

CaFe₅O₇ Structure:

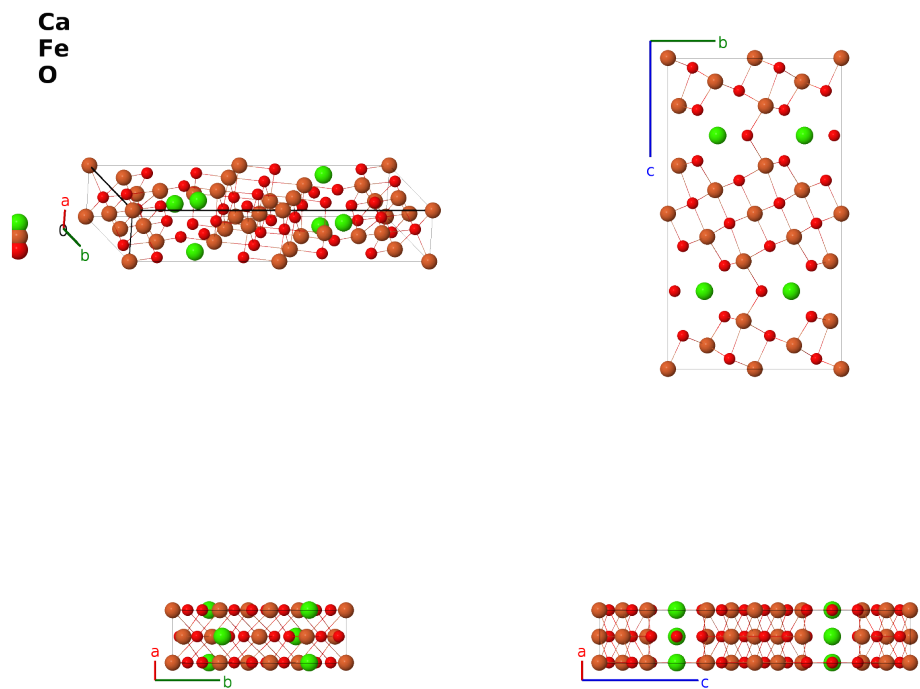
AB5C7_oC52_63_c_a2f_c3f-001

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<https://aflow.org/prototype-encyclopedia/KAT1>

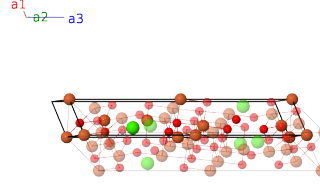
https://aflow.org/prototype-encyclopedia/AB5C7_oC52_63_c_a2f_c3f-001



Prototype	CaFe ₅ O ₇
AFLOW prototype label	AB5C7_oC52_63_c_a2f_c3f-001
ICSD	16356
CCDC	1596941
Pearson symbol	oC52
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<pre>aflow --proto=AB5C7_oC52_63_c_a2f_c3f-001 --params=a,b/a,c/a,y2,y3,y4,z4,y5,z5,y6,z6,y7,z7,y8,z8</pre>

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
$\mathbf{B}_1$	$=$	0	$=$	0	Fe I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	Fe I
$\mathbf{B}_3$	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	Ca I
$\mathbf{B}_4$	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	Ca I
$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	O I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	O I
$\mathbf{B}_7$	$=$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	Fe II
$\mathbf{B}_8$	$=$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	Fe II
$\mathbf{B}_9$	$=$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	Fe II
$\mathbf{B}_{10}$	$=$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	Fe II
$\mathbf{B}_{11}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	Fe III
$\mathbf{B}_{12}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	Fe III
$\mathbf{B}_{13}$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	Fe III
$\mathbf{B}_{14}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	Fe III
$\mathbf{B}_{15}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{16}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	O II
$\mathbf{B}_{17}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	O II
$\mathbf{B}_{18}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	O II
$\mathbf{B}_{19}$	$=$	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	O III
$\mathbf{B}_{20}$	$=$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	O III
$\mathbf{B}_{21}$	$=$	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	O III
$\mathbf{B}_{22}$	$=$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	O III
$\mathbf{B}_{23}$	$=$	$-y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{24}$	$=$	$y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{25}$	$=$	$-y_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{26}$	$=$	$y_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	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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