$K_3Cu_3P_2$: A3B3C2_hR8_166_d_ac_c-001

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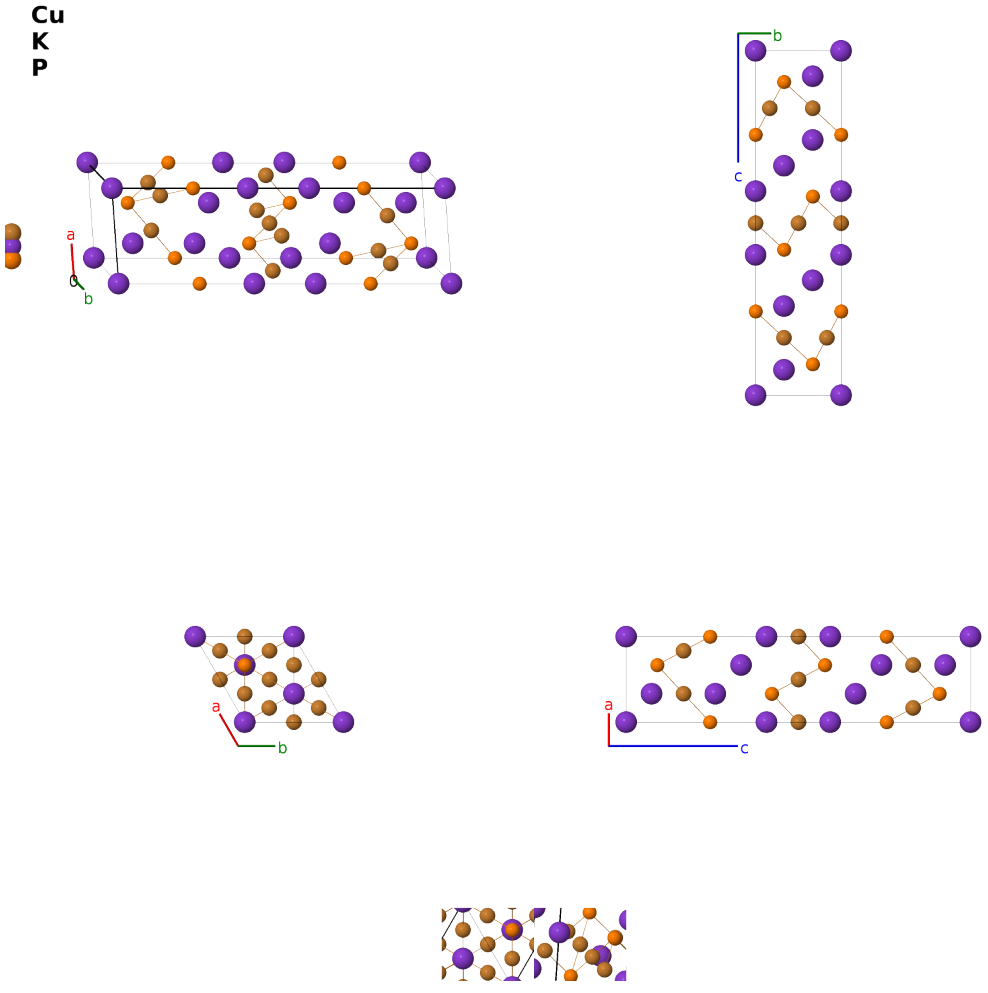
https://aflow.org/prototype-encyclopedia/V94K

https://aflow.org/prototype-encyclopedia/A3B3C2_hR8_166_d_ac_c-001



Prototype	$Cu_3K_3P_2$
AFLOW prototype label	A3B3C2_hR8_166_d_ac_c-001
ICSD	12163
CCDC	1595407
Pearson symbol	hR8
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A3B3C2_hR8_166_d_ac_c-001 --params=`$a, c/a, x_2, x_3$

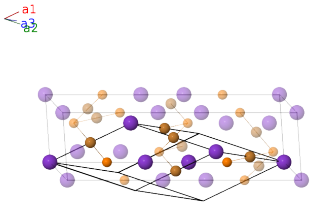
Other compounds with this structure

$K_3Ag_3As_2$, $K_3Au_3Sb_2$, $K_3Cu_3As_2$, $Rb_3Au_3Sb_2$, $Rb_3Cu_3As_2$

- The AFLOW prototype label protocol moves the K I atom from the (1b) site, as given in (Savelsberg, 1978) to the (1a) site, shifting all atomic coordinates by (0 , 0 , 1/2 c).
- This structure is given in the rhombohedral setting of space group $R\bar{3}m$ #166. The hexagonal setting may be obtained by adding `--hex` to the aflow command.

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	(1a)	K I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	K II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	K II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Cu I

References

[1] G. Savelsberg and H. Schäfer, *Darstellung und Kristallstruktur von $K_3Cu_3P_2$*, Z. Naturforsch. B **33**, 590–592 (1978), doi:10.1515/znb-1978-0604.

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