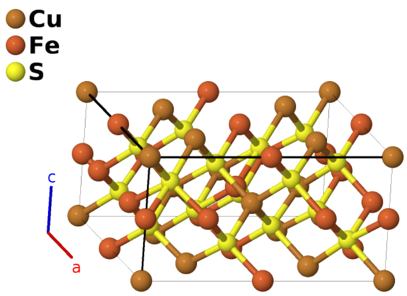
# Mooihoekite ($Cu_9Fe_9S_{16}$) Structure: A9B9C16_tP34_111_ajn_bcdek_2no-001

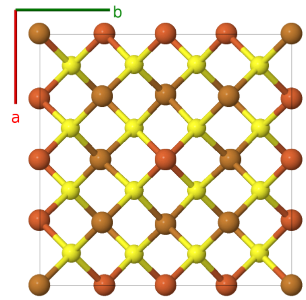
Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

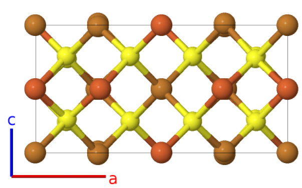
---

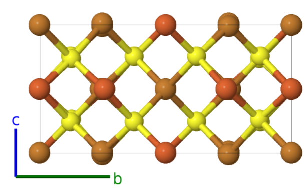
https://aflow.org/p/2KD6

https://aflow.org/p/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 |
| **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=`$a, c/a, x_6, x_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}$ |

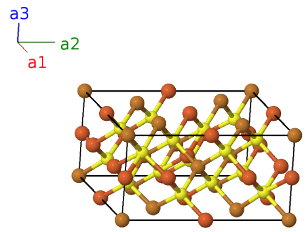
---

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

---

**Simple Tetragonal primitive vectors**

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | 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 |

## References


[1] S. R. Hall and J. F. Rowland, *The crystal structure of synthetic mooihoekite $Cu_9Fe_9S_{16}$*, Acta Crystallogr. Sect. B **29**, 2365–2372 (1973), doi:10.1107/S0567740873006710.


## Found in


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