$CrCl_3(H_2O)_6$ ($J2_2$) Structure: A3BC6_hR20_167_e_b_f-001

This structure originally had the label `A3BC6_hR20_167_e_b_f`. Calls to that address will be redirected here.

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https://aflow.org/p/YFN8

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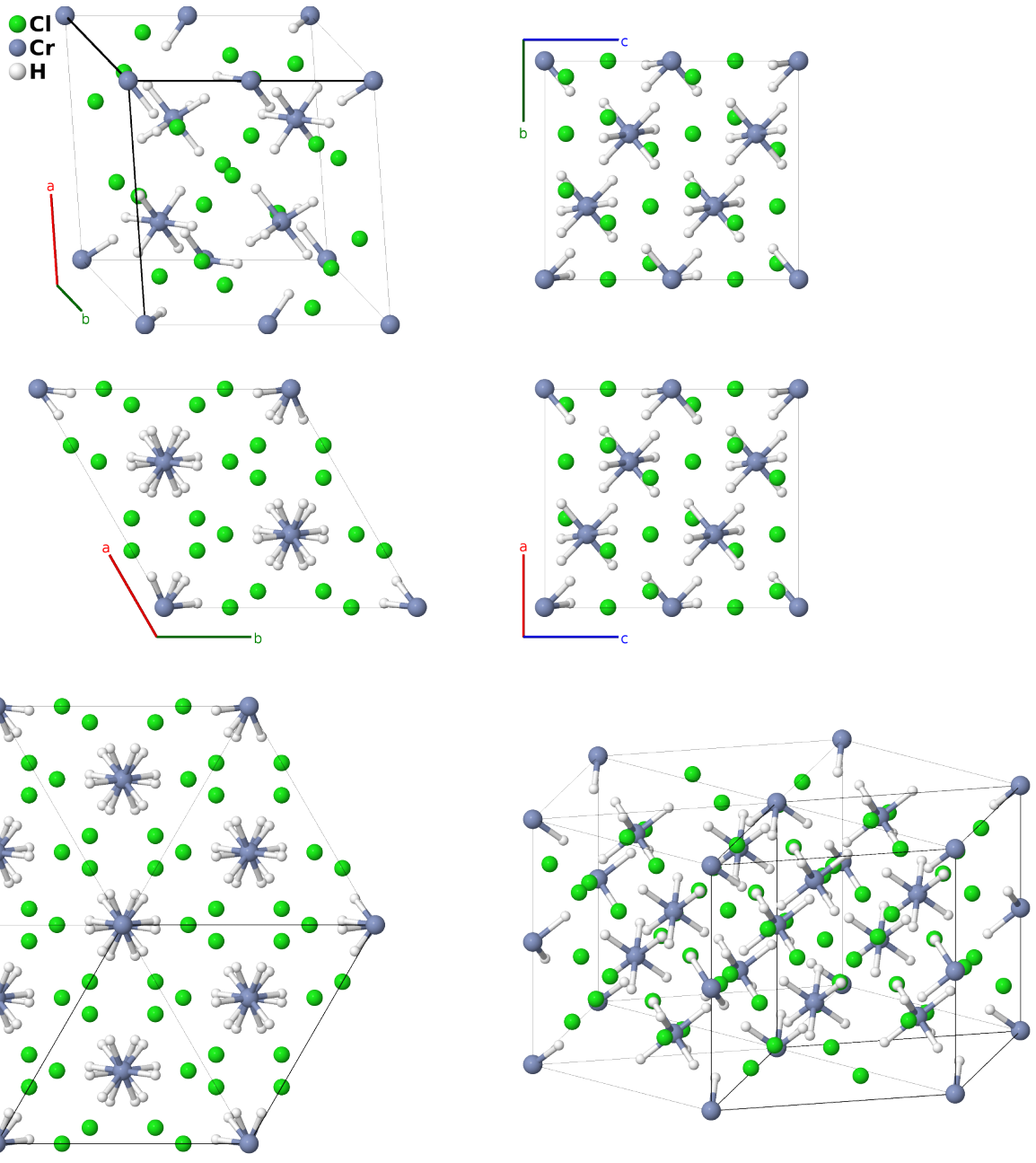


Prototype $CrCl_3(H_2O)_6$

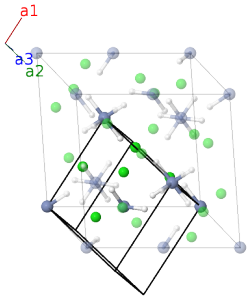
AFLOW prototype label	A3BC6_hR20_167_e_b_f-001
***Strukturbericht* designation**	$J2_2$
ICSD	26138
Pearson symbol	hR20
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A3BC6_hR20_167_e_b_f-001 --params=`$a, c/a, x_2, x_3, y_3, z_3$

Other compounds with this structure
$AlCl_3(H_2O)_6$

- 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 H_2O).

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_2 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_2 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_2 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_2 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{12}}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_3 + 2y_3 + 2z_3 - 3)\,\hat{\mathbf{z}}$	(12f)	H I

$$\mathbf{B_{13}} = -\left(y_3-\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_3-\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_3-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}}-\tfrac{1}{6}c\left(2x_3+2y_3+2z_3-3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{14}} = -\left(x_3-\tfrac{1}{2}\right)\mathbf{a}_1-\left(z_3-\tfrac{1}{2}\right)\mathbf{a}_2-\left(y_3-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}}-\tfrac{1}{6}c\left(2x_3+2y_3+2z_3-3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{15}} = -x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}}-\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{16}} = -z_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2-y_3\,\mathbf{a}_3 = \tfrac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}}-\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{17}} = -y_3\,\mathbf{a}_1-z_3\,\mathbf{a}_2-x_3\,\mathbf{a}_3 = \tfrac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}}-\tfrac{1}{3}c\left(x_3+y_3+z_3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{18}} = \left(z_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_3+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_3-z_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{19}} = \left(y_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_3+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_3-z_3\right)\hat{\mathbf{x}}+\tfrac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

$$\mathbf{B_{20}} = \left(x_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(z_3+\tfrac{1}{2}\right)\mathbf{a}_2+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_3-y_3\right)\hat{\mathbf{x}}-\tfrac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\hat{\mathbf{y}}+\tfrac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\hat{\mathbf{z}} \quad (12f) \quad \text{H I}$$

References

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Found in

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