Chalcanthite ($CuSO_4{\cdot}5H_2O$, $H4_{10}$) Structure: AB10C9D_aP42_2_bc_10i_9i_i-001

This structure originally had the label `AB10C9D_aP42_2_ae_10i_9i_i`. Calls to that address will be redirected here.

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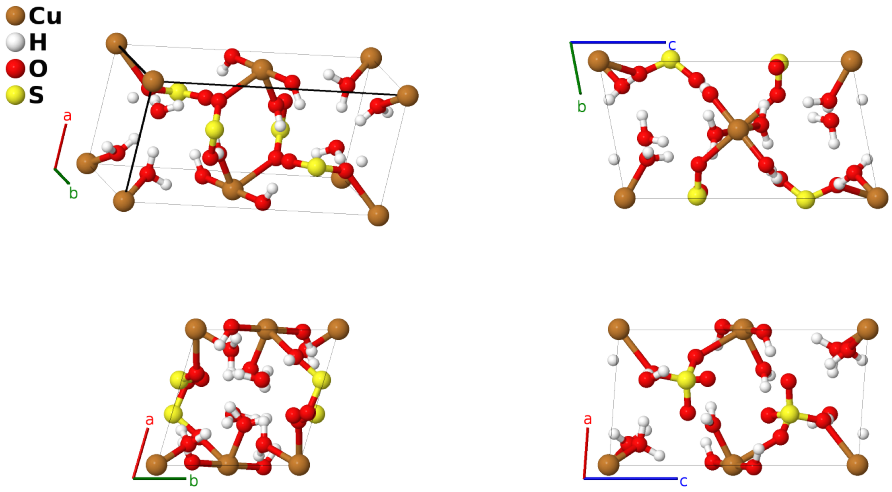
https://aflow.org/p/NQQF

https://aflow.org/p/AB10C9D_aP42_2_bc_10i_9i_i-001

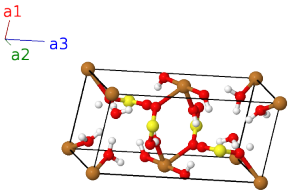


Prototype	$CuH_{10}O_9S$
AFLOW prototype label	AB10C9D_aP42_2_bc_10i_9i_i-001
***Strukturbericht* designation**	$H4_{10}$
Mineral name	chalcanthite
ICSD	4305
Pearson symbol	aP42
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=AB10C9D_aP42_2_bc_10i_9i_i-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$

- We reference (Bacon, 1975) in order to include the positions of the hydrogen atoms.

Triclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}} \\
c_x &= c\cos\beta \\
c_y &= c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c_x\,\hat{\mathbf{x}} + \frac{1}{2}c_y\,\hat{\mathbf{y}} + \frac{1}{2}c_z\,\hat{\mathbf{z}}$	(1b)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\cos\gamma\,\hat{\mathbf{x}} + \frac{1}{2}b\sin\gamma\,\hat{\mathbf{y}}$	(1c)	Cu II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} + c_zz_3\,\hat{\mathbf{z}}$	(2i)	H I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} - c_zz_3\,\hat{\mathbf{z}}$	(2i)	H I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} + c_zz_4\,\hat{\mathbf{z}}$	(2i)	H II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} - c_zz_4\,\hat{\mathbf{z}}$	(2i)	H II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} + c_zz_5\,\hat{\mathbf{z}}$	(2i)	H III
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} - c_zz_5\,\hat{\mathbf{z}}$	(2i)	H III
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} + c_zz_6\,\hat{\mathbf{z}}$	(2i)	H IV
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} - c_zz_6\,\hat{\mathbf{z}}$	(2i)	H IV
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} + c_zz_7\,\hat{\mathbf{z}}$	(2i)	H V
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} - c_zz_7\,\hat{\mathbf{z}}$	(2i)	H V
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} + c_zz_8\,\hat{\mathbf{z}}$	(2i)	H VI
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} - c_zz_8\,\hat{\mathbf{z}}$	(2i)	H VI
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_xz_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_yz_9)\,\hat{\mathbf{y}} + c_zz_9\,\hat{\mathbf{z}}$	(2i)	H VII
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + by_9\cos\gamma + c_xz_9)\,\hat{\mathbf{x}} - (by_9\sin\gamma + c_yz_9)\,\hat{\mathbf{y}} - c_zz_9\,\hat{\mathbf{z}}$	(2i)	H VII
$\mathbf{B_{17}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + by_{10}\cos\gamma + c_xz_{10})\,\hat{\mathbf{x}} + (by_{10}\sin\gamma + c_yz_{10})\,\hat{\mathbf{y}} + c_zz_{10}\,\hat{\mathbf{z}}$	(2i)	H VIII
$\mathbf{B_{18}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + by_{10}\cos\gamma + c_xz_{10})\,\hat{\mathbf{x}} - (by_{10}\sin\gamma + c_yz_{10})\,\hat{\mathbf{y}} - c_zz_{10}\,\hat{\mathbf{z}}$	(2i)	H VIII
$\mathbf{B_{19}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + by_{11}\cos\gamma + c_xz_{11})\,\hat{\mathbf{x}} + (by_{11}\sin\gamma + c_yz_{11})\,\hat{\mathbf{y}} + c_zz_{11}\,\hat{\mathbf{z}}$	(2i)	H IX

$$\mathbf{B_{20}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -\left(ax_{11} + by_{11}\cos\gamma + c_x z_{11}\right)\hat{\mathbf{x}} - \left(by_{11}\sin\gamma + c_y z_{11}\right)\hat{\mathbf{y}} - c_z z_{11}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{H IX}$$

$$\mathbf{B_{21}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} + \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{H X}$$

