# Low Temperature Pyrite ($FeS_2$) Structure: AB2_oP12_29_a_2a-001

This structure originally had the label `AB2_oP12_29_a_2a`. Calls to that address will be redirected here.

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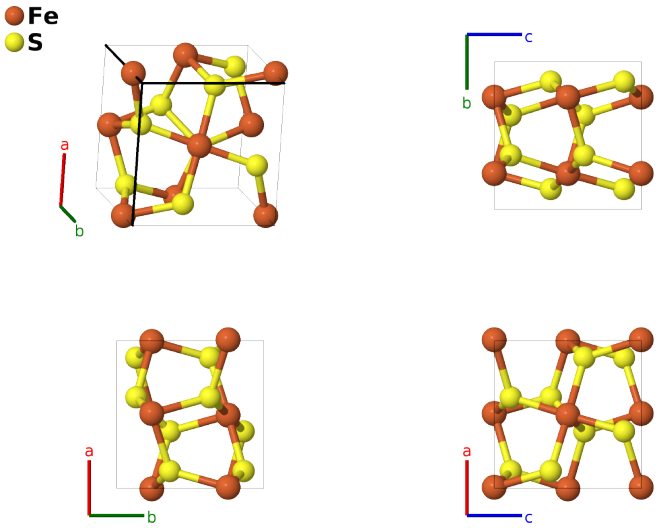
https://aflow.org/p/09UM

https://aflow.org/p/AB2_oP12_29_a_2a-001

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|---|---|
| **Prototype** | $FeS_2$ |
| **AFLOW prototype label** | AB2_oP12_29_a_2a-001 |
| **Mineral name** | pyrite |
| **ICSD** | none |
| **Pearson symbol** | oP12 |
| **Space group number** | 29 |
| **Space group symbol** | $Pca2_1$ |
| **AFLOW prototype command** | `aflow --proto=AB2_oP12_29_a_2a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$ |

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- $FeS_2$ has been found in at least four forms:
  - a triclinic ($P1$ #1) phase,
  - a low temperature orthorhombic pyrite phase (this structure),
  - the most commonly observed state, cubic pyrite ($C2$), and
  - orthorhombic martensite ($C18$).
- (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.

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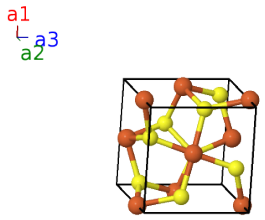
**Simple Orthorhombic primitive vectors**

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

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**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).