

CaFe₄O₆ Structure:

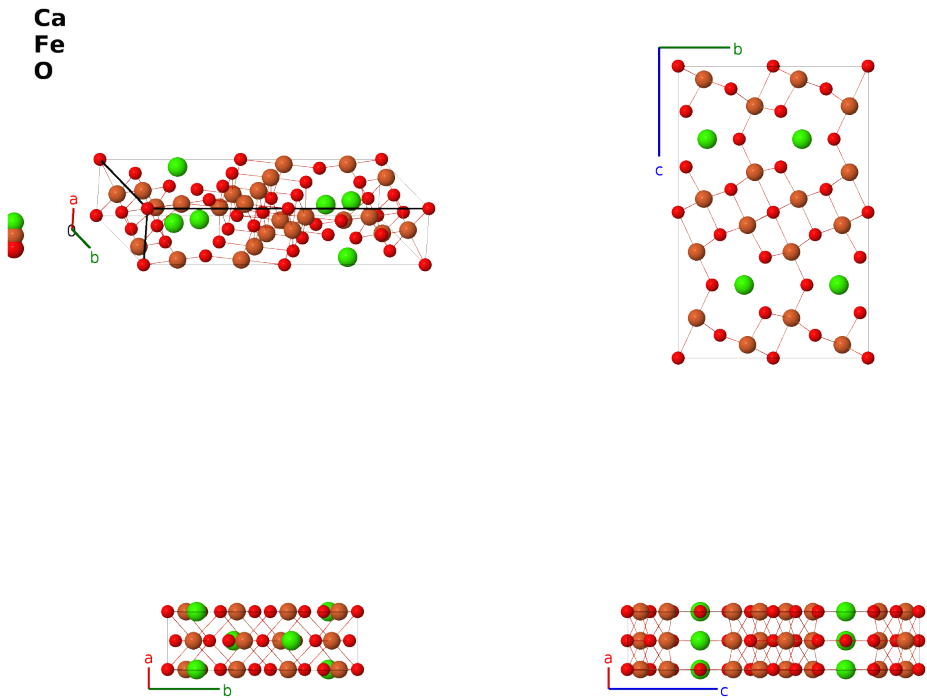
AB4C6_oC44_63_c_2f_ac2f-001

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<https://aflow.org/prototype-encyclopedia/8HU9>

https://aflow.org/prototype-encyclopedia/AB4C6_oC44_63_c_2f_ac2f-001



Prototype	CaFe ₄ O ₆
AFLOW prototype label	AB4C6_oC44_63_c_2f_ac2f-001
ICSD	16355
CCDC	1596940
Pearson symbol	oC44
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB4C6_oC44_63_c_2f_ac2f-001</code> <code>--params=a, b/a, c/a, y₂, y₃, y₄, z₄, y₅, z₅, y₆, z₆, y₇, z₇</code>

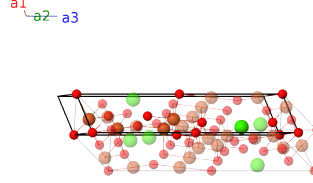
Other compounds with this structure

Fe₅O₆

- We have shifted the origin so that the O-I atom is at the origin, Wyckoff position (4a), rather than (0 0 1/2), Wyckoff position (4b) as found in (Evrard, 1980).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B ₁	=	0	=	0	(4a) O I
B ₂	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(4a) O I
B ₃	=	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c) Ca I
B ₄	=	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c) Ca I
B ₅	=	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c) O II
B ₆	=	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c) O II
B ₇	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f) Fe I
B ₈	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Fe I
B ₉	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Fe I
B ₁₀	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f) Fe I
B ₁₁	=	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f) Fe II
B ₁₂	=	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Fe II
B ₁₃	=	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Fe II
B ₁₄	=	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f) Fe II
B ₁₅	=	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f) O III
B ₁₆	=	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) O III
B ₁₇	=	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	=	$by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) O III
B ₁₈	=	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8f) O III
B ₁₉	=	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8f) O IV
B ₂₀	=	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) O IV
B ₂₁	=	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	=	$by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) O IV
B ₂₂	=	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8f) O IV

References

- [1] O. Evrard, B. Malaman, F. Jeannot, A. Courtois, H. Alebouyeh, and R. Gerardin, *Mise en évidence de CaFe_4O_6 et détermination des structures cristallines des ferrites de calcium $\text{CaFe}_{2+n}\text{O}_{4+n}$ ($n = 1, 2, 3$): nouvel exemple d'intercroissance*, J. Solid State Chem. **35**, 112–119 (1980), doi:10.1016/0022-4596(80)90471-5.

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