# Pyrite ($FeS_2$, $C2$) Structure: AB2_cP12_205_a_c-001

This structure previously used the label(s) `AB2_cP12_205_a_c`. Calls to these addresses will be redirected here.

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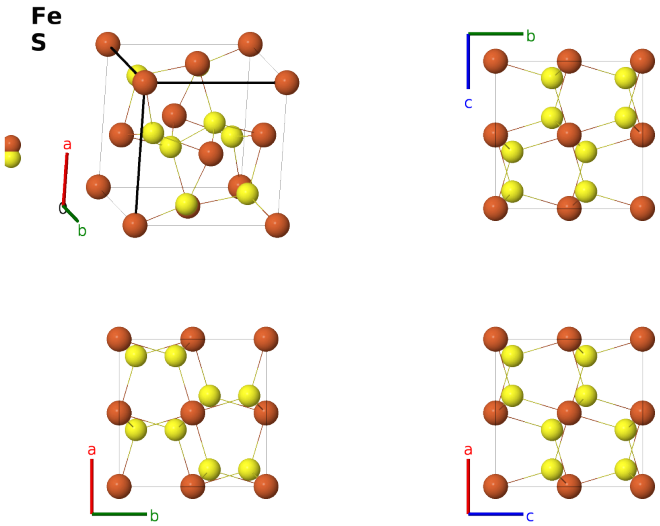
https://aflow.org/prototype-encyclopedia/M44S

https://aflow.org/prototype-encyclopedia/AB2_cP12_205_a_c-001




| | |
|---|---|
| **Prototype** | $FeS_2$ |
| **AFLOW prototype label** | AB2_cP12_205_a_c-001 |
| ***Strukturbericht* designation** | $C2$ |
| **Mineral name** | pyrite |
| **ICSD** | 15012 |
| **CCDC** | 1595797 |
| **Pearson symbol** | cP12 |
| **Space group number** | 205 |
| **Space group symbol** | $Pa\bar{3}$ |
| **AFLOW prototype command** | `aflow --proto=AB2_cP12_205_a_c-001 --params=`$a, x_2$ |

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**Other compounds with this structure**

$AuN_2$, $AuSb_2$, $BeO_2$, $BeS_2$, $CaC_2$, $CdO_2$, $CdS_2$, $CdSe_2$, CoAsS, $CoS_2$, $CoSe_2$, $CoTe_2$, $CuS_2$, $CuSe_2$, $CuTe_2$, $FeO_2$, $FeS_2$, $FeSe_2$, $FeTe_2$, $GeN_2$, $HfN_2$, $IrN_2$, $IrO_2$, $IrS_2$, $IrTe_2$, $MgO_2$, $MgSe_2$, $MgTe_2$, $MnF_2$, $MnS_2$, $MnSe_2$, $MnTe_2$, $NaO_2$, $NiAs_2$, $NiN_2$, $NiP_2$, $NiS_2$

(vaesite), $NiSe_2$, $NiTe_2$, $OsN_2$, $OsS_2$, $OsSe_2$, $OsTe_2$, $PN_2$, $PaO_2$, $PdAs_2$, $PdN_2$, $PdSb_2$, $PtAs_2$ (sperrylite), $PtBi_2$, $PtN_2$, $PtO_2$, $PtP_2$, $PtSb_2$, $RhN_2$, $RhS_2$, $RhSe_2$, $RhTe_2$, $RuN_2$, $RuS_2$, $RuSe_2$, $RuTe_2$, $SiAs_2$, $SiC_2$, $SiN_2$, $SiP_2$, $SnN_2$, $ThC_2$, $TiS_2$, $UO_2$, $ZnO_2$, $ZnS_2$, $ZnSe_2$, Co(SSe), Cu(SeTe), Ir(AsS), Ir(AsSe), Ir(AsTe), Ir(BiTe), Ir(PS), Ni(AsS), Ni(AsSe), Ni(PS), Ni(SSe), Pd(AsSb), Pd(SbTe), Pt(AsP), Pt(AsS), Pt(BiSb), Pt(GeTe), Pt(PbTe), Pt(SbTe), Pt(SeSn), Pt(SnS), Pt(SnTe), Rh(AsS), Rh(AsSe), Rh(AsTe), Rh(BiTe), Rh(PS), Rh(SbTe), Ru(SSe), Ru(SeTe), $(Co_{0.5}Ru_{0.5})S_2$, $(Fe_{0.5}Ni_{0.5})S_2$, $(Fe_{0.5}Ni_{0.5})Se_2$, $(Fe_{0.5}Ni_{0.5})Te_2$, $(Rh_{0.5}Ru_{0.5})S_2$

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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 (Bayliss, 1977),
  - The most commonly observed state, cubic pyrite ($C2$) (this structure), and
  - Orthorhombic martensite ($C18$).
- Compounds of the form A(BC) place the A atom on the Fe I (4a) site with the B and C atoms alloyed on the S I (8c) site. Compounds of the form $(A_{0.5}B_{0.5})C_2$ have the A and B atoms alloyed on the (4a) site with the C atom on the (8c) site.
- We have rewritten this page to include the original source of the data from (Brostigen, 1969). Previously we only referenced (Bayliss, 1977).

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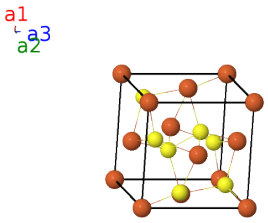
**Simple Cubic primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$ | (4a) | Fe I |
| $\mathbf{B_5}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_6}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_7}$ | = | $-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_8}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_9}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_{10}}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_{11}}$ | = | $x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | S I |
| $\mathbf{B_{12}}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (8c) | S I |

## References

[1] G. Brostigen and A. Kjekshus, *Redetermined Crystal Structure of $FeS_2$ (Pyrite)*, Acta Chem. Scand. **23**, 2186–2188 (1969), doi:10.3891/acta.chem.scand.23-2186.

## Found in

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

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

## First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017