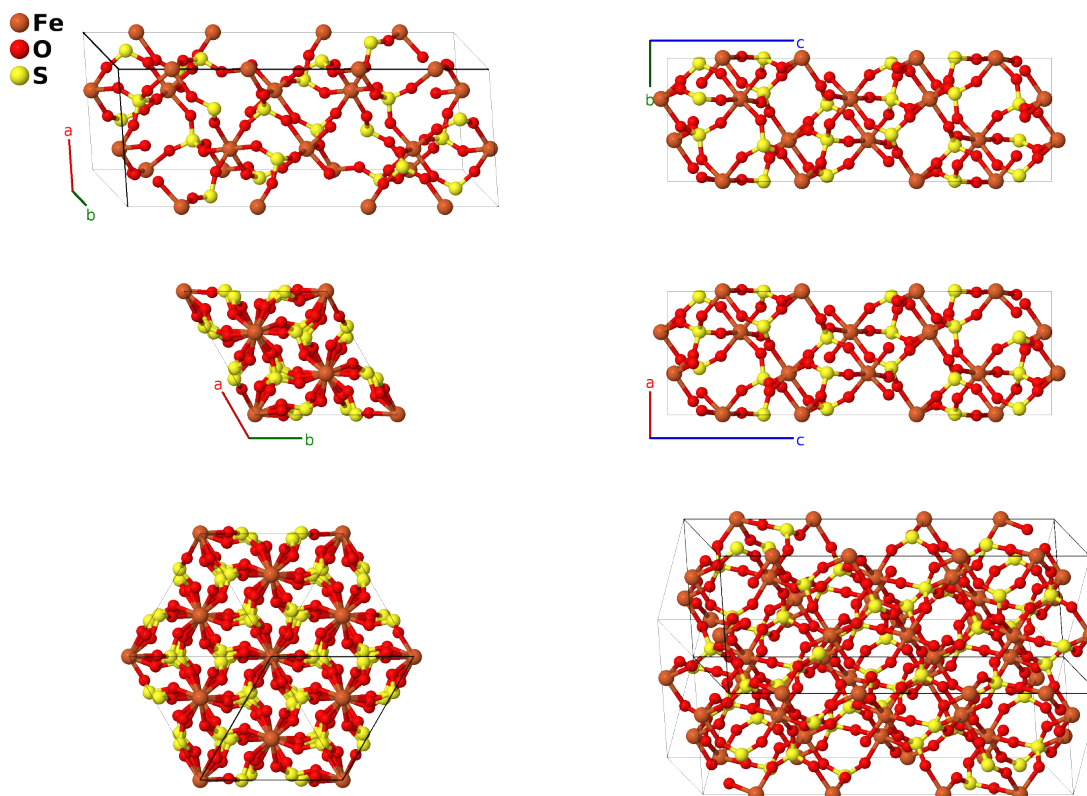


Mikasaite (Rhombohedral $\text{Fe}_2(\text{SO}_4)_3$) Structure: A2B12C3_hR34_148_2c_4f_f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/GHH0>

https://aflow.org/p/A2B12C3_hR34_148_2c_4f_f-001



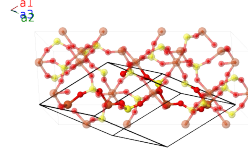
Prototype	$\text{Fe}_2\text{O}_{12}\text{S}_3$
AFLOW prototype label	A2B12C3_hR34_148_2c_4f_f-001
Mineral name	mikasaite
ICSD	22368
Pearson symbol	hR34
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=A2B12C3_hR34_148_2c_4f_f-001</code> <code>--params=a, c/a, x1, x2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7</code>

Other compounds with this structure
 $\text{Al}_2(\text{SO}_4)_3$

- $\text{Fe}_2\text{O}_{12}\text{S}_3$ also forms a monoclinic crystal.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	Fe I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	Fe I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Fe II
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Fe II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_6	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_7	$= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_8	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_9	$= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{10}	$= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{11}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{12}	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{13}	$= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{15}	$= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{16}	$= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O III
\mathbf{B}_{18}	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O III
\mathbf{B}_{19}	$= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O III

$$\begin{aligned}
\mathbf{B}_{20} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) & \text{O III} \\
\mathbf{B}_{21} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 &= \frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) & \text{O III} \\
\mathbf{B}_{22} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) & \text{O III} \\
\mathbf{B}_{23} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{24} &= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 &= -\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{25} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{26} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{27} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= \frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{28} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) & \text{O IV} \\
\mathbf{B}_{29} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I} \\
\mathbf{B}_{30} &= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3 &= -\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I} \\
\mathbf{B}_{31} &= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I} \\
\mathbf{B}_{32} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I} \\
\mathbf{B}_{33} &= -z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3 &= \frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I} \\
\mathbf{B}_{34} &= -y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) & \text{S I}
\end{aligned}$$

References

- [1] P. C. Christidis and P. J. Rentzeperis, *The crystal structure of rhombohedral $Fe_2(SO_4)_3$* , zkr **144**, 341-352 (1976), doi:10.1524/zkri.1976.144.16.341.