$Mg_6Si_7Cu_{16}$ Structure: A16B6C7_cF116_225_2f_e_ad-001

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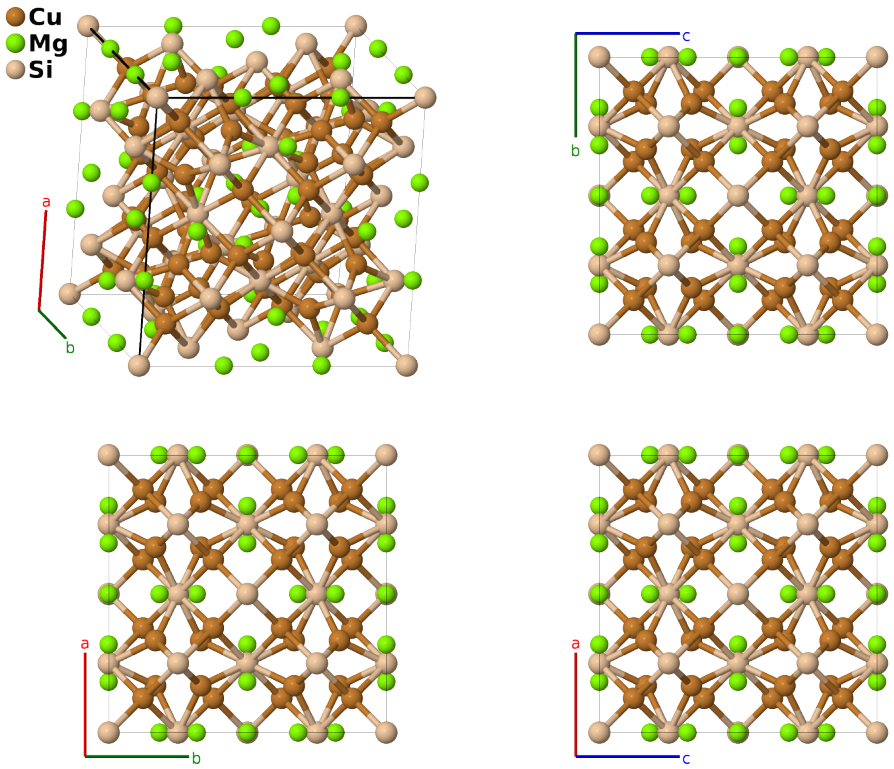
https://aflow.org/p/NHP2

https://aflow.org/p/A16B6C7_cF116_225_2f_e_ad-001



Prototype	$Cu_{16}Mg_6Si_7$
AFLOW prototype label	A16B6C7_cF116_225_2f_e_ad-001
ICSD	16624
Pearson symbol	cF116
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A16B6C7_cF116_225_2f_e_ad-001 --params=`a, x_3, x_4, x_5

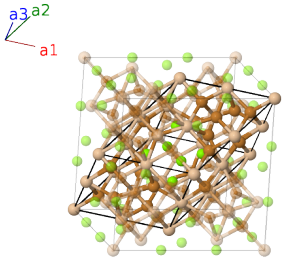
Other compounds with this structure

$Hf_6Ge_7Co_{16}$, $Hf_6Ge_7Ni_{16}$, $Hf_6Si_7Co_{16}$, $Hf_6Si_7Ni_{16}$, $Mg_6Ge_7Ni_{16}$, $Mg_6Si_7Co_{16}$, $Mg_6Si_7Cu_{16}$, $Mg_6Si_7Ni_{16}$, $Mn_6Ge_7Ni_{16}$, $Mn_6Si_7Ni_{16}$, $Nb_6Ge_7Co_{16}$, $Nb_6Ge_7Ni_{16}$, $Nb_6Si_7Co_{16}$, $Nb_6Si_7Ni_{16}$, $Sc_6Ge_7Ni_{16}$, $Sc_6Si_7Co_{16}$, $Sc_6Si_7Ni_{16}$, $Ta_6Ge_7Co_{16}$, $Ta_6Ge_7Ni_{16}$, $Ta_6Si_7Co_{16}$, $Ta_6Si_7Ni_{16}$, $Ti_6Ge_7Ni_{16}$, $Ti_6Si_7Co_{16}$, $Ti_6Si_7Ni_{16}$, $V_6Si_7Ni_{16}$, $Zr_6Ge_7Co_{16}$, $Zr_6Ge_7Ni_{16}$, $Zr_6Si_7Co_{16}$, $Zr_6Si_7Ni_{16}$

- This is the ternary version of Th_6Mn_{23} ($D8_a$).

Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Si I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Si II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Si II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Si II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Si II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(24d)	Si II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Si II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(24e)	Mg I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(24e)	Mg I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(24e)	Mg I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(24e)	Mg I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{z}}$	(24e)	Mg I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{z}}$	(24e)	Mg I
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - 3x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - 3x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{17}}$	=	$-3x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + 3x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1 + 3x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{21}}$	=	$3x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{22}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - 3x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{24}}$	=	$x_5\,\mathbf{a}_1 - 3x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{25}}$	=	$-3x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{26}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + 3x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{27}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II
$\mathbf{B_{28}}$	=	$-x_5\,\mathbf{a}_1 + 3x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(32f)	Cu II

$$\mathbf{B_{29}} = 3x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad \text{(32f)} \quad \text{Cu II}$$

References

[1] G. Bergman and J. L. T. Waugh, *The crystal structure of the intermetallic compound $Mg_6Si_7Cu_{16}$*, Acta Cryst. **9**, 214–217 (1956), doi:10.1107/S0365110X56000632.

Found in

[1] K. L. Holman, E. Morosan, P. A. Casey, L. Li, N. P. Ong, T. Klimczuk, C. Felser, and R. J. Cava, *Crystal structure and physical properties of $Mg_6Cu_{16}Si_7$-type $M_6Ni_{16}Si_7$, for M = Mg, Sc, Ti, Nb, and Ta*, Mater. Res. Bull. **43**, 9–15 (2008), doi:10.1016/j.materresbull.2007.09.023.