β-$RuCl_3$ Structure: A3B_hP8_158_d_a-001

This structure originally had the label `A3B_hP8_158_d_a`. Calls to that address will be redirected here.

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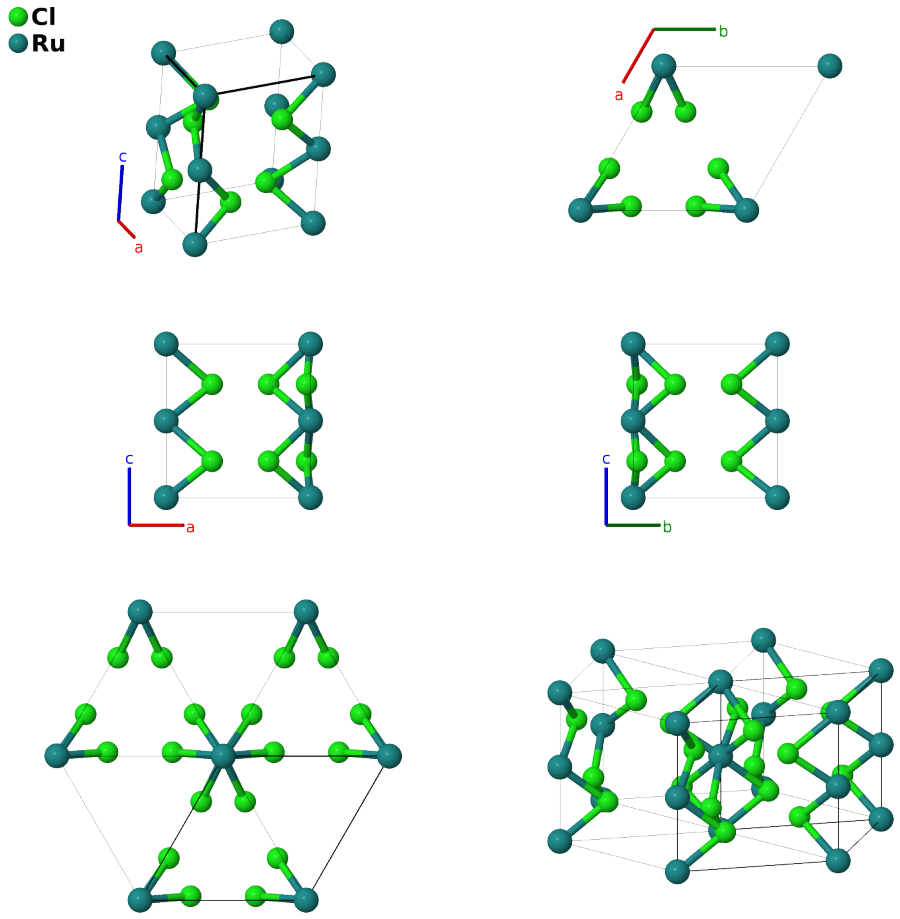
https://aflow.org/p/KC70

https://aflow.org/p/A3B_hP8_158_d_a-001

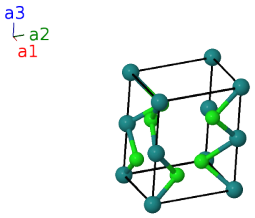


Prototype	Cl_3Ru
AFLOW prototype label	A3B_hP8_158_d_a-001
ICSD	22093
Pearson symbol	hP8
Space group number	158
Space group symbol	$P3c1$
AFLOW prototype command	`aflow --proto=A3B_hP8_158_d_a-001 --params=`$a, c/a, z_1, x_2, y_2, z_2$

- The crystal structure of both α- and β-$RuCl_3$ is somewhat uncertain:
- α-$RuCl_3$ has been reported in the trigonal $CrCl_3$ ($D0_4$) structure (Fletcher, 1967) and in the monoclinic $AlCl_3$ structure (Johnson, 2015).
- (Fletcher, 1967) states that the structure of β-$RuCl_3$ is consistent with the hexagonal space groups $P6_3cm$ #185, $P6c2$ #188, and $P6_3/mcm$ #193, in addition to the trigonal space group $P3c1$ #158, which we present here. We also provide the structure with space group #185: hexagonal β-$RuCl_3$ (A3B_hP8_185_c_a).
- Space group $P3c1$ #158 allows an arbitary choice of the origin of the z-axis. Here we set $z_1 = 0$ for the ruthenium (2a) atoms.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ru I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ru I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6d)	Cl I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 + (x_2-y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2-2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6d)	Cl I
$\mathbf{B_5}$	=	$-(x_2-y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6d)	Cl I
$\mathbf{B_6}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6d)	Cl I
$\mathbf{B_7}$	=	$-(x_2-y_2)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_2+2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6d)	Cl I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 + (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6d)	Cl I

References

[1] J. M. Fletcher, W. E. Gardner, A. C. Fox, and G. Topping, *X-Ray, infrared, and magnetic studies of - and -ruthenium trichloride*, J. Chem. Soc. A pp. 1038–1045 (1967), doi:10.1039/J19670001038.

[2] R. D. Johnson, S. C. Williams, A. A. Haghighirad, J. Singleton, V. Zapf, P. Manuel, I. I. Mazin, Y. Li, H. O. Jeschke, R. Valentí, and R. Coldea, *Monoclinic crystal structure of α-RuCl$_3$ and the zigzag antiferromagnetic ground state*, Phys. Rev. B **92**, 235119 (2015), doi:10.1103/PhysRevB.92.235119.