$NaFeS_2$ Structure: ABC2_oI16_23_ac_e_k-001

This structure previously used the label(s) `ABC2_oI16_23_ab_i_k`. Calls to these addresses will be redirected here.

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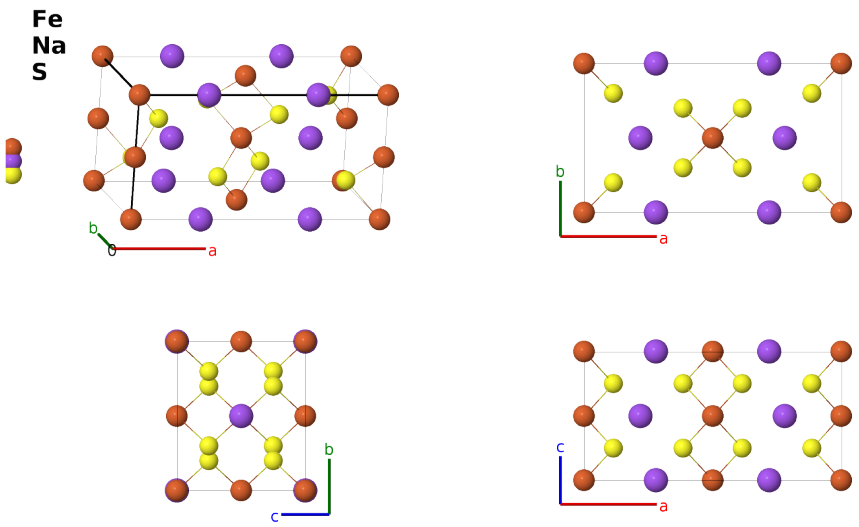
https://aflow.org/prototype-encyclopedia/J362

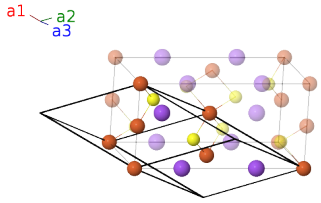
https://aflow.org/prototype-encyclopedia/ABC2_oI16_23_ac_e_k-001



Prototype	$FeNaS_2$
AFLOW prototype label	ABC2_oI16_23_ac_e_k-001
ICSD	37026
CCDC	1608390
Pearson symbol	oI16
Space group number	23
Space group symbol	$I222$
AFLOW prototype command	`aflow --proto=ABC2_oI16_23_ac_e_k-001 --params=`$a, b/a, c/a, x_3, x_4, y_4, z_4$

Body-centered Orthorhombic primitive vectors

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



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.

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