Mooihoekite ($Cu_9Fe_9S_{16}$) Structure: A9B9C16_tP34_111_ajn_bcdek_2no-001

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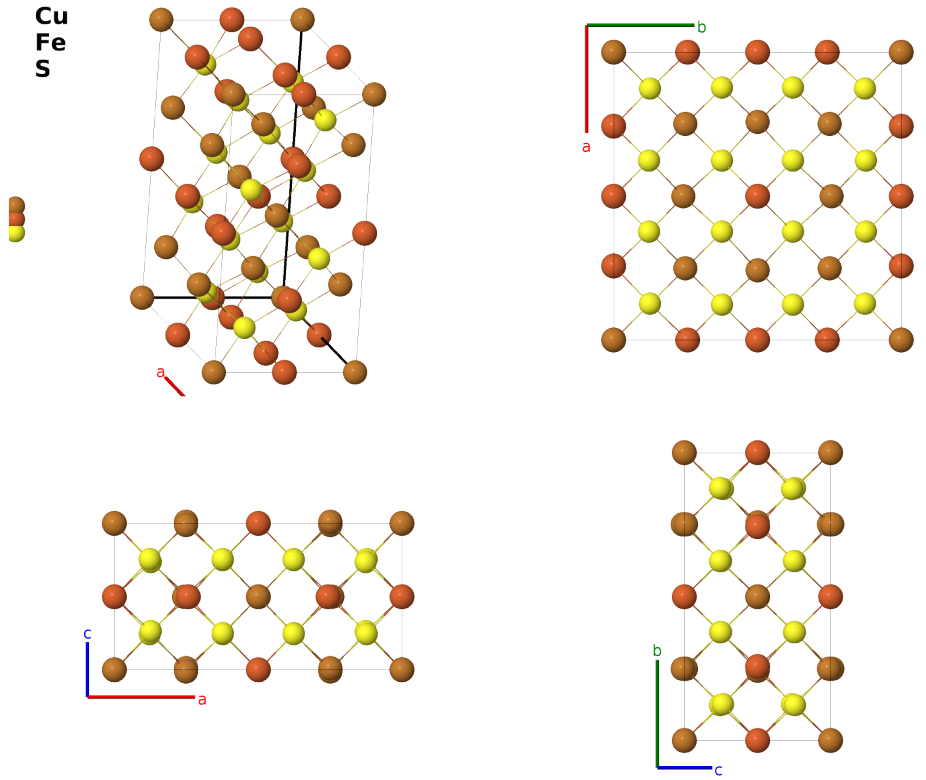
https://aflow.org/prototype-encyclopedia/2KD6

https://aflow.org/prototype-encyclopedia/A9B9C16_tP34_111_ajn_bcdek_2no-001

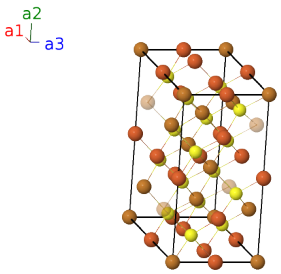


Prototype	$Cu_9Fe_9S_{16}$
AFLOW prototype label	A9B9C16_tP34_111_ajn_bcdek_2no-001
Mineral name	mooihoekite
ICSD	2649
CCDC	1592517
Pearson symbol	tP34
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	`aflow --proto=A9B9C16_tP34_111_ajn_bcdek_2no-001 --params=`$a, c/a, x_6, x_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- We have shifted the origin by $a/2(\hat{x}+\hat{y})$ from that used by (Hall, 1973).

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1c)	Fe II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}$	(1d)	Fe III
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2e)	Fe IV
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(2e)	Fe IV
$\mathbf{B_7}$	=	$x_6\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Cu II
$\mathbf{B_8}$	=	$-x_6\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Cu II
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Cu II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	Cu II
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	Fe V
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	Fe V
$\mathbf{B_{13}}$	=	$-x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	Fe V
$\mathbf{B_{14}}$	=	$x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	Fe V
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(4n)	Cu III
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1-x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(4n)	Cu III
$\mathbf{B_{17}}$	=	$x_8\,\mathbf{a}_1-x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(4n)	Cu III
$\mathbf{B_{18}}$	=	$-x_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(4n)	Cu III
$\mathbf{B_{19}}$	=	$x_9\,\mathbf{a}_1+x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(4n)	S I
$\mathbf{B_{20}}$	=	$-x_9\,\mathbf{a}_1-x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(4n)	S I
$\mathbf{B_{21}}$	=	$x_9\,\mathbf{a}_1-x_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(4n)	S I
$\mathbf{B_{22}}$	=	$-x_9\,\mathbf{a}_1+x_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(4n)	S I
$\mathbf{B_{23}}$	=	$x_{10}\,\mathbf{a}_1+x_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+ax_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(4n)	S II
$\mathbf{B_{24}}$	=	$-x_{10}\,\mathbf{a}_1-x_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-ax_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(4n)	S II
$\mathbf{B_{25}}$	=	$x_{10}\,\mathbf{a}_1-x_{10}\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}-ax_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(4n)	S II
$\mathbf{B_{26}}$	=	$-x_{10}\,\mathbf{a}_1+x_{10}\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}+ax_{10}\,\hat{\mathbf{y}}-cz_{10}\,\hat{\mathbf{z}}$	(4n)	S II

$\mathbf{B_{27}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{28}}$	=	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{29}}$	=	$y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$ay_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{30}}$	=	$-y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-ay_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{31}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{32}}$	=	$x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{33}}$	=	$-y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ay_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III
$\mathbf{B_{34}}$	=	$y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ay_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8o)	S III

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