$Cu_2Ta_4O_{11}$ Structure: A3B11C4_hR36_167_d_cef_be-001

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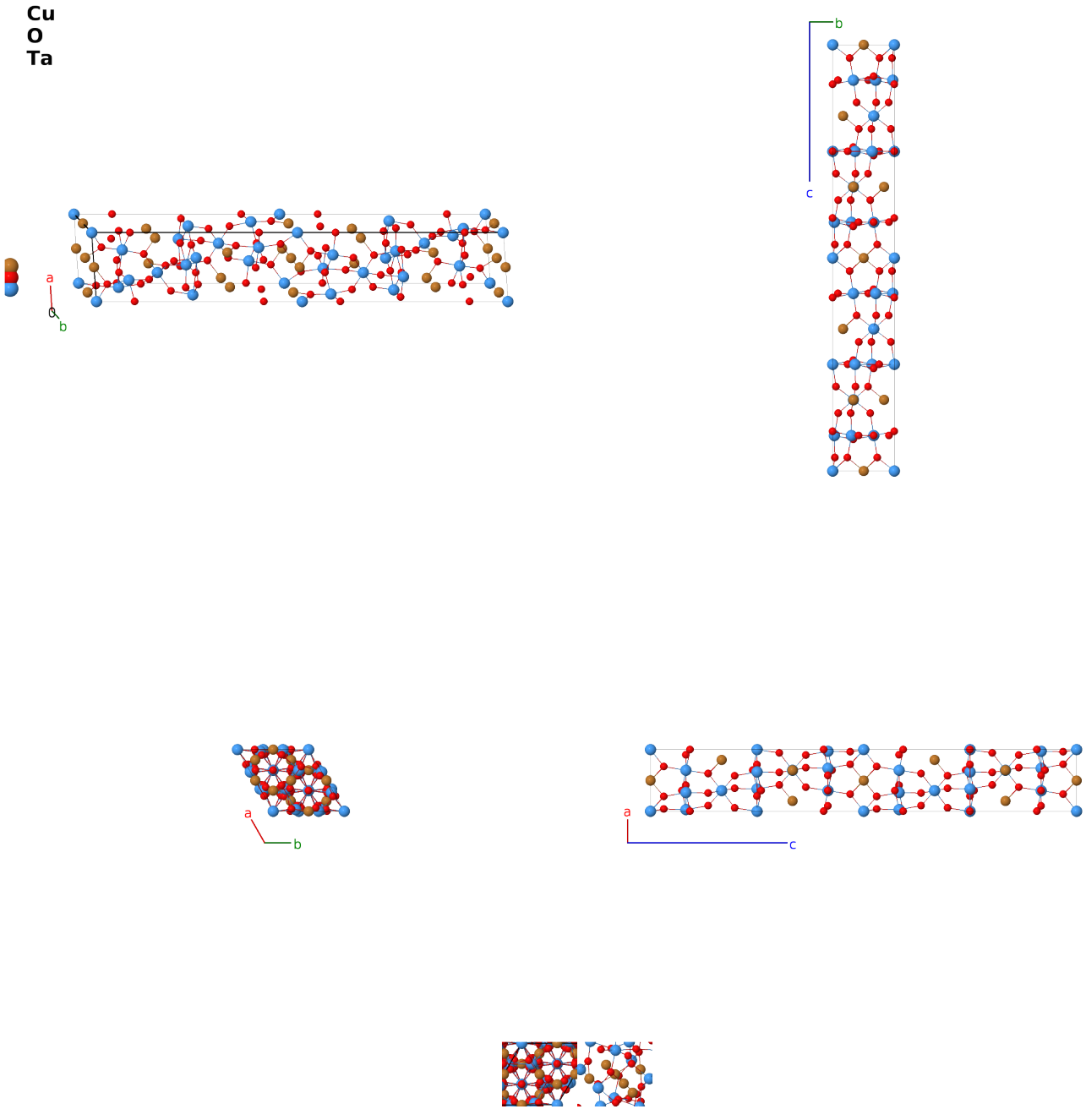
https://aflow.org/prototype-encyclopedia/AGLP

https://aflow.org/prototype-encyclopedia/A3B11C4_hR36_167_d_cef_be-001

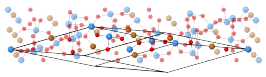


Prototype	$Cu_2O_{11}Ta_4$
AFLOW prototype label	A3B11C4_hR36_167_d_cef_be-001
ICSD	194463
CCDC	1703148
Pearson symbol	hR36
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A3B11C4_hR36_167_d_cef_be-001 --params=`$a, c/a, x_2, x_4, x_5, x_6, y_6, z_6$

- Only two-thirds of the (6d) site are filled with copper atoms.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Ta I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ta I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6d)	Cu I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\left(4x_4 - 1\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II

$\mathbf{B_{14}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,(4x_4 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_4 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{15}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{16}}$	$=$	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_4 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_4 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{17}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_4 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_4 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{18}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O II
$\mathbf{B_{19}}$	$=$	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,(4x_5 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_5 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{20}}$	$=$	$\frac{1}{4}\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{8}a\,(4x_5 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_5 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{21}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{22}}$	$=$	$-x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_5 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_5 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{23}}$	$=$	$\frac{3}{4}\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{8}a\,(4x_5 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_5 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{24}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Ta II
$\mathbf{B_{25}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{26}}$	$=$	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{27}}$	$=$	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{28}}$	$=$	$-\left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{29}}$	$=$	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{30}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 - 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{31}}$	$=$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{32}}$	$=$	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{33}}$	$=$	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{34}}$	$=$	$\left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{35}}$	$=$	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B_{36}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_6 + 2y_6 + 2z_6 + 3)\,\hat{\mathbf{z}}$	(12f)	O III

References

[1] N. King, R. D. Sommer, P. Watkins-Curry, J. Y. Chan, and P. A. Maggard, *Synthesis, Structure, and Thermal Instability of the $Cu_2Ta_4O_{11}$ Phase*, Crystal Growth & Design **15**, 552–558 (2015), doi:10.1021/cg500987c.

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