Low temperature FeS Structure: AB_oF8_22_a_c-001

This structure originally had the label `AB_oF8_22_a_c`. Calls to that address will be redirected here.

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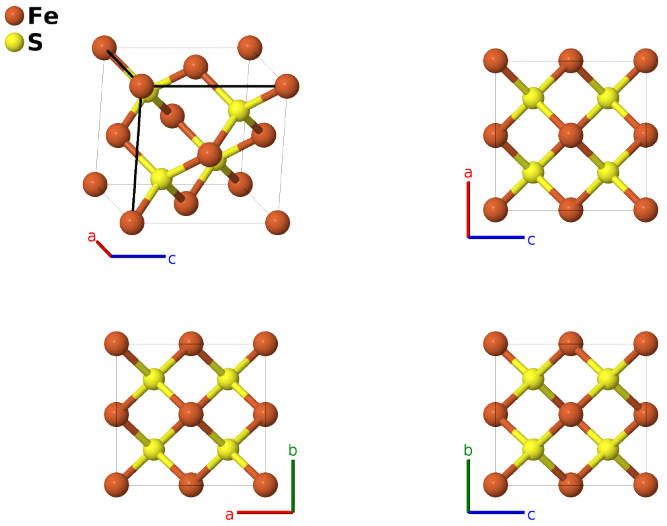
https://aflow.org/p/H691

https://aflow.org/p/AB_oF8_22_a_c-001

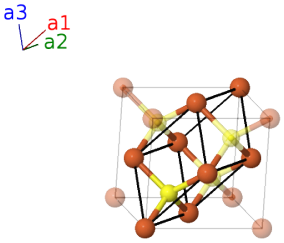


Prototype	FeS
AFLOW prototype label	AB_oF8_22_a_c-001
ICSD	none
Pearson symbol	oF8
Space group number	22
Space group symbol	$F222$
AFLOW prototype command	`aflow --proto=AB_oF8_22_a_c-001 --params=`$a, b/a, c/a$

- This is the stable structure of iron sulfide below 242K. Above that temperature it is in the zincblende ($B3$) structure. (Wintenberger, 1978).
- This data was taken at 81K. We follow (Villars, 2016) and rearrange the axis, as well as reversing the positions of the iron and sulfur atoms.

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	S I

References

[1] M. Wintenberger and J. L. Buevoz, *Structure magnetique du sulfure de fer FeS de type blende*, Solid State Commun. **27**, 511–513 (1978), doi:10.1016/0038-1098(78)90383-6.

Found in

[1] P. Villars, *FeS Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database).