$CaFe_3O_5$ Structure: AB3C5_oC36_63_c_af_c2f-001

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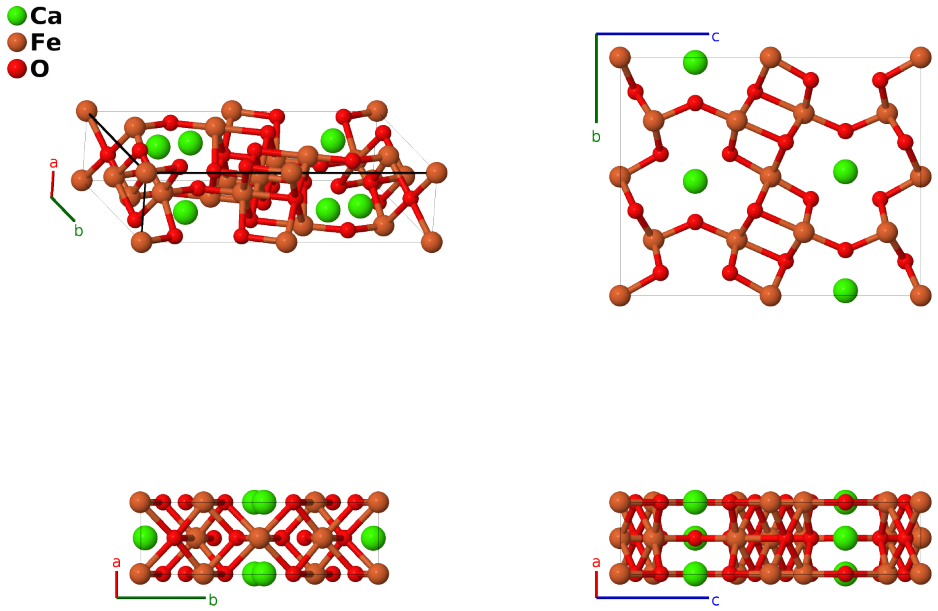
https://aflow.org/p/8XTL

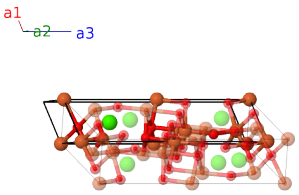
https://aflow.org/p/AB3C5_oC36_63_c_af_c2f-001



Prototype	$CaFe_3O_5$
AFLOW prototype label	AB3C5_oC36_63_c_af_c2f-001
ICSD	16354
Pearson symbol	oC36
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB3C5_oC36_63_c_af_c2f-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, z_4, y_5, z_5, y_6, z_6$

Base-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B_{11}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{14}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{15}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{16}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{17}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{18}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	O III

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 $CaFe_{2+n}O_{4+n}$ (n = 1, 2, 3): nouvel exemple d'intercroissance*, Journal of Solid State Chemistry **35**, 112–119 (1980), doi:10.1016/0022-4596(80)90471-5.