$Cu_3(P_2O_6OH)_2$ Structure: A3B12C2D4_aP21_2_ai_6i_i_2i-001

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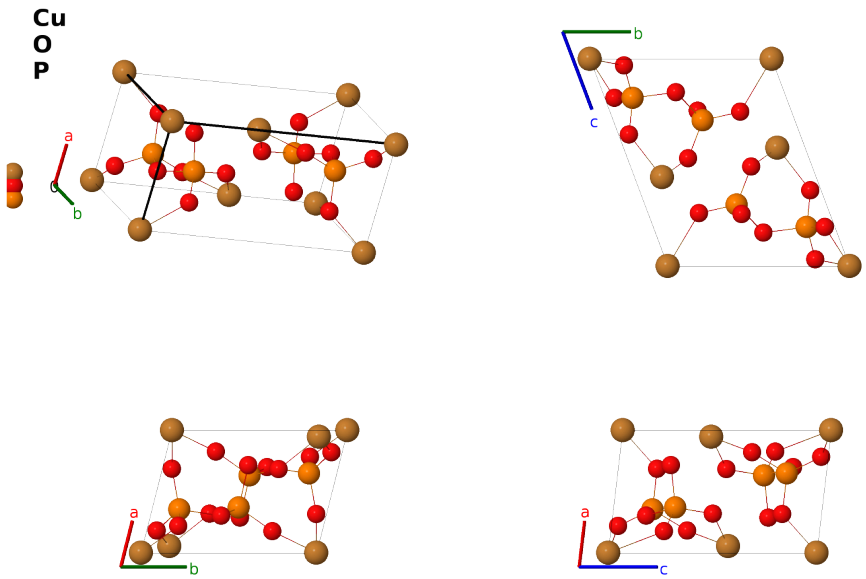
https://aflow.org/prototype-encyclopedia/L1KQ

https://aflow.org/prototype-encyclopedia/A3B12C2D4_aP21_2_ai_6i_i_2i-001

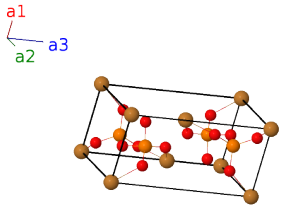


Prototype	$Cu_3O_{12}(OH)_2P_4$
AFLOW prototype label	A3B12C2D4_aP21_2_ai_6i_i_2i-001
ICSD	170128
CCDC	1685757
Pearson symbol	aP21
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A3B12C2D4_aP21_2_ai_6i_i_2i-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- The positions of the hydrogen atoms in the OH radicals were not determined. While we list the radical as a separate species, OH I, (Baies, 2005) simply list it as O7.
- The positions of the oxygen atoms in the ICSD entry do not precisely match the positions in Table 2 of (Baies, 2005).

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(2i)	Cu II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} - (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} - c_z z_2\,\hat{\mathbf{z}}$	(2i)	Cu II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} - c_z z_4\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} - c_z z_5\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} - c_z z_6\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_{12}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B_{13}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} - c_z z_7\,\hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B_{15}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} - c_z z_8\,\hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B_{16}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} + c_z z_9\,\hat{\mathbf{z}}$	(2i)	OH I
$\mathbf{B_{17}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} - (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} - c_z z_9\,\hat{\mathbf{z}}$	(2i)	OH I

$\mathbf{B_{18}}$	$=$	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	$=$	$(ax_{10} + by_{10}\cos\gamma + c_x z_{10})\,\hat{\mathbf{x}} +$ $(by_{10}\sin\gamma + c_y z_{10})\,\hat{\mathbf{y}} + c_z z_{10}\,\hat{\mathbf{z}}$	(2i)	P I
$\mathbf{B_{19}}$	$=$	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	$=$	$-(ax_{10} + by_{10}\cos\gamma + c_x z_{10})\,\hat{\mathbf{x}} -$ $(by_{10}\sin\gamma + c_y z_{10})\,\hat{\mathbf{y}} - c_z z_{10}\,\hat{\mathbf{z}}$	(2i)	P I
$\mathbf{B_{20}}$	$=$	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$(ax_{11} + by_{11}\cos\gamma + c_x z_{11})\,\hat{\mathbf{x}} +$ $(by_{11}\sin\gamma + c_y z_{11})\,\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}}$	(2i)	P II
$\mathbf{B_{21}}$	$=$	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	$=$	$-(ax_{11} + by_{11}\cos\gamma + c_x z_{11})\,\hat{\mathbf{x}} -$ $(by_{11}\sin\gamma + c_y z_{11})\,\hat{\mathbf{y}} - c_z z_{11}\,\hat{\mathbf{z}}$	(2i)	P II

References

[1] R. Baies, V. Caignaert, V. Pralong, and B. Raveau, *Copper Hydroxydiphosphate with a One-Dimensional Arrangement of Copper Polyhedra: $Cu_3[P_2O_6OH]_2$*, Inorganic Chemistry **44**, 2376–2380 (2005), doi:10.1021/ic0485209.

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