$$\mathbf{B_{22}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -\left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} - \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} - c_z z_{12}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{H X}$$

$$\mathbf{B_{23}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} + \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} + c_z z_{13}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O I}$$

$$\mathbf{B_{24}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -\left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} - \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} - c_z z_{13}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O I}$$

$$\mathbf{B_{25}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} + \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} + c_z z_{14}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O II}$$

$$\mathbf{B_{26}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -\left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} - \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} - c_z z_{14}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O II}$$

$$\mathbf{B_{27}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = \left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} + \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} + c_z z_{15}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O III}$$

$$\mathbf{B_{28}} = -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -\left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} - \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} - c_z z_{15}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O III}$$

$$\mathbf{B_{29}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = \left(ax_{16} + by_{16}\cos\gamma + c_x z_{16}\right)\hat{\mathbf{x}} + \left(by_{16}\sin\gamma + c_y z_{16}\right)\hat{\mathbf{y}} + c_z z_{16}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O IV}$$

$$\mathbf{B_{30}} = -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -\left(ax_{16} + by_{16}\cos\gamma + c_x z_{16}\right)\hat{\mathbf{x}} - \left(by_{16}\sin\gamma + c_y z_{16}\right)\hat{\mathbf{y}} - c_z z_{16}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O IV}$$

$$\mathbf{B_{31}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = \left(ax_{17} + by_{17}\cos\gamma + c_x z_{17}\right)\hat{\mathbf{x}} + \left(by_{17}\sin\gamma + c_y z_{17}\right)\hat{\mathbf{y}} + c_z z_{17}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O V}$$

$$\mathbf{B_{32}} = -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -\left(ax_{17} + by_{17}\cos\gamma + c_x z_{17}\right)\hat{\mathbf{x}} - \left(by_{17}\sin\gamma + c_y z_{17}\right)\hat{\mathbf{y}} - c_z z_{17}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O V}$$

$$\mathbf{B_{33}} = x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = \left(ax_{18} + by_{18}\cos\gamma + c_x z_{18}\right)\hat{\mathbf{x}} + \left(by_{18}\sin\gamma + c_y z_{18}\right)\hat{\mathbf{y}} + c_z z_{18}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VI}$$

$$\mathbf{B_{34}} = -x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -\left(ax_{18} + by_{18}\cos\gamma + c_x z_{18}\right)\hat{\mathbf{x}} - \left(by_{18}\sin\gamma + c_y z_{18}\right)\hat{\mathbf{y}} - c_z z_{18}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VI}$$

$$\mathbf{B_{35}} = x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = \left(ax_{19} + by_{19}\cos\gamma + c_x z_{19}\right)\hat{\mathbf{x}} + \left(by_{19}\sin\gamma + c_y z_{19}\right)\hat{\mathbf{y}} + c_z z_{19}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VII}$$

$$\mathbf{B_{36}} = -x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -\left(ax_{19} + by_{19}\cos\gamma + c_x z_{19}\right)\hat{\mathbf{x}} - \left(by_{19}\sin\gamma + c_y z_{19}\right)\hat{\mathbf{y}} - c_z z_{19}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VII}$$

$$\mathbf{B_{37}} = x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = \left(ax_{20} + by_{20}\cos\gamma + c_x z_{20}\right)\hat{\mathbf{x}} + \left(by_{20}\sin\gamma + c_y z_{20}\right)\hat{\mathbf{y}} + c_z z_{20}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VIII}$$

$$\mathbf{B_{38}} = -x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3 = -\left(ax_{20} + by_{20}\cos\gamma + c_x z_{20}\right)\hat{\mathbf{x}} - \left(by_{20}\sin\gamma + c_y z_{20}\right)\hat{\mathbf{y}} - c_z z_{20}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O VIII}$$

$$\mathbf{B_{39}} = x_{21}\,\mathbf{a}_1 + y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3 = \left(ax_{21} + by_{21}\cos\gamma + c_x z_{21}\right)\hat{\mathbf{x}} + \left(by_{21}\sin\gamma + c_y z_{21}\right)\hat{\mathbf{y}} + c_z z_{21}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O IX}$$

$$\mathbf{B_{40}} = -x_{21}\,\mathbf{a}_1 - y_{21}\,\mathbf{a}_2 - z_{21}\,\mathbf{a}_3 = -\left(ax_{21} + by_{21}\cos\gamma + c_x z_{21}\right)\hat{\mathbf{x}} - \left(by_{21}\sin\gamma + c_y z_{21}\right)\hat{\mathbf{y}} - c_z z_{21}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{O IX}$$

$$\mathbf{B_{41}} = x_{22}\,\mathbf{a}_1 + y_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3 = \left(ax_{22} + by_{22}\cos\gamma + c_x z_{22}\right)\hat{\mathbf{x}} + \left(by_{22}\sin\gamma + c_y z_{22}\right)\hat{\mathbf{y}} + c_z z_{22}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{S I}$$

$$\mathbf{B_{42}} = -x_{22}\,\mathbf{a}_1 - y_{22}\,\mathbf{a}_2 - z_{22}\,\mathbf{a}_3 = -\left(ax_{22} + by_{22}\cos\gamma + c_x z_{22}\right)\hat{\mathbf{x}} - \left(by_{22}\sin\gamma + c_y z_{22}\right)\hat{\mathbf{y}} - c_z z_{22}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{S I}$$

References

[1] G. E. Bacon and D. H. Titterdon, *Neutron-diffraction studies of $CuSO_4 \cdot 5H_2O$ and $CuSO_4 \cdot 5D_2O$*, Z. Kristallogr. **141**, 330–341 (1975), doi:10.1524/zkri.1975.141.16.330.

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[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).