FeS_2 ($P1$) Structure: AB2_aP12_1_4a_8a-001

This structure originally had the label `AB2_aP12_1_4a_8a`. Calls to that address will be redirected here.

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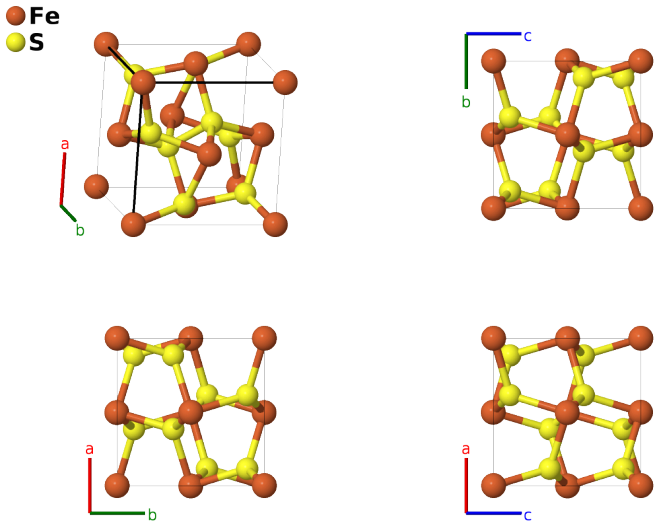
https://aflow.org/p/RHYA

https://aflow.org/p/AB2_aP12_1_4a_8a-001

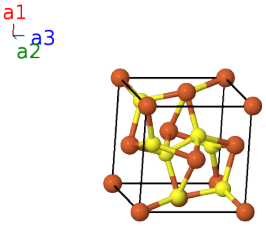


Prototype	FeS_2
AFLOW prototype label	AB2_aP12_1_4a_8a-001
ICSD	10422
Pearson symbol	aP12
Space group number	1
Space group symbol	$P1$
AFLOW prototype command	`aflow --proto=AB2_aP12_1_4a_8a-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- FeS_2 has been found in at least four forms:
  - a triclinic ($P1$ #1) phase (this structure),
  - a low temperature orthorhombic pyrite phase,
  - the most commonly observed state, cubic pyrite ($C2$), and
  - orthorhombic martensite ($C18$).
- This structure is just a slightly distorted version of pyrite ($C2$), with no rotational symmetry whatsoever.

Triclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}} \\
c_x &= c\cos\beta \\
c_y &= c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} + c_z z_1\,\hat{\mathbf{z}}$	(1a)	Fe I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(1a)	Fe II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(1a)	Fe III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(1a)	Fe IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(1a)	S II
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(1a)	S III
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(1a)	S IV
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} + c_z z_9\,\hat{\mathbf{z}}$	(1a)	S V
$\mathbf{B_{10}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + by_{10}\cos\gamma + c_x z_{10})\,\hat{\mathbf{x}} + (by_{10}\sin\gamma + c_y z_{10})\,\hat{\mathbf{y}} + c_z z_{10}\,\hat{\mathbf{z}}$	(1a)	S VI
$\mathbf{B_{11}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + by_{11}\cos\gamma + c_x z_{11})\,\hat{\mathbf{x}} + (by_{11}\sin\gamma + c_y z_{11})\,\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}}$	(1a)	S VII
$\mathbf{B_{12}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + by_{12}\cos\gamma + c_x z_{12})\,\hat{\mathbf{x}} + (by_{12}\sin\gamma + c_y z_{12})\,\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}}$	(1a)	S VIII

References

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