

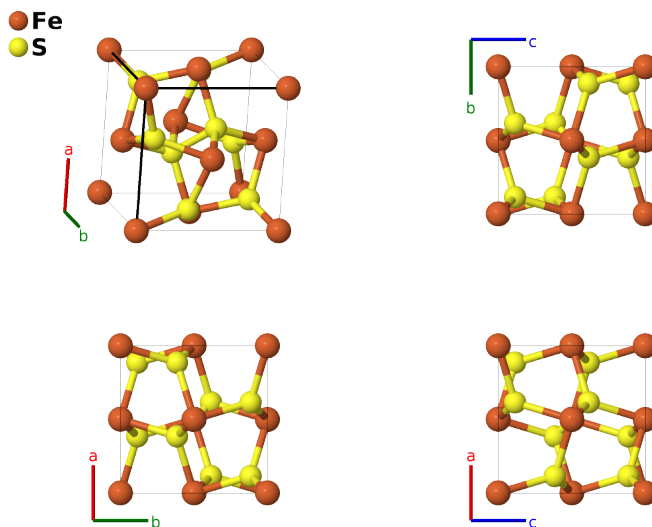
Pyrite (FeS_2 , $C2$) Structure: AB2_cP12_205_a_c-001

This structure originally had the label AB2_cP12_205_a_c. Calls to that address will be redirected here.

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<https://aflow.org/p/M44S>

https://aflow.org/p/AB2_cP12_205_a_c-001



Prototype	FeS_2
AFLOW prototype label	AB2_cP12_205_a_c-001
<i>Strukturbericht</i> designation	$C2$
Mineral name	pyrite
ICSD	15012
Pearson symbol	cP12
Space group number	205
Space group symbol	$P\bar{a}3$
AFLOW prototype command	<code>aflow --proto=AB2_cP12_205_a_c-001 --params=a, x2</code>

Other compounds with this structure

AuSb_2 , CaC_2 , CoS_2 , CoSe_2 , FeS_2 , MnS_2 , MnSe_2 , MnTe_2 , NiS_2 (vaesite), NiSe_2 , OsS_2 , OsSe_2 , OsTe_2 , PdAs_2 , PdSb_2 , PtAs_2 , PtBi_2 , PtP_2 , PtSb_2 , RhS_2 , RhSe_2 , RuS_2 , RuSe_2 , RuTe_2

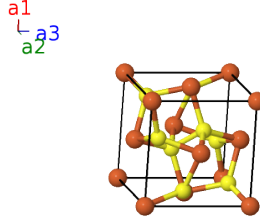
- FeS_2 has been found in at least four forms:
 - a triclinic ($P1 \#1$) phase,
 - a low temperature orthorhombic pyrite phase (Bayliss, 1977),

- the most commonly observed state, cubic pyrite (*C2*) (this structure), and
- orthorhombic martensite (*C18*).

- We have rewritten this page to include the original source of the data from (Brostigen, 1969). Previously we only referenced (Bayliss, 1977).

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



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	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	S I
\mathbf{B}_7	$-x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	S I
\mathbf{B}_8	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(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}	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	S I
\mathbf{B}_{11}	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	S I
\mathbf{B}_{12}	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	S I