# Marcasite ($FeS_2$, $C18$) Structure: AB2_oP6_58_a_g-003

This structure previously used the label(s) `AB2_oP6_58_a_g.FeS2`. Calls to these addresses will be redirected here.

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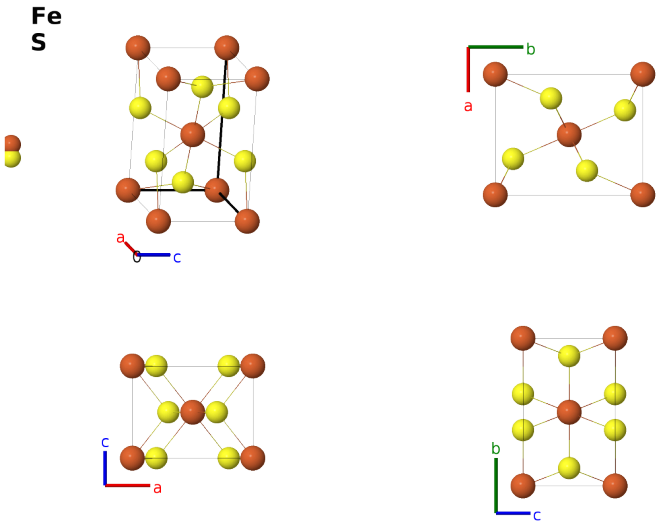
https://aflow.org/prototype-encyclopedia/USY5

https://aflow.org/prototype-encyclopedia/AB2_oP6_58_a_g-003




| | |
|---|---|
| **Prototype** | $FeS_2$ |
| **AFLOW prototype label** | AB2_oP6_58_a_g-003 |
| ***Strukturbericht* designation** | $C18$ |
| **Mineral name** | marcasite |
| **ICSD** | 109374 |
| **CCDC** | 1666987 |
| **Pearson symbol** | oP6 |
| **Space group number** | 58 |
| **Space group symbol** | $Pnnm$ |
| **AFLOW prototype command** | `aflow --proto=AB2_oP6_58_a_g-003 --params=`$a, b/a, c/a, x_2, y_2$ |

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**Other compounds with this structure**

$BeH_2$, $CoAs_2$, $CoSb_2$, $CoSe_2$, $CoTe_2$, $CrSb_2$, $CuS_2$, $CuSe_2$, $FeAs_2$, $FeP_2$, $FeS_2$, $FeSb_2$, $FeSe_2$, $FeTe_2$, $MnS_2$, $NiAs_2$ (rammelsbergite), $NiS_2$, $NiSb_2$, $NiSe_2$, $OsAs_2$, $OsP_2$, $OsSb_2$, $PdI_2$, $RuAs_2$, $RuP_2$, $RuSb_2$, $RuTe_2$, $TiS_2$

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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,
  - the most commonly observed state, cubic pyrite ($C2$), and
  - orthorhombic martensite ($C18$) (this structure).
- Hydrophilite ($CaCl_2$, $C35$), $\eta$–$Fe_2C$, and marcasite ($FeS_2$, $C18$) have the same AFLOW prototype label, AB2_oP6_58_a_g. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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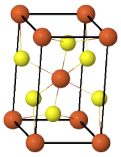
**Simple Orthorhombic primitive vectors**


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



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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2a) | Fe I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$ | = | $ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$ | (4g) | S I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$ | = | $-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$ | (4g) | S I |
| $\mathbf{B_5}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4g) | S I |
| $\mathbf{B_6}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4g) | S I |

**References**


[1] M. Rieder, J. C. Crelling, O. Šustai, M. Drábek, Z. Weiss, and M. Klementová, *Arsenic in iron disulfides in a brown coal from the North Bohemian Basin, Czech Republic*, Int. J. Coal Geology **71**, 115–121 (2007), doi:10.1016/j.coal.2006.07.003.


**Found in**


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


**First cited in**


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