

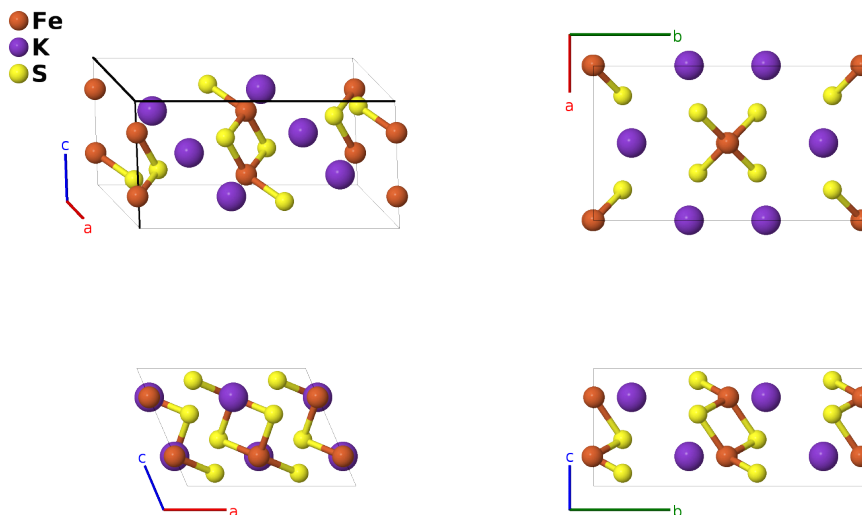
KFeS₂ (*F*5_{*a*}) Structure: ABC2_mC16_15_e_e_f-004

This structure originally had the label ABC2_mC16_15_e_e_f. Calls to that address will be redirected here.

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<https://aflow.org/p/G8C6>

https://aflow.org/p/ABC2_mC16_15_e_e_f-004



Prototype	FeKS ₂
AFLOW prototype label	ABC2_mC16_15_e_e_f-004
<i>Strukturbericht</i> designation	<i>F</i> 5 _{<i>a</i>}
ICSD	202380
Pearson symbol	mC16
Space group number	15
Space group symbol	<i>C</i> 2/ <i>c</i>
AFLOW prototype command	<code>aflow --proto=ABC2_mC16_15_e_e_f-004 --params=a, b/a, c/a, β, y₁, y₂, x₃, y₃, z₃</code>

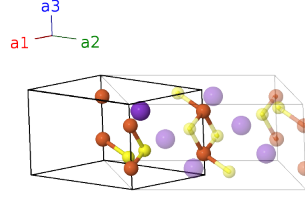
Other compounds with this structure

RbFeS₂, KFeSe₂, RbFeSe₂, CsGaS₂, CsGaSe₂

- This structure forms cages of Fe atoms surrounded by tetrahedra of S atoms.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Fe I
\mathbf{B}_2	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Fe I
\mathbf{B}_3	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	K I
\mathbf{B}_4	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	K I
\mathbf{B}_5	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_6	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_7	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_8	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	S I

References

- [1] W. Bronger, A. Kyas, and P. Müller, *The antiferromagnetic structures of $KFeS_2$, $RbFeS_2$, $KFeSe_2$, and $RbFeSe_2$ and the correlation between magnetic moments and crystal field calculations*, J. Solid State Chem. **70**, 262–270 (1987), doi:10.1016/0022-4596(87)90065-X.