

CrCl₃ Structure:

A3B_hP24_153_3c_2a-001

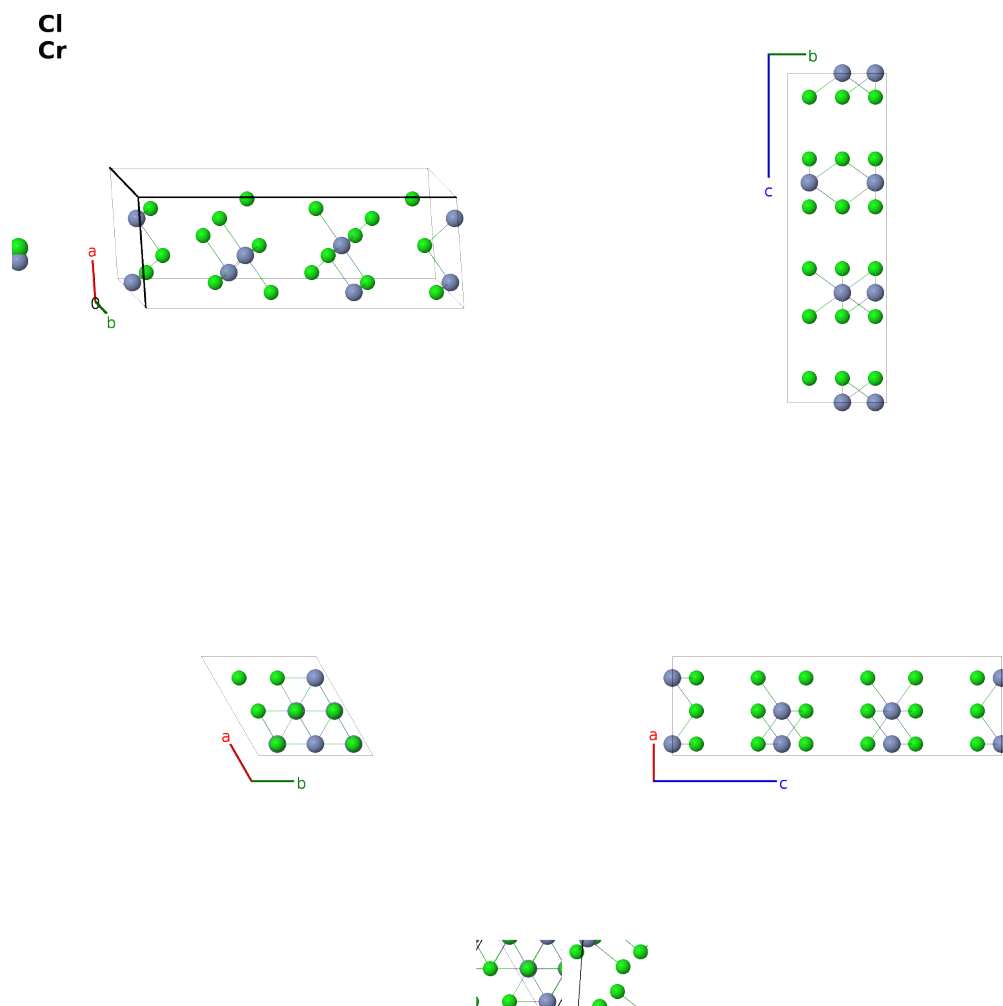
This structure previously used the label(s) **A3B_hP24_153_3c_2b**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/Z0S9>

https://aflow.org/prototype-encyclopedia/A3B_hP24_153_3c_2a-001



Prototype	Cl ₃ Cr
AFLOW prototype label	A3B_hP24_153_3c_2a-001
ICSD	33578
CCDC	1606339
Pearson symbol	hP24

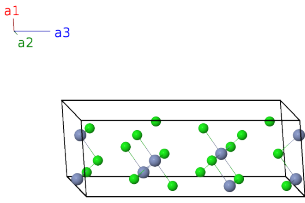
Space group number	153
Space group symbol	$P3_212$
AFLOW prototype command	<code>aflow --proto=A3B_hP24_153_3c_2a-001</code> <code>--params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

Other compounds with this structure

CrI₃

- This structure is the enantiomorph of the $D0_4$ (A3B_hP24_151_3c_2a) structure, and was generated by reflecting the coordinates of space group $P3_112$ #151 structure through the $z = 0$ plane.

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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	=	$-\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Cr I
$\mathbf{B}_2$	$x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	=	$\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	=	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Cr II
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	=	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_9$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{10}$	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{11}$	$-(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	Cl II

$$\begin{aligned}
\mathbf{B}_{15} &= - (x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{Cl II} \\
\mathbf{B}_{16} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right) \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}} - c\left(z_4 - \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{Cl II} \\
\mathbf{B}_{17} &= - (x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} & (6c) & \text{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) & \text{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) & \text{Cl III} \\
\mathbf{B}_{20} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{2}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (6c) & \text{Cl III} \\
\mathbf{B}_{21} &= - (x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{3}\right) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{Cl III} \\
\mathbf{B}_{22} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{3}\right) \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}} - c\left(z_5 - \frac{1}{3}\right) \hat{\mathbf{z}} & (6c) & \text{Cl III} \\
\mathbf{B}_{23} &= - (x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{2}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}} & (6c) & \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}} & (6c) & \text{Cl III}
\end{aligned}$$

References

- [1] N. Wooster, *The Structure of Chromium Trichloride CrCl_3* , 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).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043