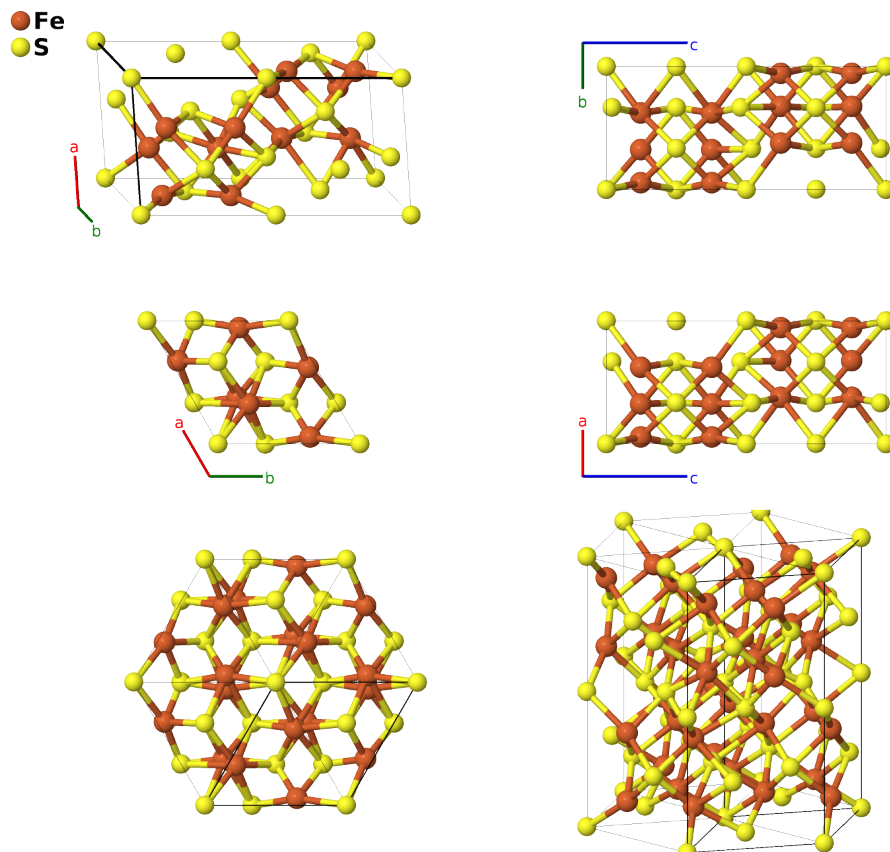# Troilite (FeS) Structure: AB_hP24_190_i_afh-001

This structure originally had the label **AB_hP24_190_i_afh**. Calls to that address will be redirected here.

https://aflow.org/p/6ZXP

https://aflow.org/p/AB_hP24_190_i_afh-001

Prototype	FeS
AFLOW prototype label	AB_hP24_190_i_afh-001
Mineral name	troilite
ICSD	633296
Pearson symbol	hP24
Space group number	190
Space group symbol	$P\bar{6}2c$
AFLOW prototype command	`aflow --proto=AB_hP24_190_i_afh-001` `--params=`$a, c/a, z_2, x_3, y_3, x_4, y_4, z_4$

Hexagonal primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
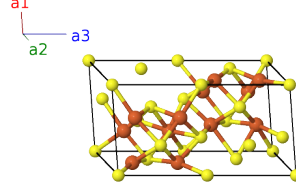
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	S I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B_3}$	$=$	$\tfrac{1}{3}\,\mathbf{a_1} + \tfrac{2}{3}\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	S II
$\mathbf{B_4}$	$=$	$\tfrac{1}{3}\,\mathbf{a_1} + \tfrac{2}{3}\,\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	S II
$\mathbf{B_5}$	$=$	$\tfrac{2}{3}\,\mathbf{a_1} + \tfrac{1}{3}\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	S II
$\mathbf{B_6}$	$=$	$\tfrac{2}{3}\,\mathbf{a_1} + \tfrac{1}{3}\,\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	S II
$\mathbf{B_7}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_8}$	$=$	$-y_3\,\mathbf{a_1} + \left(x_3 - y_3\right)\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_9}$	$=$	$-\left(x_3 - y_3\right)\mathbf{a_1} - x_3\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{10}}$	$=$	$y_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{11}}$	$=$	$\left(x_3 - y_3\right)\mathbf{a_1} - y_3\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{12}}$	$=$	$-x_3\,\mathbf{a_1} - \left(x_3 - y_3\right)\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	S III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{14}}$	$=$	$-y_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{15}}$	$=$	$-\left(x_4 - y_4\right)\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{16}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{17}}$	$=$	$-y_4\,\mathbf{a_1} + \left(x_4 - y_4\right)\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{18}}$	$=$	$-\left(x_4 - y_4\right)\mathbf{a_1} - x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{19}}$	$=$	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{20}}$	$=$	$\left(x_4 - y_4\right)\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{21}}$	$=$	$-x_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{22}}$	$=$	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 + y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{23}}$	$=$	$\left(x_4 - y_4\right)\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4 - 2y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I
$\mathbf{B_{24}}$	$=$	$-x_4\,\mathbf{a_1} - \left(x_4 - y_4\right)\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_4 - y_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	Fe I

References

[1] N. Morimoto, H. Nakazawa, K. Nishigucmi, and M. Tokonami, *Pyrrhotites: Stoichiometric Compounds with Composition $Fe_{n-1}S_n$ (n ≥ 8)*, Science **168**, 964–966 (1970), doi:10.1126/science.168.3934.964.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.