Cu_4SnMg Structure: A4BC_cF24_216_e_a_c-001

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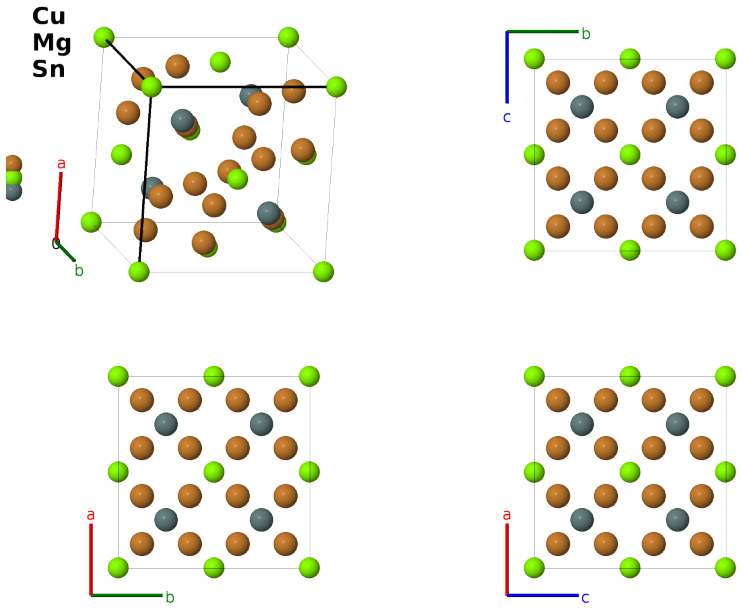
https://aflow.org/prototype-encyclopedia/VFWF

https://aflow.org/prototype-encyclopedia/A4BC_cF24_216_e_a_c-001



Prototype	Cu_4MgSn
AFLOW prototype label	A4BC_cF24_216_e_a_c-001
ICSD	103055
CCDC	1661013
Pearson symbol	cF24
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4BC_cF24_216_e_a_c-001 --params=`a, x_3

Other compounds with this structure

Co_4CeMg, Co_4TbMg, Co_4USn, Co_4YMg, Cu_4AgZr, Cu_4CaIn, Cu_4DyAg, Cu_4DyAu, Cu_4DyIn, Cu_4ErAg, Cu_4ErAu, Cu_4ErCd, Cu_4ErPd, Cu_4GdAg, Cu_4GdAu, Cu_4GdIn, Cu_4GdPd, Cu_4HoAg, Cu_4HoAu, Cu_4HoCd, Cu_4HoIn, Cu_4InCa, Cu_4InMg, Cu_4InYb, Cu_4LuAu, Cu_4MnSn, Cu_4NdAg, Cu_4NdAu, Cu_4NdMg, Cu_4NdPd, Cu_4ScIn, Cu_4ScSn, Cu_4SmAg, Cu_4SmPd, Cu_4TbAg, Cu_4TbAu, Cu_4TbIn, Cu_4TmAg, Cu_4TmBe, Cu_4TmCd, Cu_4UAg, Cu_4UAu, Cu_4UPd, Cu_4YIn, Cu_4YMg, Cu_4YbAg, Cu_4YbAu, Cu_4YbCd, Cu_4YbIn, Cu_4YbNi, Cu_4YbPd, Ni_4AlU, Ni_4CaMg, Ni_4CeCd, Ni_4CeMg, Ni_4CeMn, Ni_4DyAu, Ni_4DyCd, Ni_4ErAu,

Ni_4ErCd, Ni_4ErMn, Ni_4GdAu, Ni_4GdCd, Ni_4GdIn, Ni_4GdMg, Ni_4HoAu, Ni_4HoCd, Ni_4InU, Ni_4InZr, Ni_4LaMg, Ni_4LuAu, Ni_4LuCd, Ni_4LuSn, Ni_4NdCd, Ni_4NdMg, Ni_4PrCd, Ni_4PrMg, Ni_4ScAu, Ni_4ScCd, Ni_4ScSn, Ni_4SmCd, Ni_4SmMg, Ni_4SnU, Ni_4SnZr, Ni_4TbAu, Ni_4TbCd, Ni_4TbMg, Ni_4TmAu, Ni_4TmCd, Ni_4TmIn, Ni_4UIn, Ni_4USn, Ni_4UZn, Ni_4YAu, Ni_4YCd, Ni_4YIn, Ni_4YMg, Ni_4YMn, Ni_4YbAu, Ni_4YbCd, Ni_4ZnZr, Pt_4CeIn, Pt_4DyIn, Pt_4ErIn, Pt_4EuIn, Pt_4GdIn, Pt_4HoIn, Pt_4LaIn, Pt_4NdIn, Pt_4PrIn, Pt_4SmIn, Pt_4TbIn, Pt_4UAu, Pt_4UIr, Cu_4InMg, Cu_4SnMg, Cu_4SnMn, Ni_4CaMg, Ni_4CeMg, Ni_4DyMg, Ni_4ErMg, Ni_4HoMg, Ni_4LaMg, Ni_4LuMg, Ni_4NdMg, Ni_4PrMg, Ni_4ScMg, Ni_4SmMg, Ni_4TbMg, Ni_4TmMg, Ni_4YMg, Ni_4YbMg

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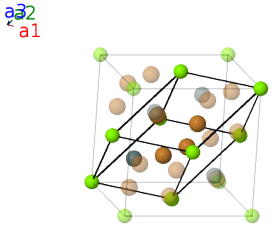
- This is the ternary form of $AuBe_5$, *Strukturbericht* $C15_b$. The original NRL *Crystal Lattice Structure Page* listed it as the prototype $C15_b$. Later we listed both binary and ternary compounds on the same page, but now we have separated them.
- (Osamura, 1978) put the tin atom Sn I on the (4a) site. The AFLOW standard label protocol moves the origin so that the magnesium Mg I atom is on the (4a) site.

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)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	Sn I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Cu I
$\mathbf{B_6}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Cu I

References

[1] K. Osamura and Y. Murakami, *Crystal structures of CuSnMg and Cu_4SnMg ternary compounds*, J. Less-Common Met. **60**, 311–313 (1978), doi:10.1016/0022-5088(78)90185-6.

Found in

[1] ICSD, *Inorganic Crystal Structure Database [MgSnCu4]*. ID 103055.

First cited in

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