

Covellite (CuS, *B18*) Structure: AB_hP12_194_cf_de-001

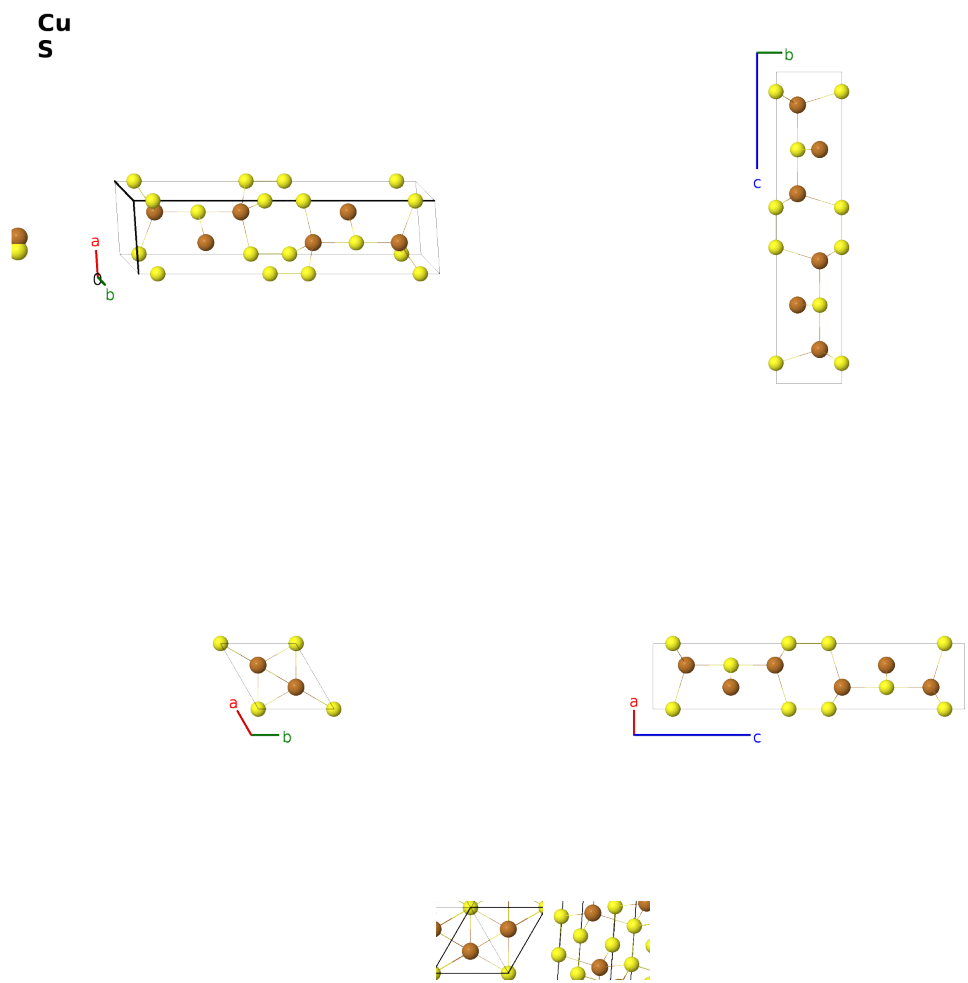
This structure previously used the label(s) **AB_hP12_194_df_ce**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/QP0Q>

https://aflow.org/prototype-encyclopedia/AB_hP12_194_cf_de-001



Prototype	CuS
AFLOW prototype label	AB_hP12_194_cf_de-001
<i>Strukturbericht</i> designation	<i>B18</i>
Mineral name	covellite
ICSD	41975

CCDC	1611696
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	aflow --proto=AB_hP12_194_cf_de-001 --params= $a, c/a, z_3, z_4$

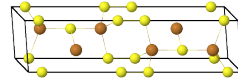
Other compounds with this structure

CuSe

- We did not find an ICSD entry for (Ohmasa, 1977), so we one from (Kalbskopf, 1975) which is quoted our source paper.
- The AFLOW Prototype Label Protocol moves the origin so that the Cu I atom is on the (2c) Wyckoff site rather than the (2d).

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
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Cu I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_6$	$= (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_7$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_8$	$= -(z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f)	Cu II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cu II
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f)	Cu II
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cu II

References

- [1] M. Ohmasa, M. Suzuki, and Y. Takéuchi, *A refinement of the crystal structure of covellite, CuS*, Mineralogical Journal **8**, 311–319 (1977), doi:10.2465/minerj.8.311.
- [2] R. Kalbskopf, F. Pertlik, and J. Zeman, *Verfeinerung des Kristallstruktur des Covellins, Cu S, mit Einkristalldaten*, TMPM Tschermaks Min. Petr. Mitt. **22**, 242–249 (1975).

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