$Cu_2Ta_4O_{12}$ Structure: A3B12C4_oP38_47_bcdefg_uvwxyz_A-001

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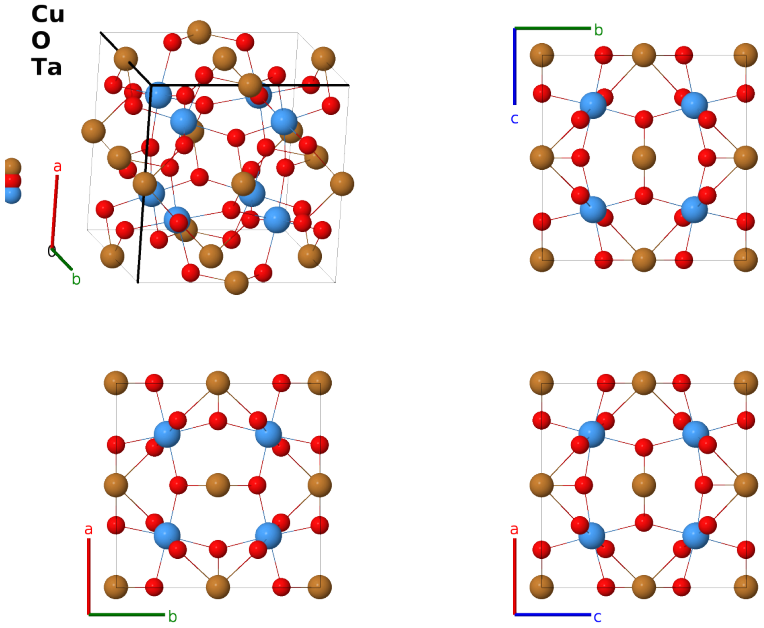
https://aflow.org/prototype-encyclopedia/TM8T

https://aflow.org/prototype-encyclopedia/A3B12C4_oP38_47_bcdefg_uvwxyz_A-001

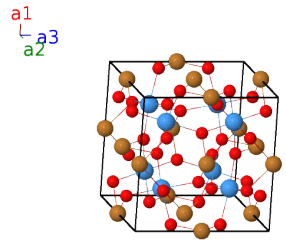


Prototype	$Cu_2Ta_4O_{12}$
AFLOW prototype label	A3B12C4_oP38_47_bcdefg_uvwxyz_A-001
ICSD	160741
CCDC	1677155
Pearson symbol	oP38
Space group number	47
Space group symbol	$Pmmm$
AFLOW prototype command	`aflow --proto=A3B12C4_oP38_47_bcdefg_uvwxyz_A-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, y_8, z_8, y_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, y_{12}, x_{13}, y_{13}$

- This structure is nearly cubic. An uncertainty of 0.2Å in the atomic positions transforms it into a structure resembling $CaCu_3Mn_4O_{12}$ with the calcium ions removed. This is a body-centered cubic structure in space group $Im\bar{3}$ #204.
- (Ebbinghaus, 2007) gives the stoichiometry of the sample as $Cu_{2+x}Ta_4O_{12+\delta}$, with x=0.125 and no information on δ. This value of x indicates that about 72% of the copper sites are occupied. The published site-occupancy factors (SOF) do not add up to anything near this result. The ICSD uses a completely different set of SOF with occupations between 42 and 100%, yielding a final composition of $Cu_{3.976}Ta_4O_{12}$. The CIF associated with this page lists the ICSD SOF.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_8}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8A)	Ta I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(1b)	Cu I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1c)	Cu II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Cu III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(1e)	Cu IV
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(1f)	Cu V
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1g)	Cu VI
$\mathbf{B_{15}}$	=	$y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4u)	O I
$\mathbf{B_{16}}$	=	$-y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4u)	O I
$\mathbf{B_{17}}$	=	$y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4u)	O I
$\mathbf{B_{18}}$	=	$-y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4u)	O I
$\mathbf{B_{19}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4v)	O II
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4v)	O II
$\mathbf{B_{21}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4v)	O II
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4v)	O II
$\mathbf{B_{23}}$	=	$x_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(4w)	O III
$\mathbf{B_{24}}$	=	$-x_{10}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(4w)	O III
$\mathbf{B_{25}}$	=	$-x_{10}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(4w)	O III
$\mathbf{B_{26}}$	=	$x_{10}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(4w)	O III
$\mathbf{B_{27}}$	=	$x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4x)	O IV
$\mathbf{B_{28}}$	=	$-x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4x)	O IV

$\mathbf{B_{29}}$	=	$-x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(4x)	O IV
$\mathbf{B_{30}}$	=	$x_{11}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(4x)	O IV
$\mathbf{B_{31}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2$	=	$ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}}$	(4y)	O V
$\mathbf{B_{32}}$	=	$-x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2$	=	$-ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}}$	(4y)	O V
$\mathbf{B_{33}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2$	=	$-ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}}$	(4y)	O V
$\mathbf{B_{34}}$	=	$x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2$	=	$ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}}$	(4y)	O V
$\mathbf{B_{35}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4z)	O VI
$\mathbf{B_{36}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4z)	O VI
$\mathbf{B_{37}}$	=	$-x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4z)	O VI
$\mathbf{B_{38}}$	=	$x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4z)	O VI

References

[1] S. G. Ebbinghaus, *Influence of composition and thermal treatment on the properties of* $Cu_{2+x}\,Ta_4O_{12} + \delta$, Prog. Solid State Chem. **35**, 421–431 (2007), doi:10.1016/j.progsolidstchem.2007.01.032.

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