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

This structure originally had the label `AB2_oP6_58_a_g.FeS2`. Calls to that address will be redirected here.

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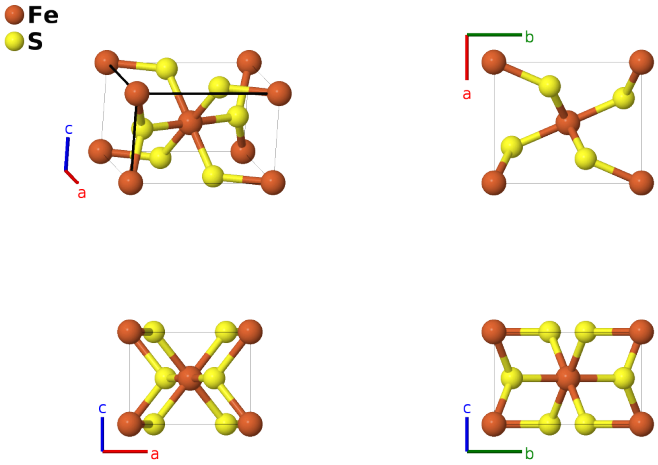
https://aflow.org/p/USY5

https://aflow.org/p/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
Pearson symbol	oP6
Space group number	58
Space group symbol	$Pnnm$
AFLOW prototype command	`aflow --proto=AB2_oP6_58_a_g-003 --params=`$a, b/a, c/a, x_2, y_2$

Other compounds with this structure
$CoAs_2$, $CoTe_2$, $CrSb_2$, CuS_2, $FeAs_2$, FeP_2, $FeSb_2$, $FeSe_2$, $FeTe_2$, $NiAs_2$ (rammelsbergite), NiS_2, $NiSb_2$, $OsAs_2$, OsP_2, $OsSb_2$, $RuAs_2$, RuP_2, $RuSb_2$, $RuTe_2$

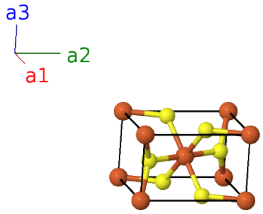
- FeS_2 has been found in at least four forms:
  - a triclinic ($P1$ #1) phase,
  - a low temperature orthorhombic pyrite phase,
  - the most commonly observed state, cubic pyrite ($C2$), and

– orthorhombic martensite ($C18$) (this structure).

- Hydrophilite ($CaCl_2$, $C35$), η–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.

Simple Orthorhombic primitive vectors

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



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).