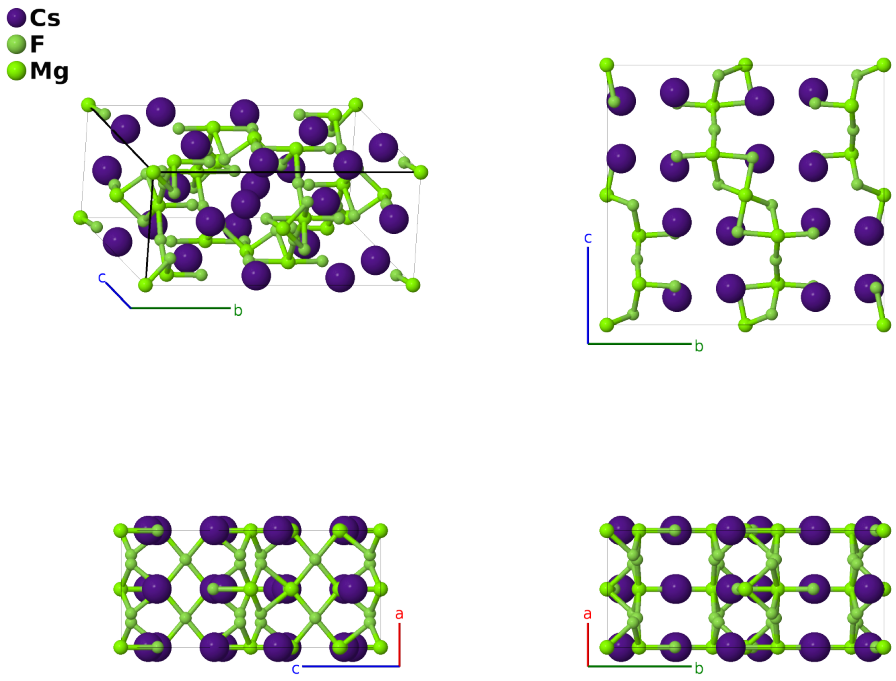
$Cs_4Mg_3F_{10}$ Structure: A4B10C3_oC68_64_2f_e2fg_af-001

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/B9LX

https://aflow.org/p/A4B10C3_oC68_64_2f_e2fg_af-001



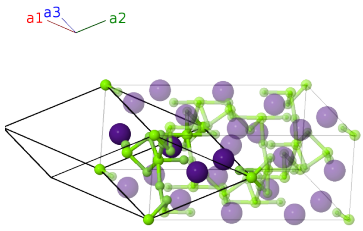
Prototype	$Cs_4F_{10}Mg_3$
AFLOW prototype label	A4B10C3_oC68_64_2f_e2fg_af-001
ICSD	16084
Pearson symbol	oC68
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=A4B10C3_oC68_64_2f_e2fg_af-001 --params=`$a, b/a, c/a, y_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, x_8, y_8, z_8$

Other compounds with this structure

$Ba_4Ir_3F_{10}$, $Ba_4Mn_3O_{10}$, $Ba_4Ru_3O_{10}$, $Ba_4Sn_3O_{10}$, $Cs_4Fe_3F_{10}$, $Cs_4Ni_3F_{10}$, $Cs_4Zn_3F_{10}$, $Rb_4Mg_3H_{10}$, $Sr_4Mn_3O_{10}$, $Ba_4Ti_2PtO_{10}$

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)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B_3}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	F I
$\mathbf{B_4}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	F I
$\mathbf{B_5}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	F I
$\mathbf{B_6}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	F I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Cs I
$\mathbf{B_8}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Cs I
$\mathbf{B_9}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Cs I
$\mathbf{B_{10}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Cs I
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Cs II
$\mathbf{B_{12}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Cs II
$\mathbf{B_{13}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Cs II
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Cs II
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_{16}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_{17}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_{18}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{20}}$	=	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{21}}$	=	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{22}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	F III

$\mathbf{B_{23}}$	=	$-y_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_{24}}$	=	$\left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_{25}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_{26}}$	=	$y_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B_{27}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{28}}$	=	$\left(-x_8 + y_8 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_8 + y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{29}}$	=	$-\left(x_8 + y_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_8 + y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{30}}$	=	$(x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{31}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{32}}$	=	$\left(x_8 - y_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 + y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{33}}$	=	$\left(x_8 + y_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 - y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	F IV
$\mathbf{B_{34}}$	=	$-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16g)	F IV

References

[1] H. Steinfink and G. D. Burton, *The Crystal Structure of $Cs_4Mg_3F_{10}$*, Inorg. Chem. **8**, 1665–1668 (1969), doi:10.1021/ic50078a019.