

La₃CuSiS₇ Structure: AB3C7D_hP24_173_a_c_b2c_b-001

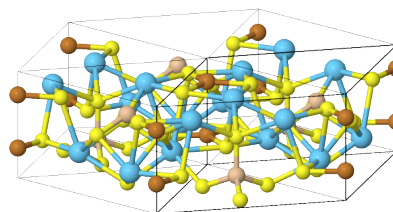
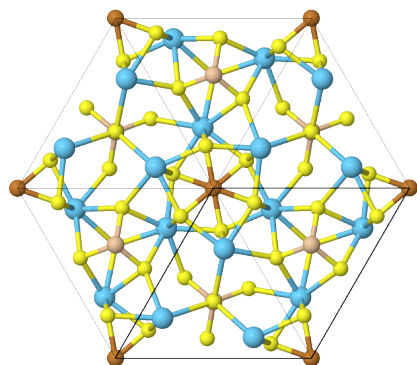
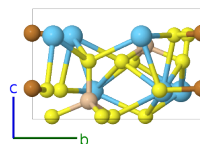
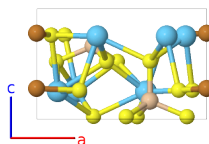
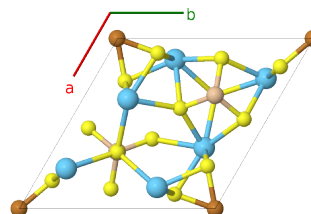
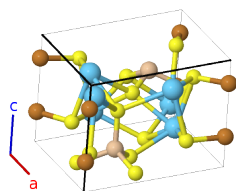
This structure originally had the label AB3C7D_hP24_173_a_c_b2c_b. Calls to that address will be redirected here.

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<https://aflow.org/p/H1TU>

https://aflow.org/p/AB3C7D_hP24_173_a_c_b2c_b-001

● Cu
● La
● S
● Si



Prototype	CuLa ₃ S ₇ Si
AFLOW prototype label	AB3C7D_hP24_173_a_c_b2c_b-001
ICSD	23519
Pearson symbol	hP24
Space group number	173
Space group symbol	<i>P</i> 6 ₃

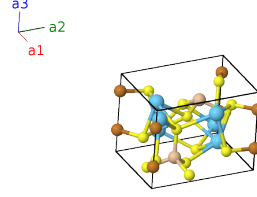
AFLOW prototype command `aflow --proto=AB3C7D_hP24_173_a_c_b2c_b-001`
`--params=a, c/a, z1, z2, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6`

Other compounds with this structure

Ce₃CuGeS₇, Ce₃CuGeSe₇, Ce₃CuSnSe₇, Dy₃CuGeS₇, Gd₃CuGeS₇, Gd₃CuGeSe₇, Ho₃CuGeSe₇, La₃MnFeS₇, Nd₃CuGeS₇, Nd₃CuGeSe₇, Pr₃CuGeS₇, Pr₃CuGeSe₇, Sm₃CuGeS₇, Sm₃CuGeSe₇, Tb₃CuGeS₇, Tb₃CuGeSe₇, Y₃CuSiS₇, Y₃CuSiSe₇

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Cu I
\mathbf{B}_2	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Cu I
\mathbf{B}_3	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	S I
\mathbf{B}_4	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	S I
\mathbf{B}_5	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2b)	Si I
\mathbf{B}_6	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Si I
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_8	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_9	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{11}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{12}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	La I
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{14}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{15}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{16}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{17}	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{18}	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II
\mathbf{B}_{19}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	S III
\mathbf{B}_{20}	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	S III
\mathbf{B}_{21}	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	S III
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S III
\mathbf{B}_{23}	$= y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S III

$$\mathbf{B}_{24} = (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (6c) \quad \text{S III}$$

References

- [1] G. Collin and P. Laruelle, *Structure de $\text{La}_6\text{Cu}_2\text{Si}_2\text{S}_{14}$* , Bull. Soc. fr. Minéral. Cristallogr. **94**, 175–176 (1971), doi:10.3406/bulmi.1971.6576.

Found in

- [1] L. D. Gulay, D. Kaczorowski, and A. Pietraszko, *Crystal structure and magnetic properties of $\text{Ce}_3\text{CuSnSe}_7$* , J. Alloys Compd. **403**, 49–52 (2005), doi:10.1016/j.jallcom.2005.05.030.