

CrCl₃(H₂O)₆ (*J*2₂) Structure: A3BC6_hR20_167_e_b_f-001

This structure previously used the label(s) **A3BC6_hR20_167_e_b_f**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/YFN8>

https://aflow.org/prototype-encyclopedia/A3BC6_hR20_167_e_b_f-001

Prototype	CrCl ₃ (H ₂ O) ₆
AFLOW prototype label	A3BC6_hR20_167_e_b_f-001
<i>Strukturbericht</i> designation	<i>J</i> 2 ₂
ICSD	26138
CCDC	1601578
Pearson symbol	hR20
Space group number	167
Space group symbol	<i>R</i> $\bar{3}c$
AFLOW prototype command	<code>aflow --proto=A3BC6_hR20_167_e_b_f-001 --params=<i>a</i>, <i>c/a</i>, <i>x</i>₂, <i>x</i>₃, <i>y</i>₃, <i>z</i>₃</code>

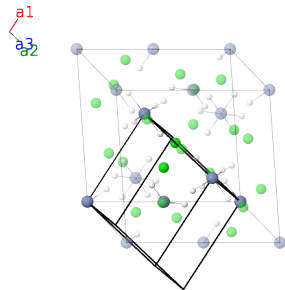
Other compounds with this structure

AlCl₃(H₂O)₆

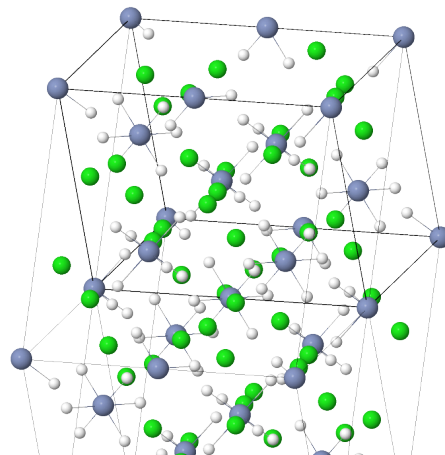
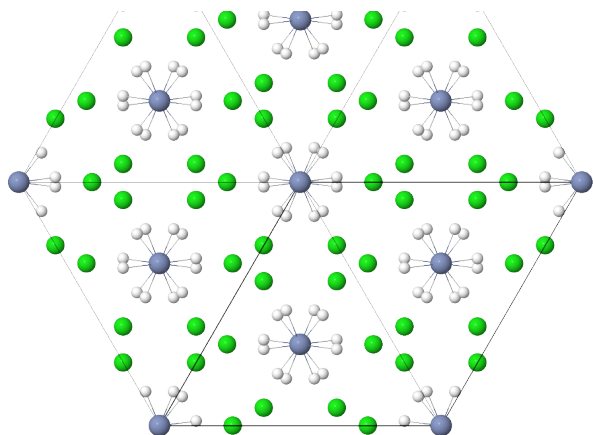
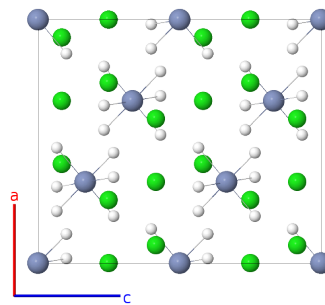
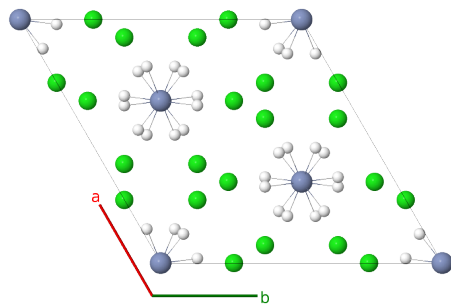
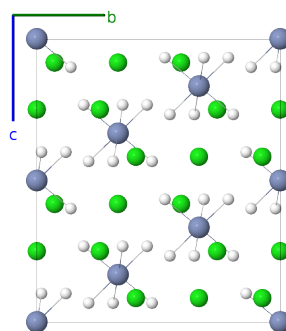
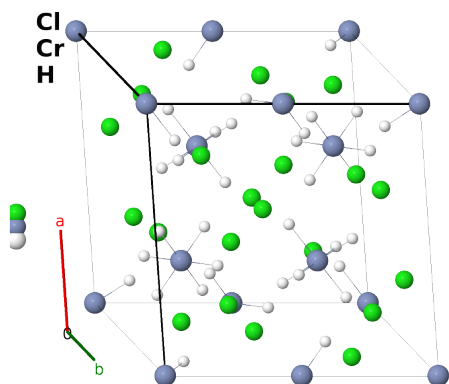
- The positions of the hydrogen atoms in the water molecules were not determined, so we only provide the positions of the oxygen atoms (labeled as H₂O).

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors



	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2b) Cr I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b) Cr I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8} a (4x_2 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8} a (4x_2 - 1) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_4$	$=$	$\frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{8} a (4x_2 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8} a (4x_2 - 1) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_6$	$=$	$-x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8} a (4x_2 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24} a (12x_2 + 1) \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_7$	$=$	$\frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{8} a (4x_2 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24} a (12x_2 + 5) \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_8$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + \frac{5}{12} c \hat{\mathbf{z}}$	(6e) Cl I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{10}$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2} a (y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{11}$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2} a (x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{12}$	$=$	$-(z_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 - 3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{13}$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2} a (y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 - 3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{14}$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2} a (x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 - 3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{15}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2} a (x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{16}$	$=$	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a (y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{17}$	$=$	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3} c (x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{18}$	$=$	$(z_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2} a (x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{19}$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a (y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a (2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(12f) H I
$\mathbf{B}_{20}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a (x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a (x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{6} c (2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(12f) H I

References

- [1] K. R. Andress and C. Carpenter, *Die Struktur von Chromchlorid- und Aluminiumchloridhexahydrat*, Z. Krystallogr. **87**, 446–463 (1934), doi:10.1524/zkri.1934.87.1.446.

Found in

- [1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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