

UCl₃ Structure: A3B_hP8_176_h_c-001

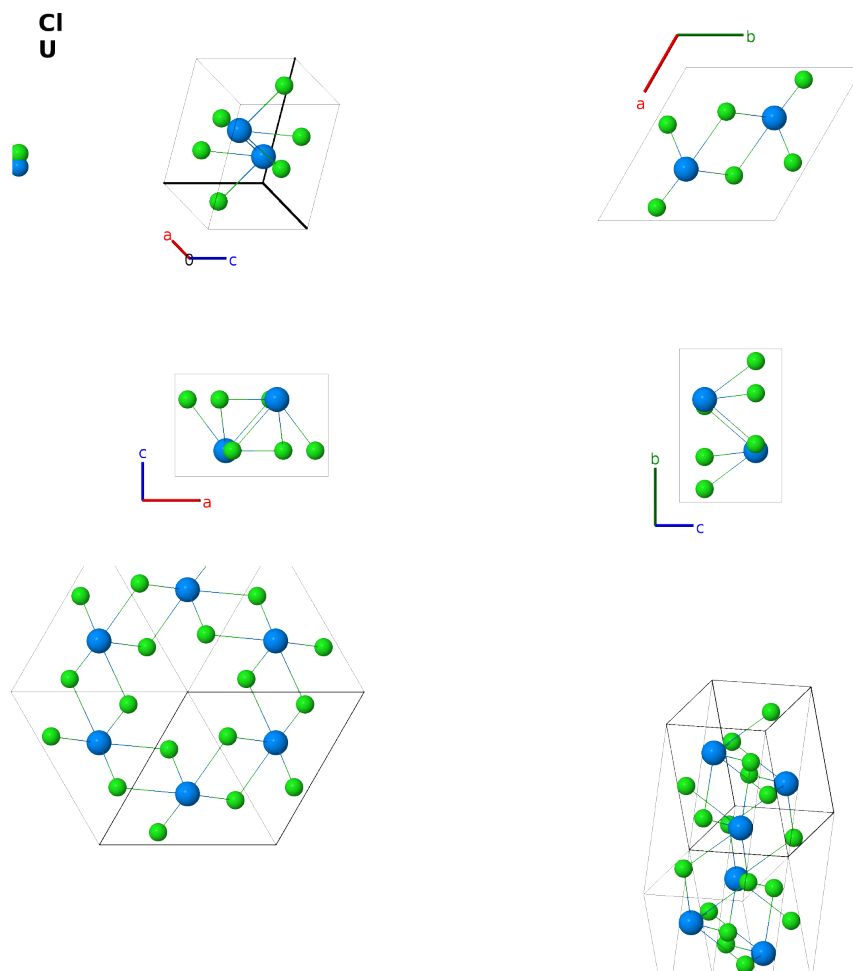
This structure previously used the label(s) **A3B_hP8_176_h_c**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A3B_hP8_176_h_c-001



Prototype	Cl ₃ U
AFLOW prototype label	A3B_hP8_176_h_c-001
ICSD	27857
CCDC	1603035
Pearson symbol	hP8
Space group number	176

Space group symbol $P6_3/m$

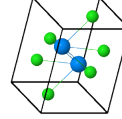
AFLOW prototype command `aflow --proto=A3B_hP8_176_h_c-001`
`--params=a, c/a, x2, y2`

Other compounds with this structure

AcBr₃, AgCl₃, AmCl₃, CeBr₃, CeCl₃, La(OH)₃, LaCl₃, NbCl₃, Nd(OH)₃, NdCl₃, NpBr₃, NpCl₃, α -NpBr₃, Pr(OH)₃, PrBr₃, PrCl₃, PuCl₃, UBr₃

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
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	U I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	U I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
$\mathbf{B}_5$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_2 - y_2) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Cl I

References

- [1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. I. New structure types*, Acta Cryst. **1**, 265–268 (1948), doi:10.1107/S0365110X48000703.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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