg, Ag_2InNd, Ag_2InPr, Ag_2InSc, Ag_2InSm, Ag_2InTb, Ag_2InTm, Ag_2InY, Ag_2LiGe, Ag_2LiIn, Ag_2LiSn, Ag_2MgTm, Ag_2MgZn, Al_2IrLi, Al_2LiPd, Al_2LiPt, Al_2LiRh, Al_2MnNi, Al_2MnOs, Al_2NiPt, Au_2AgMn, Au_2AlHf, Au_2AlMn, Au_2AlSc, Au_2AlTi, Au_2CeIn, Au_2CuMn, Au_2DyIn, Au_2ErIn, Au_2GdIn, Au_2HfIn, Au_2HoIn, Au_2InLu, Au_2InNd, Au_2InPr, Au_2InSc, Au_2InSm, Au_2InTb, Au_2InTh, Au_2InTi, Au_2InTm, Au_2InU, Au_2InY, Au_2InYb, Au_2InZr, Au_2SnU, Ba_2AsAu, Ba_2AuBi, Ba_2AuSb, Ba_2HgPb, Ba_2HgSn, Ba_2MgTl, C_2CrK, C_2KTi, C_2KV, Ca_2AsAu, Ca_2AuBi, Ca_2AuSb, Ca_2HgPb, Ca_2HgSn, Cd_2AgAu, Cd_2AgCe, Cd_2FeS, Cd_2FeSe, Co_2AgSi, Co_2AlCr, Co_2AlFe, Co_2AlHf, Co_2AlMn, Co_2AlMo, Co_2AlNb, Co_2AlRh, Co_2AlRu, Co_2AlTa, Co_2AlTc, Co_2AlTi, Co_2AlV, Co_2AlY, Co_2AlZr, Co_2AsLa, Co_2AsMn, Co_2AsSc, Co_2AsV, Co_2AsY, Co_2BCr, Co_2BMn, Co_2BTi, Co_2BV, Co_2BZr, Co_2BeGe, Co_2BeSi, Co_2BiMn, Co_2BiY, Co_2CrGa, Co_2CrGe, Co_2CrIn, Co_2CrMg, Co_2CrSi, Co_2CrSn, Co_2FeGa, Co_2FeGe, Co_2FeIn, Co_2FeSi, Co_2GaHf, Co_2GaMn, Co_2GaNb, Co_2GaNi, Co_2GaTa, Co_2GaTi, Co_2GaV, Co_2GaZr, Co_2GeLa, Co_2GeLi, Co_2GeMn, Co_2GeSc, Co_2GeTa, Co_2GeTi, Co_2GeV, Co_2GeY, Co_2GeZn, Co_2GeZr, Co_2HfSb, Co_2HfSn, Co_2InMn, Co_2InNb, Co_2InTi, Co_2InV, Co_2InZr, Co_2LaP, Co_2LaSb, Co_2MgV, Co_2MnP, Co_2MnPb, Co_2MnSb, Co_2MnSi, Co_2MnSn, Co_2MnTl, Co_2NbSi, Co_2NbSn, Co_2PSc, Co_2PY, Co_2PdSi, Co_2SY, Co_2SbSc, Co_2SbTi, Co_2SbV, Co_2SbY, Co_2ScSi, Co_2ScSn, Co_2SeV, Co_2SeY, Co_2SiTa, Co_2SiTi, Co_2SiV, Co_2SiY, Co_2SiZr, Co_2SnTi, Co_2SnV, Co_2SnY, Co_2SnZr, Co_2TaTi, Cr_2GdGe, Cr_2GdSi, Cr_2GeTa, Cr_2PSc, Cr_2PY, Cr_2SnTa, Cr_2SnTi, Cu_2AlCr, Cu_2AlHf, Cu_2AlMn, Cu_2AlSc, Cu_2AlTi, Cu_2AlZr, Cu_2CdZr, Cu_2CeIn, Cu_2CoSn, Cu_2DyIn, Cu_2ErIn, Cu_2FeSn, Cu_2GaLi, Cu_2GaMn, Cu_2GaSc, Cu_2GdIn, Cu_2GeLi, Cu_2HfAl, Cu_2HfIn, Cu_2HoIn, Cu_2InLa, Cu_2InLu, Cu_2InMn, Cu_2InNd, Cu_2InPr, Cu_2InSc, Cu_2InSm, Cu_2InTb, Cu_2InTi, Cu_2InTm, Cu_2InY, Cu_2InZr, Cu_2LaIn, Cu_2LiSi, Cu_2LuIn, Cu_2MgRu, Cu_2MnAl, Cu_2MnIn, Cu_2MnPt, Cu_2MnSb, Cu_2MnSn, Cu_2NdIn, Cu_2NiSn, Cu_2ZrZn, Fe_2AlCo, Fe_2AlCr, Fe_2AlMn, Fe_2AlMo, Fe_2AlNb, Fe_2AlNi, Fe_2AlSc, Fe_2AlTa, Fe_2AlTi, Fe_2AlV, Fe_2AlY, Fe_2AlZn, Fe_2AlZr, Fe_2AsMn, Fe_2AsNb, Fe_2AsSc, Fe_2AsTi, Fe_2AsV, Fe_2AsY, Fe_2AsZr, Fe_2B Ti, Fe_2BSc, Fe_2BTa, Fe_2BZr, Fe_2CoGa, Fe_2CoGe, Fe_2CrGa, Fe_2CrGe, Fe_2CrSi, Fe_2CrSn, Fe_2GaMn, Fe_2GaNb, Fe_2GaNi, Fe_2GaSc, Fe_2GaTa, Fe_2GaTi, Fe_2GaV, Fe_2GaY, Fe_2GeMn, Fe_2GeNb, Fe_2GeSc, Fe_2GeTa, Fe_2GeTi, Fe_2GeV, Fe_2GeZr, Fe_2InTa, Fe_2InTi, Fe_2InV, Fe_2InZr, Fe_2IrRh, Fe_2MgTi, Fe_2MgV, Fe_2MnP, Fe_2MnSb, Fe_2MnSi, Fe_2MoAl, Fe_2MoSi, Fe_2NbSi, Fe_2NbSn, Fe_2P Ti, Fe_2PNb, Fe_2PSc, Fe_2PV, Fe_2PZr, Fe_2SbSc, Fe_2SbTi, Fe_2SbV, Fe_2SbY, Fe_2SbZr, Fe_2ScSe, Fe_2ScSi, Fe_2SiTa, Fe_2SiTi, Fe_2SiV, Fe_2SiY, Fe_2SiZr, Fe_2SnTa, Fe_2SnTi, Fe_2SnV, Fe_2SnY, Fe_2SnZr, Ga_2CoMn, Ga_2IrLi, Ga_2LiPd, Ga_2LiPt, Ga_2LiRh, Ga_2LiRu, Ga_2MnNi, Hf_2BCr, Hf_2CrGa, Hf_2CrGe, Hf_2CrIn, Hf_2CrSi, Hf_2CrSn, Hf_2OsV, Hf_2ReV, Hg_2CeLi, Hg_2ScTi, In_2IrLi, In_2LiPd, In_2LiPt, In_2LiRh, In_2LiRu, Ir_2AlMn, Ir_2GaMn, K_2CsSb, Li_2AgMg, Li_2AgSn, Li_2AuMg, Li_2AuSn, Li_2BiMg, Li_2BiTl, Li_2CSr, Li_2CaC, Li_2CaPb, Li_2CaSn, Li_2CdGe, Li_2CdMg, Li_2CdPb, Li_2CdSb, Li_2CdSn, Li_2CuGe, Li_2CuSn, Li_2DyIn, Li_2GaMg, Li_2GeHg, Li_2GeMg, Li_2GePd, Li_2GeZn, Li_2HgMg, Li_2InMg, Li_2IrSn, Li_2MgPb, Li_2MgSb, Li_2MgSn, Li_2MgTl, Li_2NaSb, Li_2PbPd, Li_2PdSn, Li_2PtSn, Li_2SbTl, Li_2SbZn, Li_2SnZn, Mg_2AgCe, Mg_2AgGd, Mg_2AgNd, Mg_2AgPr, Mg_2AgSm, Mg_2CeCu, Mg_2GaLi, Mg_2GeLi, Mg_2LiPb, Mg_2LiSi, Mg_2LiTl, Mn_2AlCr, Mn_2AlMo, Mn_2AlNb, Mn_2AlNi, Mn_2AlSc, Mn_2AlV, Mn_2AlY, Mn_2AlZr, Mn_2AsLi, Mn_2AsSc, Mn_2AsY, Mn_2AsZr, Mn_2AuPd, Mn_2AuPt, Mn_2BSc, Mn_2CoCr, Mn_2CrGa, Mn_2CuPt, Mn_2FeSi, Mn_2GaMo, Mn_2GaNb, Mn_2GaNi, Mn_2GaRh, Mn_2GaSc, Mn_2GaTa, Mn_2GaV, Mn_2GeMg, Mn_2GeNb, Mn_2GeRu, Mn_2GeSc, Mn_2GeTi, Mn_2InV, Mn_2IrRu, Mn_2