Cu_3P Structure: A3B_hP24_185_ab2c_c-001

This structure originally had the label `A3B_hP24_185_ab2c_c`. Calls to that address will be redirected here.

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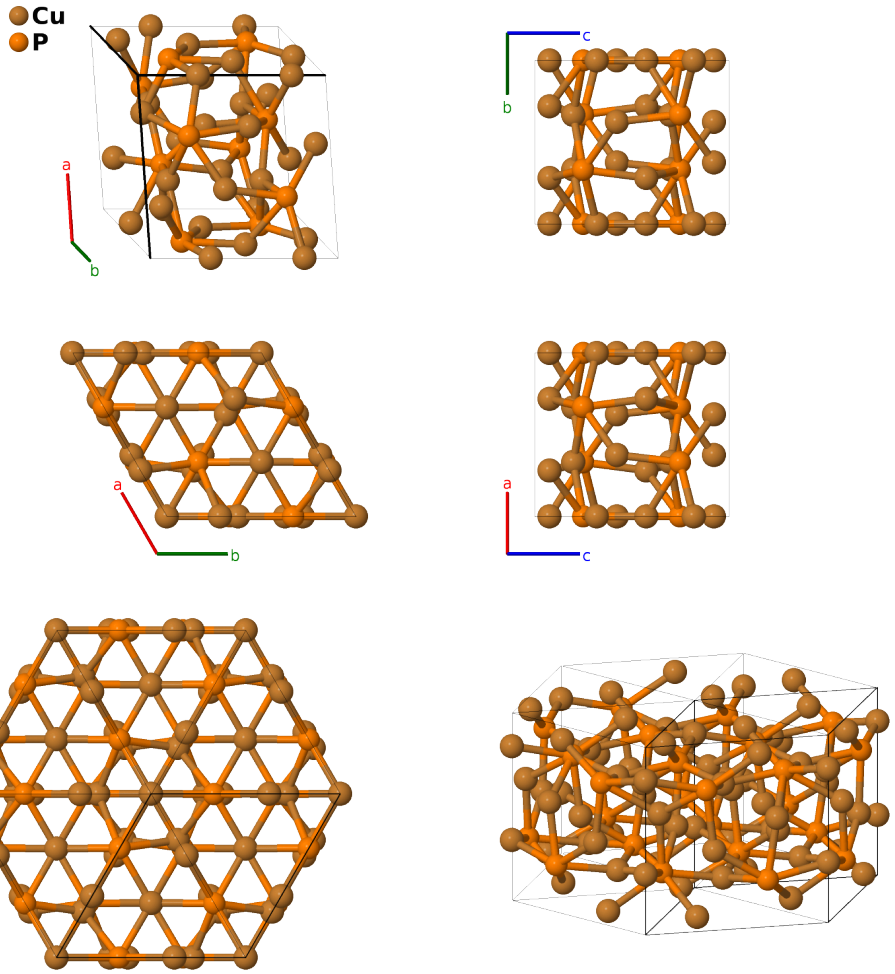
https://aflow.org/p/L8U5

https://aflow.org/p/A3B_hP24_185_ab2c_c-001



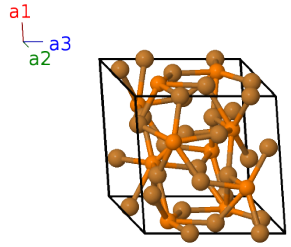
Prototype	Cu_3P
AFLOW prototype label	A3B_hP24_185_ab2c_c-001
ICSD	15056
Pearson symbol	hP24
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	`aflow --proto=A3B_hP24_185_ab2c_c-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
Mg_3Au, Mg_3Ir, Mg_3Pt, Na_3As

- (Olofsson, 1972) argues that this is the correct structure for Cu_3P rather than the structure which was originally identified as *Strukturbericht* $D0_{21}$, space group $P\bar{3}c1$ #165. Hafner and Range (Hafner, 1994) state that this is also the correct structure for Na_3As, rather than *Strukturbericht* $D0_{18}$, space group $P6_3/mmc$ #194. Finally, $AuMg_3$, $IrMg_3$ and Mg_3Pt, which have been placed in the $D0_{18}$ and $D0_{21}$ structures, are also claimed to actually be in this structure (Range, 1993).
- Space group $P6_3cm$ #185 allows an arbitary choice of the origin of the z-axis. Here we set $z_5 = 3/4$ for the phosporous (6c) atoms.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4b)	Cu II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+cz_3\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+cz_4\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cu IV
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	P I
$\mathbf{B_{21}}$	=	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+cz_5\,\hat{\mathbf{z}}$	(6c)	P I

$$\mathbf{B_{22}} = -x_5\,\mathbf{a}_1 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}ax_5\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{P I}$$

$$\mathbf{B_{23}} = -x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}ax_5\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{P I}$$

$$\mathbf{B_{24}} = x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(6c)} \quad \text{P I}$$

References

[1] O. Olofsson, *The Crystal Structure of Cu_3P*, Acta Chem. Scand. **26**, 2777–2787 (1972), doi:10.3891/acta.chem.scand.26-2771.

[2] P. Hafner and K.-J. Range, *Na_3As revisited: high-pressure synthesis of single crystals and structure refinement*, J. Alloys Compd. **216**, 7–10 (1994), doi:10.1016/0925-8388(94)91033-2.

[3] K.-J. Range and P. Hafner, *Structure refinement of $AuMg_3$, $IrMg_3$ and $IrMg_{2.8}$*, J. Alloys Compd. **191**, L5–L7 (1993), doi:10.1016/0925-8388(93)90053-P.