KCu_4S_3 Structure: A4BC3_tP8_123_i_a_bh-001

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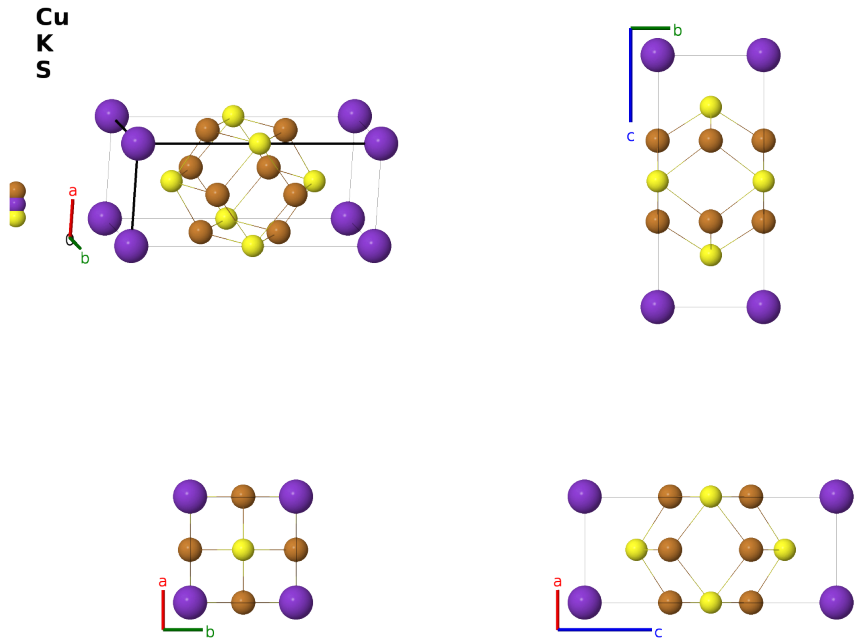
https://aflow.org/prototype-encyclopedia/RPTR

https://aflow.org/prototype-encyclopedia/A4BC3_tP8_123_i_a_bh-001



Prototype	Cu_4KS_3
AFLOW prototype label	A4BC3_tP8_123_i_a_bh-001
ICSD	23336
CCDC	1599462
Pearson symbol	tP8
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A4BC3_tP8_123_i_a_bh-001 --params=`$a, c/a, z_3, z_4$

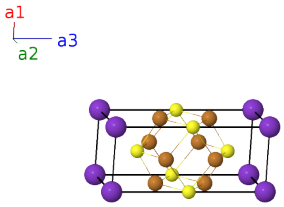
Other compounds with this structure

$CsCu_4S_3$, $CsCu_4Se_3$, KCu_4Se_3, $RbCu_4S_3$, $RbCu_4Se_3$, $TlCu_4S_3$, $TlCu_4Se_3$

- The standard AFLOW label moves the origin from the S-I atom reported by (Brown, 1980) to the K-I atom.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	S I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2h)	S II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2h)	S II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4i)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4i)	Cu I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4i)	Cu I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(4i)	Cu I

References

[1] D. B. Brown, J. A. Zubieta, P. A. Vella, J. T. Wrobleski, T. Watt, W. E. Hatfield, and P. Day, *Solid-state structure and electronic properties of a mixed-valence two-dimensional metal, potassium copper sulfide (KCu_4S_3)*, Inorg. Chem. **19**, 1945–1950 (1980), doi:10.1021/ic50209a024.

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