

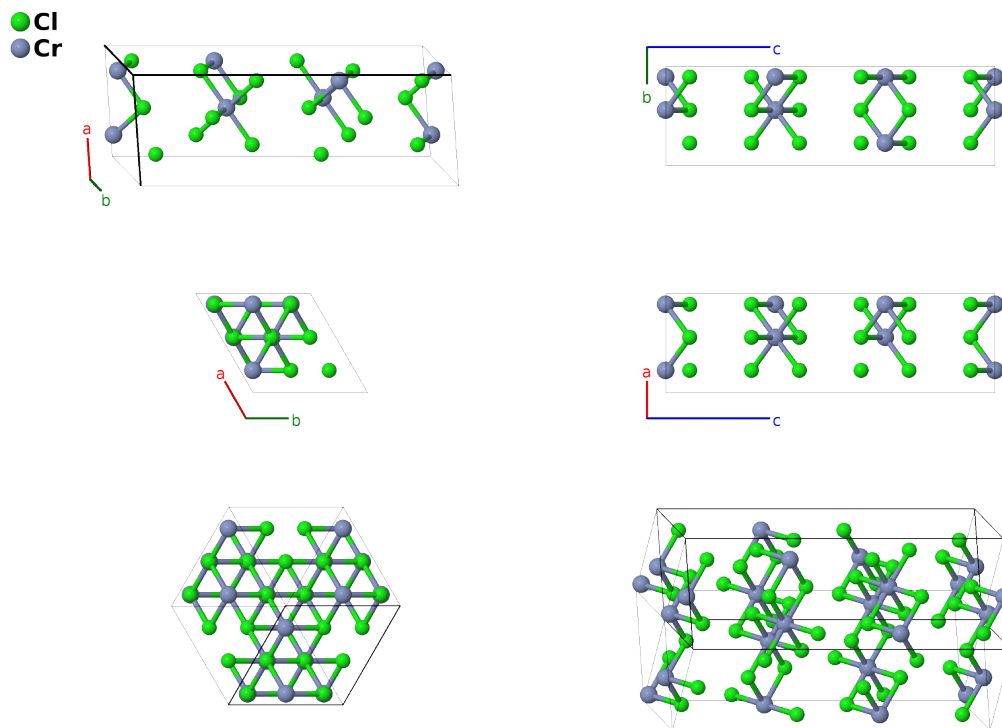
CrCl₃ (*D*₀₄) Structure: A3B_hP24_151_3c_2a-001

This structure originally had the label A3B_hP24_151_3c_2a. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

<https://aflow.org/p/5EPG>

https://aflow.org/p/A3B_hP24_151_3c_2a-001



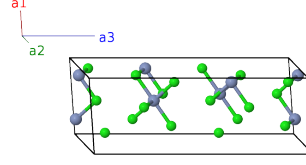
Prototype	Cl ₃ Cr
AFLOW prototype label	A3B_hP24_151_3c_2a-001
<i>Strukturbericht</i> designation	<i>D</i> ₀₄
ICSD	33578
Pearson symbol	hP24
Space group number	151
Space group symbol	<i>P</i> 3 ₁ 12
AFLOW prototype command	<code>aflow --proto=A3B_hP24_151_3c_2a-001 --params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

Other compounds with this structure
CrBr₃, CrI₃, α-AlCl₃, α-RuCl₃

- This structure may also be found in the enantiomorphic space group $P3_212$ #153. The ICSD entry for this structure is in that space group.

Trigonal (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	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Cr I
\mathbf{B}_2	$= x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Cr I
\mathbf{B}_3	$= -2x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(3a)	Cr I
\mathbf{B}_4	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Cr II
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Cr II
\mathbf{B}_6	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(3a)	Cr II
\mathbf{B}_7	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_8	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_9	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_{10}	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_{11}	$= -(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_{12}	$= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6c)	Cl I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{14}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{15}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{16}	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{17}	$= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{18}	$= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(6c)	Cl II
\mathbf{B}_{19}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{20}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{21}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{22}	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}}$	(6c)	Cl III

$$\mathbf{B}_{23} = \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \\ (z_5 - \frac{1}{3}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}} \quad (6c) \quad \text{Cl III}$$

$$\mathbf{B}_{24} = x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (6c) \quad \text{Cl III}$$

References

- [1] N. Wooster, *The Structure of Chromium Trichloride CrCl₃*, *Z. Kristallogr* **74**, 363–374 (1930), doi:10.1524/zkri.1930.74.1.363.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).