

Low Temperature Pyrite (FeS₂) Structure: AB2_oP12_29_a_2a-001

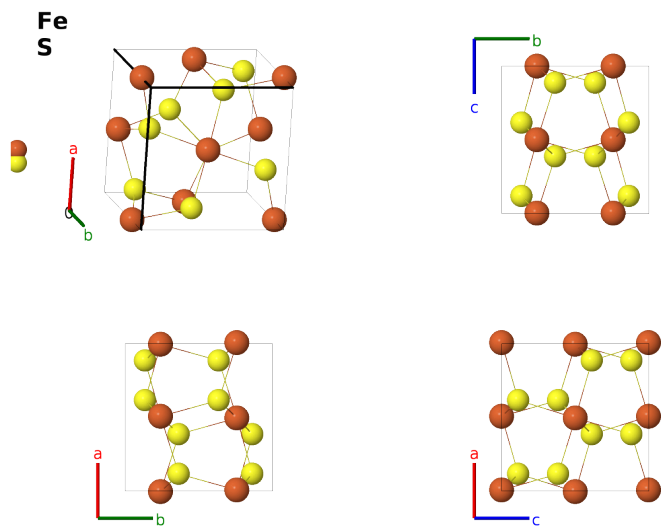
This structure previously used the label(s) **AB2_oP12_29_a_2a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/09UM>

https://aflow.org/prototype-encyclopedia/AB2_oP12_29_a_2a-001



Prototype	FeS ₂
AFLOW prototype label	AB2_oP12_29_a_2a-001
Mineral name	pyrite
Pearson symbol	oP12
Space group number	29
Space group symbol	<i>Pca</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=AB2_oP12_29_a_2a-001 --params=a, b/a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃</code>

- FeS₂ has been found in at least four forms:
 - a triclinic (*P*1 #1) phase,
 - a low temperature orthorhombic pyrite phase (this structure),
 - the most commonly observed state, cubic pyrite (*C*2), and
 - orthorhombic martensite (*C*18).

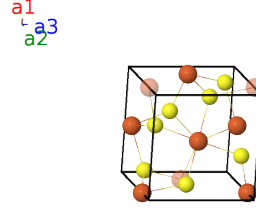
- (Bayliss, 1977) calls this “weakly anisotropic pyrite.”
- ZrO_2 (A2B_oP12_29_2a_a) and pyrite (AB2_oP12_29_a_2a) have similar AFLOW prototype labels (i.e., same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_3$	$=$	$\left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_4$	$=$	$-\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_6$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_7$	$=$	$\left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_8$	$=$	$-\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B}_{10}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B}_{11}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B}_{12}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	S II

References

- [1] P. Bayliss, *Crystal structure refinement of a weakly anisotropic pyrite*, Am. Mineral. **62**, 1168–1172 (1977).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043