

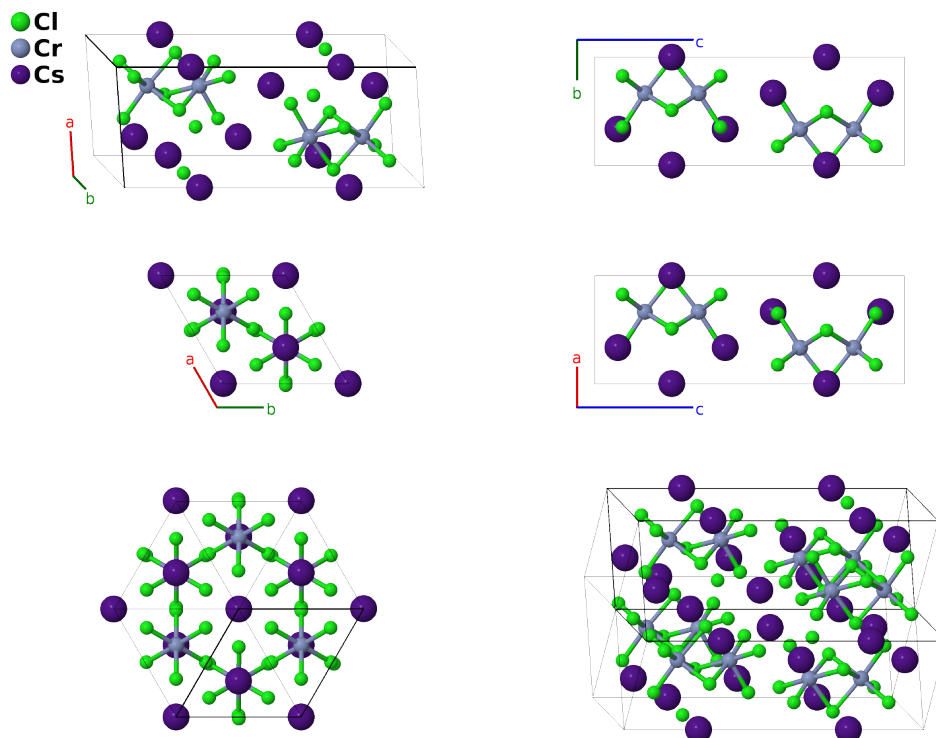
Cs₃Cr₂Cl₉ Structure: A9B2C3_hP28_194_hk_f_bf-001

This structure originally had the label A9B2C3_hP28_194_hk_f_bf. Calls to that address will be redirected here.

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<https://aflow.org/p/77Z6>

https://aflow.org/p/A9B2C3_hP28_194_hk_f_bf-001



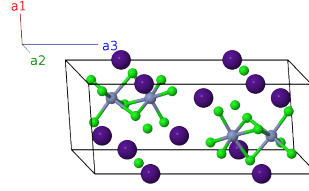
Prototype	Cl ₉ Cr ₂ Cs ₃
AFLOW prototype label	A9B2C3_hP28_194_hk_f_bf-001
ICSD	16706
Pearson symbol	hP28
Space group number	194
Space group symbol	<i>P6₃/mmc</i>
AFLOW prototype command	<code>aflow --proto=A9B2C3_hP28_194_hk_f_bf-001 --params=a, c/a, z₂, z₃, x₄, x₅, z₅</code>

Other compounds with this structure

Cs₃Cr₂Br₉, Mo₂N₃Cl₉, Rb₃Mo₂Br₉, Rb₃Nb₂Br₉, Rb₃Os₂Br₉, Rb₃Mo₂Cl₉

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Cs I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Cs I
\mathbf{B}_3	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Cr I
\mathbf{B}_4	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cr I
\mathbf{B}_5	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Cr I
\mathbf{B}_6	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cr I
\mathbf{B}_7	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Cs II
\mathbf{B}_8	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cs II
\mathbf{B}_9	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Cs II
\mathbf{B}_{10}	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Cs II
\mathbf{B}_{11}	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{12}	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{15}	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{16}	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{18}	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{19}	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{20}	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{21}	$= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{22}	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{23}	$= 2x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{24}	$= -x_5 \mathbf{a}_1 - 2x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{25}	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\sqrt{3}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{26}	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{27}	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II
\mathbf{B}_{28}	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\sqrt{3}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k)	Cl II

References

- [1] G. G. Wessel and D. J. W. IJdo, *The Crystal Structure of $Cs_3Cr_2Cl_9$* , Acta Cryst. **10**, 466–468 (1957), doi:10.1107/S0365110X57001577.

Found in

- [1] A. Dönni, A. Furrer, and H. U. Güdel, *Structure of the dimer compounds $Cs_3R_2Br_9$ ($R = Tb, Dy, Ho, Er, Yb$) at 8 and 295 K studied by neutron diffraction*, J. Solid State Chem. **81**, 278–284 (1989), doi:10.1016/0022-4596(89)90015-7.