LiSb, Mn_2MoSi, Mn_2NbSi, Mn_2NbSn, Mn_2NiPd, Mn_2NiSb, Mn_2PSc, Mn_2PZr, Mn_2PdPt, Mn_2PdRh, Mn_2PtRh, Mn_2RhSi, Mn_2RuSn, Mn_2SY, Mn_2SbSc, Mn_2SbTi, Mn_2SbZr, Mn_2ScSe, Mn_2ScSi, Mn_2SeY, Mn_2SiTi, Mn_2SiY, Mn_2SiZr, Mn_2SnTi, Mn_2SnW, N_2CrK, N_2KTi, N_2KV, N_2NbTa, N_2NbV, N_2TaV, Na_2KSb, Nb_2FeMn, Ni_2AlCo, Ni_2AlCr, Ni_2AlFe, Ni_2AlHf, Ni_2AlMn, Ni_2AlNb, Ni_2AlSc, Ni_2AlTa, Ni_2AlTi, Ni_2AlV, Ni_2AlW, Ni_2AlZr, Ni_2AsCr, Ni_2AsMn, Ni_2BeSi, Ni_2CrGa, Ni_2CrGe, Ni_2CrIn, Ni_2CrP, Ni_2CrSb, Ni_2CrSi, Ni_2CrSn, Ni_2CuSb, Ni_2CuSn, Ni_2GaFe, Ni_2GaHf, Ni_2GaMn, Ni_2GaNb, Ni_2GaSc, Ni_2GaTa, Ni_2GaTi, Ni_2GaV, Ni_2GaZr, Ni_2GeLi, Ni_2GeMn, Ni_2GeZn, Ni_2HfIn, Ni_2HfSn, Ni_2InMg, Ni_2InMn, Ni_2InSc, Ni_2InTi, Ni_2InU, Ni_2InZr, Ni_2LiSi, Ni_2LiSn, Ni_2LuSn, Ni_2MgMn, Ni_2MgRu, Ni_2MgSb, Ni_2MgSn, Ni_2MnGa, Ni_2MnP, Ni_2MnSb, Ni_2MnSi, Ni_2MnSn, Ni_2MnTi, Ni_2NbSn, Ni_2ReSn, Ni_2SbTi, Ni_2SbZr, Ni_2ScSn, Ni_2SiZn, Ni_2SnTi, Ni_2SnU, Ni_2SnV, Ni_2SnYb, Ni_2SnZr, Ni_2TiV, O_2CoCr, O_2CoCs, O_2CoCu, O_2CoFe, O_2CoMn, O_2CoNi, O_2CoSc, O_2CoTi, O_2CoV, O_2CoZn, O_2CrCs, O_2CrK, O_2CsFe, O_2CsMn, O_2CsNi, O_2CsV, O_2HeTh, O_2KTi, O_2KV, Os_2HfSn, Os_2MnSi, P_2BeSi, P_2CdGe, P_2CdSi, P_2GeZn, P_2HgSi, P_2MgSi, P_2SiZn, P_2SnZn, Pd_2AlCo, Pd_2AlCu, Pd_2AlHf, Pd_2AlMn, Pd_2AlSc, Pd_2AlTi, Pd_2AlZr, Pd_2AsMn, Pd_2AuCr, Pd_2AuMn, Pd_2BiY, Pd_2CoGa, Pd_2CrCu, Pd_2CuMn, Pd_2CuSn, Pd_2DyIn, Pd_2DySn, Pd_2ErIn, Pd_2ErSn, Pd_2GaHf, Pd_2GaMn, Pd_2GaSc, Pd_2GaTi, Pd_2GaZr, Pd_2GdIn, Pd_2GeLi, Pd_2GeMn, Pd_2HfIn, Pd_2HfSn, Pd_2HgMn, Pd_2HoSn, Pd_2InLu, Pd_2InMn, Pd_2InSc, Pd_2InTi, Pd_2InTm, Pd_2InY, Pd_2InZr, Pd_2LiPb, Pd_2LiSi, Pd_2LiSn, Pd_2LuSn, Pd_2MgRu, Pd_2MgSb, Pd_2MgTi, Pd_2MnSb, Pd_2MnSn, Pd_2PbY, Pd_2SbY, Pd_2ScSn, Pd_2SnMg, Pd_2SnTb, Pd_2SnTm, Pd_2SnY, Pd_2SnYb, Pd_2SnZr, Pd_2Tm, Pt_2AlMn, Pt_2CrCu, Pt_2CuMn, Pt_2GaMn, Pt_2InLu, Pt_2InSc, Pt_2InZr, Pt_2MnNi, Pt_2MnSc, Pt_2ScSn, Rb_2CsSb, Re_2CrSi, Rh_2AlCr, Rh_2AlFe, Rh_2