

High Temperature Cu₂Se Structure:

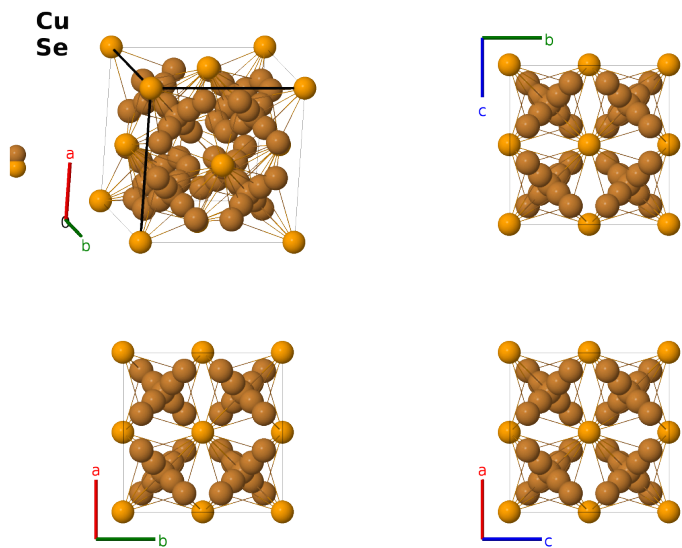
A18B_cF76_225_c2f_a-001

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<https://aflow.org/prototype-encyclopedia/7K0D>

https://aflow.org/prototype-encyclopedia/A18B_cF76_225_c2f_a-001



Prototype	Cu ₂ Se
AFLOW prototype label	A18B_cF76_225_c2f_a-001
Pearson symbol	cF76
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A18B_cF76_225_c2f_a-001</code> <code>--params=a, x₃, x₄</code>

Other compounds with this structure

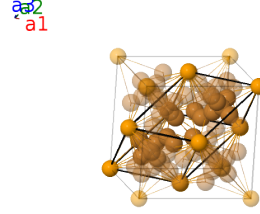
Ag₂Te (HT), Cu_{1.8}S

- Cu₂Se exists in two forms:
 - A low-temperature layered monoclinic structure, and
 - this high-temperature (above $\approx 400\text{K}$) highly disordered superionic cubic structure.
- The data for the rhombohedral phase was taken at room temperature, while the high temperature structure was examined at 415K.

- All of the copper sites in the high temperature phase are partially occupied, with the copper atoms averaging to the positions of the fluorite ($C1$) structure.
- The Cu-I (8c) site has 31% occupancy; the Cu-II (32f) site has 14% occupancy; and the Cu-III (32f) site has 3% occupancy.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Se I
$\mathbf{B}_2$	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(8c) Cu I
$\mathbf{B}_3$	=	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(8c) Cu I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_6$	=	$x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_7$	=	$-3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_8$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + 3x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_9$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_{10}$	=	$-x_3 \mathbf{a}_1 + 3x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_{11}$	=	$3x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(32f) Cu II
$\mathbf{B}_{12}$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{13}$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{14}$	=	$x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{15}$	=	$-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{16}$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + 3x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{17}$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{18}$	=	$-x_4 \mathbf{a}_1 + 3x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(32f) Cu III
$\mathbf{B}_{19}$	=	$3x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(32f) Cu III

References

- [1] L. Gulay, M. Daszkiewicz, O. Strok, and A. Pietraszko, *Crystal structure of Cu₂Se*, Chem. Met. Alloys **4**, 200–205 (2011), doi:10.30970/cma4.0184.

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