$CsCrF_4$ Structure: ABC4_hP18_189_f_g_fgj-001

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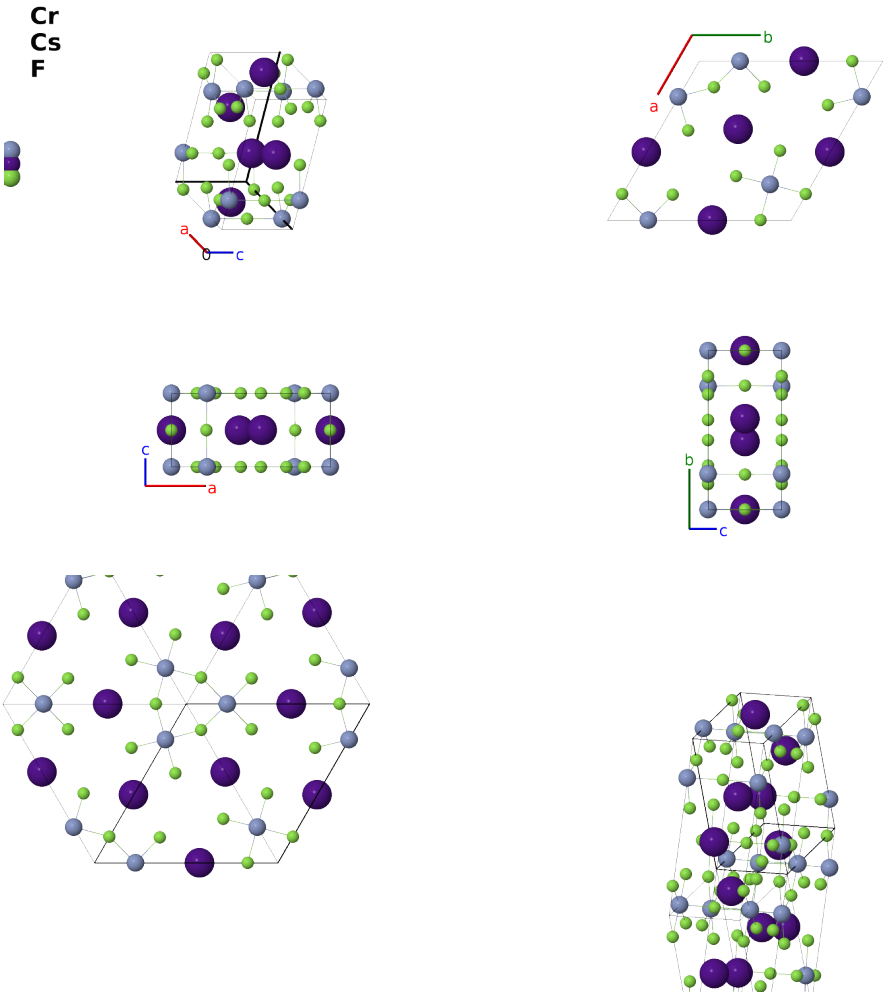
https://aflow.org/prototype-encyclopedia/6BNK

https://aflow.org/prototype-encyclopedia/ABC4_hP18_189_f_g_fgj-001



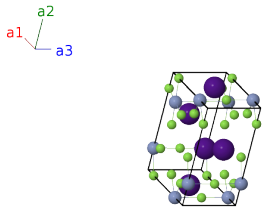
Prototype	$CrCsF_4$
AFLOW prototype label	ABC4_hP18_189_f_g_fgj-001
ICSD	2278
CCDC	1592188
Pearson symbol	hP18
Space group number	189

Space group symbol $P\bar{6}2m$

AFLOW prototype command `aflow --proto=ABC4_hP18_189_f_g_fgj-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, y_5$

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(3f)	Cr I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(3f)	Cr I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(3f)	Cr I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(3f)	F I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_2$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(3f)	F I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(3f)	F I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cs I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cs I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Cs I
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}}$	(6j)	F III
$\mathbf{B_{14}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6j)	F III
$\mathbf{B_{15}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}$	(6j)	F III
$\mathbf{B_{16}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}}$	(6j)	F III
$\mathbf{B_{17}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6j)	F III
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}$	(6j)	F III

References

[1] D. Babel and G. Knoke, *Strukturen caesiumhaltiger Fluoride. IV. Die KristallStruktur von $CsCrF_4$ - ein neuer Tetrafluorometallat-Typ mit Kettenstruktur*, Z. Anorganische und Allgemeine Chemie **442**, 151–162 (1978), doi:10.1002/zaac.19784420119.

Found in

[1] H. Manaka, Y. Hirai, Y. Hachigo, M. Mitsunaga, M. Ito, and N. Terada, *Spin-Liquid State Study of Equilateral Triangle S=3/2 Spin Tubes Formed in $CsCrF_4$*, J. Phys. Soc. Jpn. **78**, 093701 (2009), doi:10.1143/JPSJ.78.093701.

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