Cu_3P ($D0_{21}$) Structure: A3B_hP24_165_bdg_f-001

This structure previously used the label(s) `A3B_hP24_165_bdg_f`. Calls to these addresses will be redirected here.

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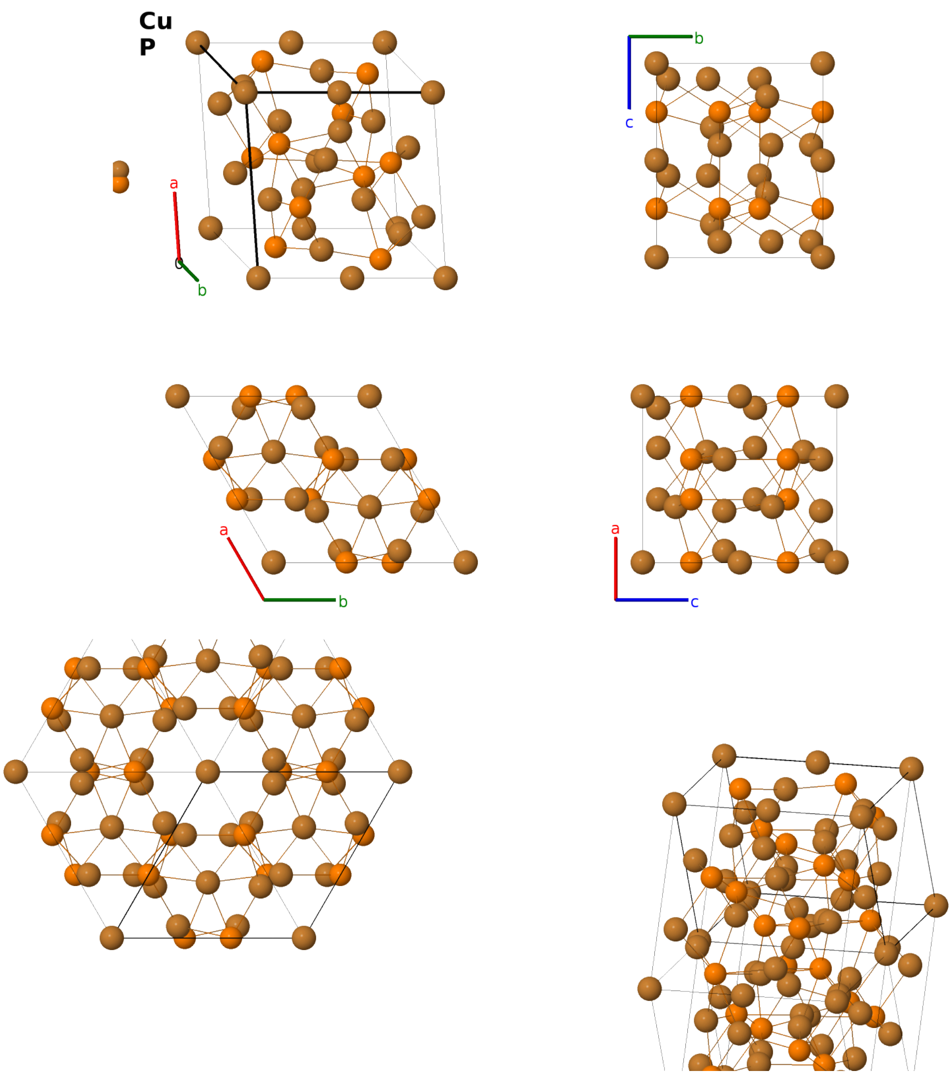
https://aflow.org/prototype-encyclopedia/Z2X0

https://aflow.org/prototype-encyclopedia/A3B_hP24_165_bdg_f-001



Prototype Cu_3P

AFLOW prototype label A3B_hP24_165_bdg_f-001

***Strukturbericht* designation** $D0_{21}$

ICSD 198370

CCDC	1925272
Pearson symbol	hP24
Space group number	165
Space group symbol	$P\overline{3}c1$
AFLOW prototype command	`aflow --proto=A3B_hP24_165_bdg_f-001` `--params=`$a, c/a, z_2, x_3, x_4, y_4, z_4$

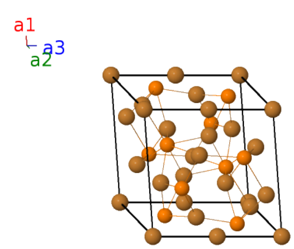
Other compounds with this structure

Cu_3As, Cd_3Au, Mg_3Au, Mg_3Ir, Mg_3Pt, Na_3As, CeF_3, LaF_3

- Range and Hafner (Range, 1993) and Olofsson (Olofsson, 1972) argue that several compounds which were previously identified as having this structure actually take on the Cu_3P structure, space group $P63cm$ #185, A3B_hP24_185_ab2c_c. These structures include Cu_3P, Na_3As, $AuMg_3$, Ir_3 and Mg_3Pt. The $D0_{21}$ structure is crystallographically equivalent to the H_3Ho structure, A3B_hP24_165_adg_f.
- We have not found any evidence in the literature showing that either the hydride structure or the fluoride structures mentioned above should be in any other space group.
- We were unable to obtain the original reference, so we use the crystallographic information presented in the American Mineralogist Crystal Structure Database (Downs, 2003).
- The original version of Pearson's Handbook (Pearson, 1958) states that the lattice constants for this structure should be slightly smaller.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\mathbf{\hat{z}}$	(2b)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(4d)	Cu II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Cu II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(4d)	Cu II
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Cu II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	P I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	P I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	P I

$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	P I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	P I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6f)	P I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4-y_4\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4-2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{15}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{17}}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - \left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4-2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4-y_4\right)\,\mathbf{a}_2 - \left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4-y_4\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4+2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{21}}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{22}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{23}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4+2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III
$\mathbf{B_{24}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4-y_4\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12g)	Cu III

References

[1] B. Steenberg, *The Crystal Structure of Cu_3As and Cu_3P*, Arkiv for Kemi, Min. Geol. **A12**, 1–15 (1938).

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, no. N.R.C. No. 4303 in International Series of Monographs on Metal Physics and Physical Metallurgy (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.

[2] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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