

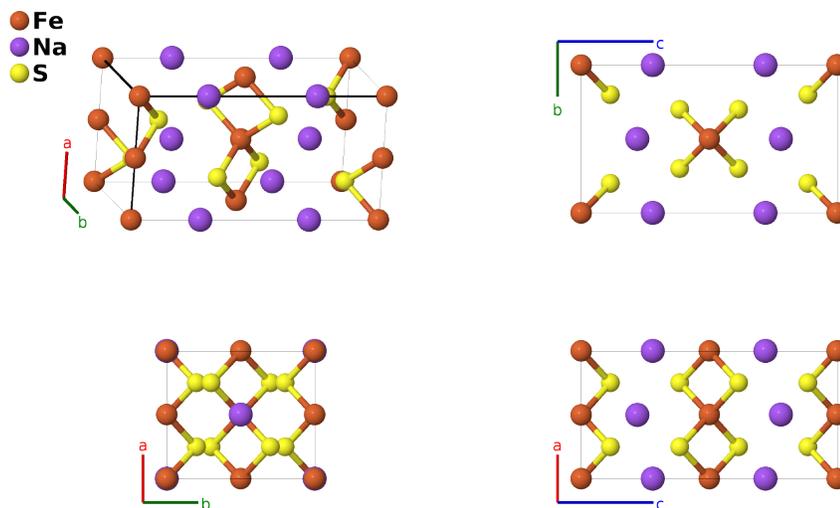
NaFeS₂ Structure: ABC2_oI16_23_ac_e_k-001

This structure originally had the label ABC2_oI16_23_ab_i_k. Calls to that address will be redirected here.

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<https://aflow.org/p/J362>

https://aflow.org/p/ABC2_oI16_23_ac_e_k-001



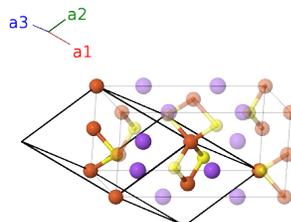
Prototype	FeNaS ₂
AFLOW prototype label	ABC2_oI16_23_ac_e_k-001
ICSD	37026
Pearson symbol	oI16
Space group number	23
Space group symbol	<i>I</i> 222
AFLOW prototype command	aflow --proto=ABC2_oI16_23_ac_e_k-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , <i>x</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄

Body-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = -\frac{1}{2}a \hat{x} + \frac{1}{2}b \hat{y} + \frac{1}{2}c \hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{x} - \frac{1}{2}b \hat{y} + \frac{1}{2}c \hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{x} + \frac{1}{2}b \hat{y} - \frac{1}{2}c \hat{z}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a) Fe I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(2c) Fe II
\mathbf{B}_3	=	$x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}}$	(4e) Na I
\mathbf{B}_4	=	$-x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}}$	(4e) Na I
\mathbf{B}_5	=	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 +$ $(x_4 + y_4) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k) S I
\mathbf{B}_6	=	$-(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 -$ $(x_4 + y_4) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8k) S I
\mathbf{B}_7	=	$(y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 -$ $(x_4 - y_4) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k) S I
\mathbf{B}_8	=	$-(y_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 +$ $(x_4 - y_4) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8k) S I

References

- [1] H. Boller and H. Blaha, *Zur Kenntnis des Natriumthioferrates(III)*, *Monatsh. Chem.* **114**, 145–154 (1983), doi:10.1007/BF00798319.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.