

Ilmenite (FeTiO_3 , $E2_2$) Structure: AB3C_hR10_148_c_f_c-001

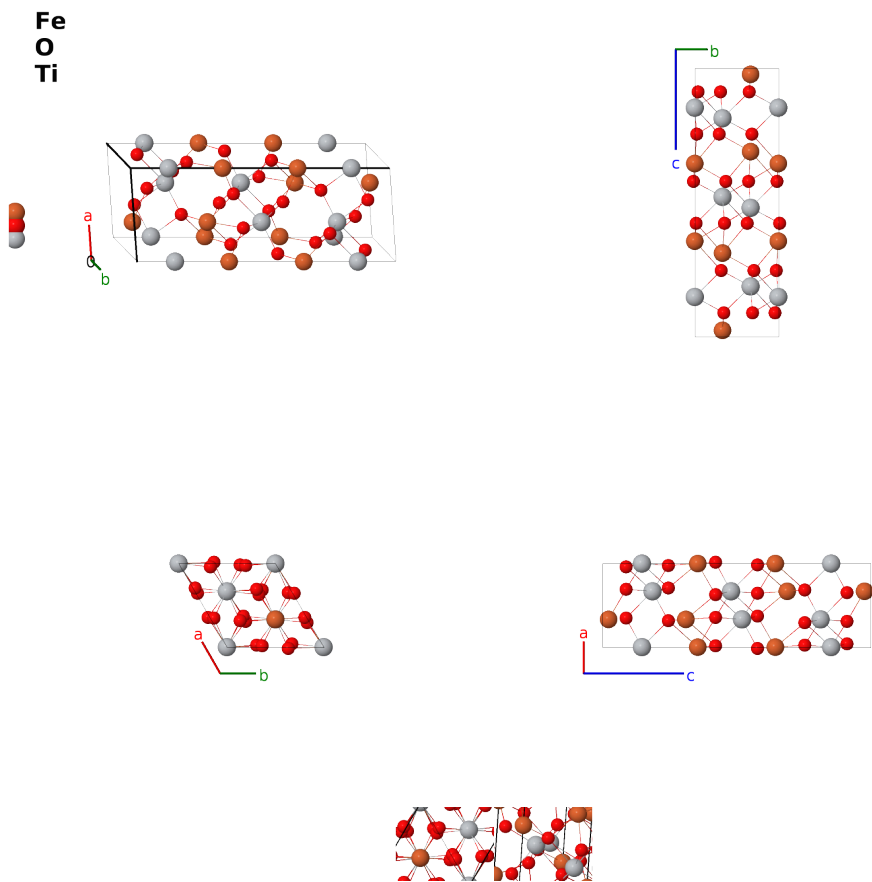
This structure previously used the label(s) **AB3C_hR10_148_c_f_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/4YUA>

https://aflow.org/prototype-encyclopedia/AB3C_hR10_148_c_f_c-001



Prototype	FeTiO_3
AFLOW prototype label	AB3C_hR10_148_c_f_c-001
<i>Strukturbericht</i> designation	$E2_2$
Mineral name	ilmenite
ICSD	30664
CCDC	1604908
Pearson symbol	hR10

Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB3C_hR10_148_c_f_c-001</code> <code>--params=a, c/a, x₁, x₂, x₃, y₃, z₃</code>

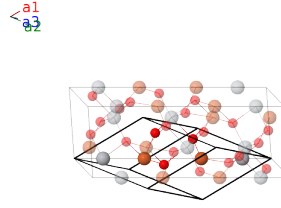
Other compounds with this structure

NiCrO₃, CoTiO₃, CrTiO₃, CrVO₃, CuVO₃, MnTiO₃, CoMnO₃, NiMnO₃, α -Na₂(GeTe)O₆, Na₂(TiTe)O₆

- If the iron and titanium atoms are replaced by a single species the structure becomes corundum.
- In the quaternary phases listed here the atoms in parentheses are alloyed onto one (2c) Wyckoff position.
- (Ewald, 1931) originally gave this the *Strukturbericht* designation *G4*.
- 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)	Ti I
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c)	Ti I
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(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

References

- [1] B. A. Wechsler and . T. Prewitt, *Crystal Structure of Ilmenite (FeTiO_3) at high temperature and high pressure*, Am. Mineral. **69**, 176–185 (1984).
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

First cited in

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