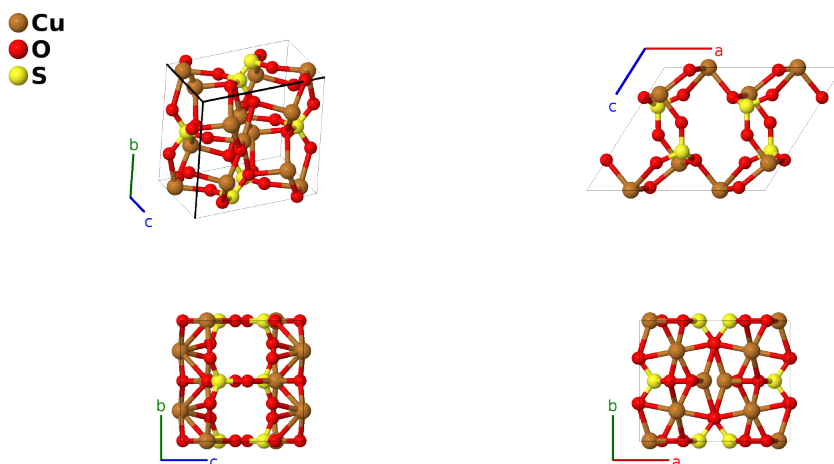


Dolerophanite [Cu₂O(SO₄)] Structure: A2B5C_mC32_12_ei_3ij_i-001

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<https://afLOW.org/p/H100>

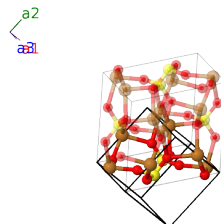
https://afLOW.org/p/A2B5C_mC32_12_ei_3ij_i-001



Prototype	Cu ₂ O ₅ S
AFLOW prototype label	A2B5C_mC32_12_ei_3ij_i-001
Mineral name	dolerophanite
ICSD	34649
Pearson symbol	mC32
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	afLOW --proto=A2B5C_mC32_12_ei_3ij_i-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>x</i> ₂ , <i>z</i> ₂ , <i>x</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>z</i> ₄ , <i>x</i> ₅ , <i>z</i> ₅ , <i>x</i> ₆ , <i>z</i> ₆ , <i>x</i> ₇ , <i>y</i> ₇ , <i>z</i> ₇

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Cu I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Cu I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cu II
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Cu II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O I
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_9	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	O III
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	O III
\mathbf{B}_{11}	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	S I
\mathbf{B}_{12}	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	S I
\mathbf{B}_{13}	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{14}	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{15}	$= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
\mathbf{B}_{16}	$= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV

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