AlMn, Rh_2AlY, Rh_2AlZr, Rh_2CrGa, Rh_2CrGe, Rh_2CrIn, Rh_2CrSn, Rh_2CuMn, Rh_2CuSb, Rh_2CuSn, Rh_2FeGa, Rh_2FeIn, Rh_2GaMn, Rh_2GaZr, Rh_2GeLi, Rh_2GeMn, Rh_2GeZr, Rh_2HfMn, Rh_2InMn, Rh_2InZr, Rh_2MnPb, Rh_2MnSn, Rh_2MnTi, Rh_2MnZr, Rh_2NiSn, Rh_2SY, Rh_2SiZr, Rh_2SnV, Rh_2SnZr, Ru_2AlCr, Ru_2AlMn, Ru_2AlNb, Ru_2AlTa, Ru_2AlV, Ru_2AsCr, Ru_2AsMn, Ru_2AsV, Ru_2AsZr, Ru_2CrGa, Ru_2CrGe, Ru_2CrIn, Ru_2CrP, Ru_2CrSb, Ru_2CrSi, Ru_2CrSn, Ru_2FeGa, Ru_2FeSi, Ru_2FeSn, Ru_2GaNb, Ru_2GaTa, Ru_2GaV, Ru_2GeMn, Ru_2GeTi, Ru_2GeV, Ru_2GeZr, Ru_2HfMn, Ru_2InNb, Ru_2MnNb, Ru_2MnP, Ru_2MnSb, Ru_2MnSi, Ru_2MnSn, Ru_2MnTa, Ru_2MnTi, Ru_2MnV, Ru_2PV, Ru_2SbTi, Ru_2SbV, Ru_2SbZr, Ru_2ScSb, Ru_2SiTi, Ru_2SiV, Ru_2SiZr, Ru_2SnTi, Ru_2SnV, Ru_2SnZr, S_2CuAl, Sc_2CMn, Sc_2CoGa, Sc_2GeMn, Sc_2MnSi, Sc_2MnSn, Se_2AlCu, Sr_2AsAu,

Sr_2AuBi, Sr_2AuSb, Sr_2HgPb, Sr_2HgSn, Ta_2FeMn, Te_2AlCu, Ti_2AlCo, Ti_2AlFe, Ti_2AlIr, Ti_2AlNb, Ti_2AsV, Ti_2BIr, Ti_2CoSi, Ti_2CrGa, Ti_2FeSb, Ti_2GaFe, Ti_2GaIr, Ti_2IrIn, Ti_2MnAl, Ti_2NiV, Ti_2OsV, Ti_2ReV, Ti_2RuV, V_2AlFe, V_2AlMn, V_2AsCo, V_2AsCu, V_2AsNi, V_2AsZn, V_2CuGa, V_2CuGe, V_2FeGa, V_2FeOs, V_2FeRe, V_2FeRu, V_2GaMn, V_2GaZn, V_2GeNi, V_2GeZn, V_2NiTi, Y_2AlMn, Y_2GaMn, Y_2GeMn, Y_2MnSb, Y_2MnSi, Y_2MnSn, Zn_2AgAu, Zn_2AuCu, Zn_2CeMg, Zr_2AlTi, Zr_2CoMn, Zr_2GaNi, Zr_2GeV, Zr_2OsV, Zr_2PbV, Zr_2SiV, Zr_2SnV, β-Zn_2AuCu

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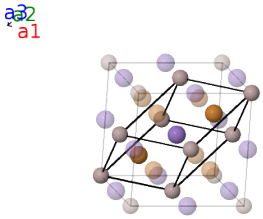
- All of the atoms are located on the sites of a body-centered cubic lattice. If we replace the Mn atom by another copper atom, the structure reduces to the crystallographically equivalent $D0_3$ (BiF_3) structure.
- If we replace one of the copper atoms by any fourth species we get the the "quaternary-Heusler," 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

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First cited in

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