

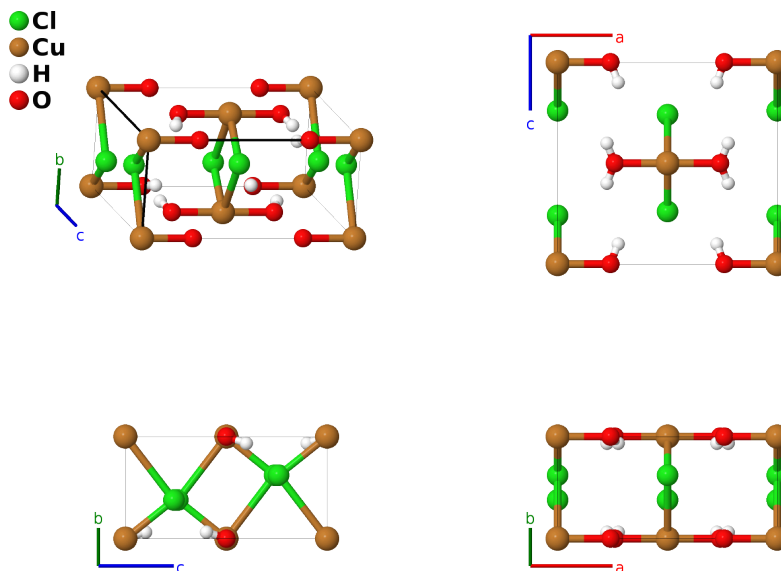
Eriochalcite ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, $C45$) Structure: A2BC4D2_oP18_53_h_a_i_e-001

This structure originally had the label `A2BC4D2_oP18_53_h_a_i_e`. Calls to that address will be redirected here.

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

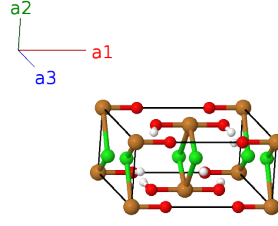
https://aflow.org/p/A2BC4D2_oP18_53_h_a_i_e-001



Prototype	$\text{Cl}_2\text{CuH}_4\text{O}_2$
AFLOW prototype label	A2BC4D2_oP18_53_h_a_i_e-001
<i>Strukturbericht</i> designation	$C45$
Mineral name	eriochalcite
ICSD	40290
Pearson symbol	oP18
Space group number	53
Space group symbol	$Pmna$
AFLOW prototype command	<code>aflow --proto=A2BC4D2_oP18_53_h_a_i_e-001 --params=a, b/a, c/a, x2, y3, z3, x4, y4, z4</code>

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Cu I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Cu I
\mathbf{B}_3	$x_2 \mathbf{a}_1$	$=$	$a x_2 \hat{\mathbf{x}}$	(4e)	O I
\mathbf{B}_4	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_5	$-x_2 \mathbf{a}_1$	$=$	$-a x_2 \hat{\mathbf{x}}$	(4e)	O I
\mathbf{B}_6	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_7	$y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4h)	Cl I
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Cl I
\mathbf{B}_9	$\frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Cl I
\mathbf{B}_{10}	$-y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4h)	Cl I
\mathbf{B}_{11}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{12}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{13}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{14}	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{15}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{16}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{17}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	H I
\mathbf{B}_{18}	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8i)	H I

References

- [1] S. Brownstein, N. F. Han, E. Gabe, and Y. LePage, *A redetermination of the crystal structure of cupric chloride dihydrate*, Z. Kristallogr. **189**, 13–15 (1989), doi:10.1524/zkri.1989.189.1-2.13.