High Temperature Cu$_2$Se Structure: A18B_cF76_225_c2f_a-001

https://aflow.org/p/7K0D

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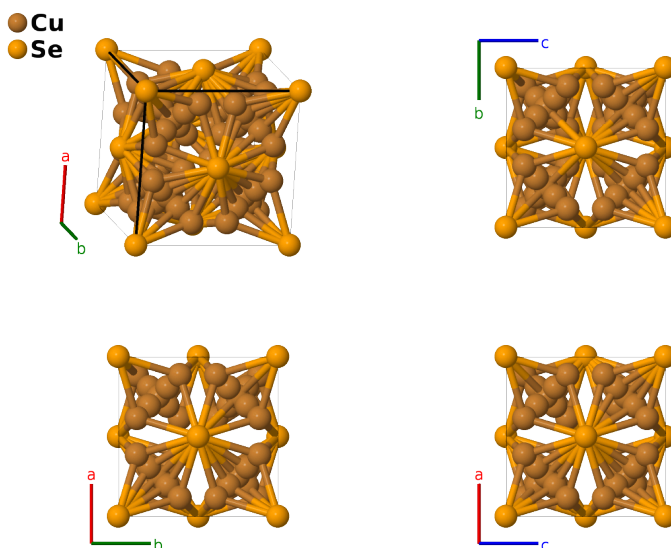
Prototype	Cu$_2$Se
AFLOW prototype label	A18B_cF76_225_c2f_a-001
ICSD	none
Pearson symbol	cF76
Space group number	225
Space group symbol	$Fm\overline{3}m$
AFLOW prototype command	aflow --proto=A18B_cF76_225_c2f_a-001 --params=a, x_3, x_4

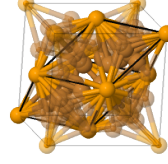**Other compounds with this structure**
Ag$_2$Te (HT), Cu$_{1.8}$S

- Cu$_2$Se exists in two forms:

    - A low-temperature layered monoclinic structure, and
    - this high-temperature (above $\approx$ 400K) 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

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

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Se I
$\mathbf{B_2}$	=	$\tfrac{1}{4}\mathbf{a_1} + \tfrac{1}{4}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_3}$	=	$\tfrac{3}{4}\mathbf{a_1} + \tfrac{3}{4}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$\tfrac{3}{4}a\,\hat{\mathbf{x}} + \tfrac{3}{4}a\,\hat{\mathbf{y}} + \tfrac{3}{4}a\,\hat{\mathbf{z}}$	(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.