

KNiCl₃ Structure:

A3BC_hP30_185_cd_c_ab-001

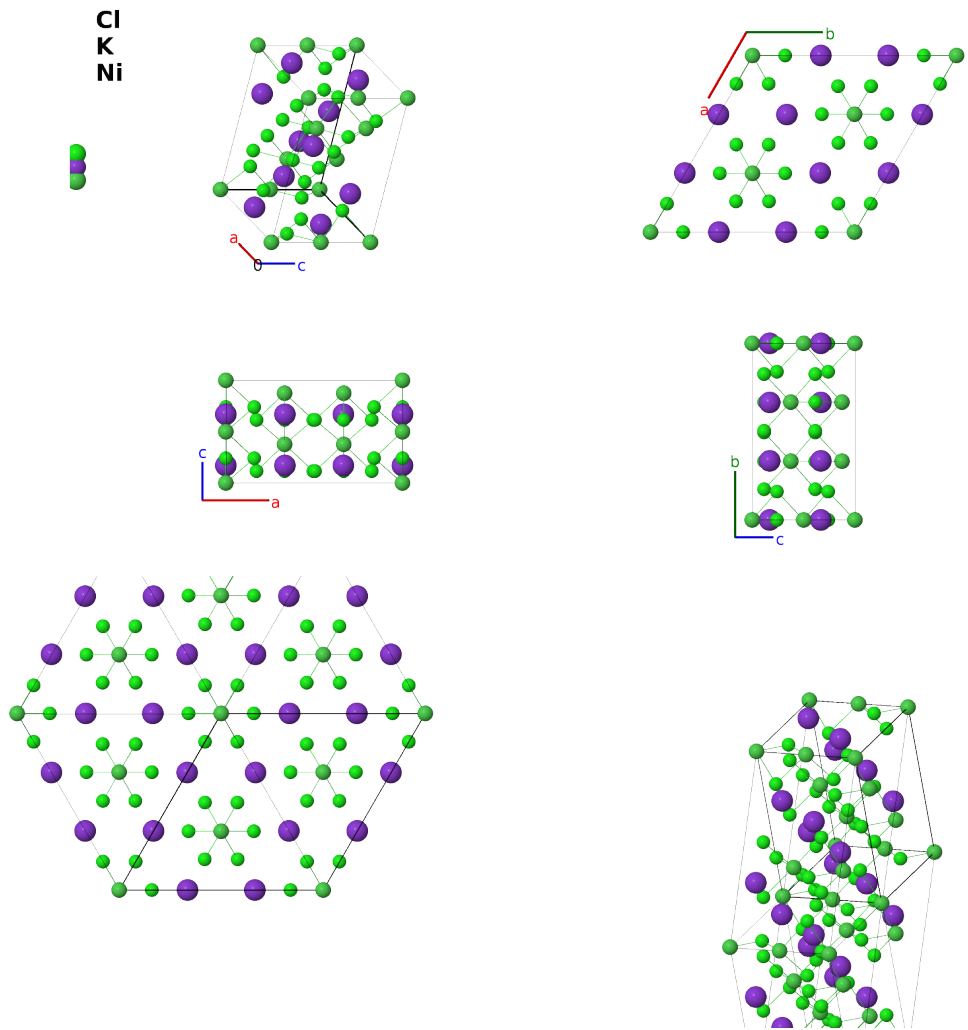
This structure previously used the label(s) **A3BC_hP30_185_cd_c_ab**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A3BC_hP30_185_cd_c_ab-001



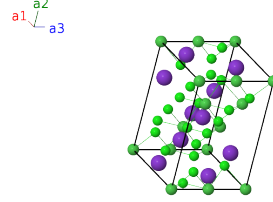
Prototype	Cl ₃ KNi
AFLOW prototype label	A3BC_hP30_185_cd_c_ab-001
ICSD	10508
CCDC	1595340
Pearson symbol	hP30

Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	<code>aflow --proto=A3BC_hP30_185_cd_c_ab-001</code> <code>--params=a, c/a, z₁, z₂, x₃, z₃, x₄, z₄, x₅, y₅, z₅</code>

- Space group $P6_3cm$ #185 allows an arbitrary choice of the origin of the z -axis. Here we set $z_1 = 0$ for the nickel (2a) atoms.

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
$\mathbf{B}_1$	$z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_2$	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B}_3$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_4$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_5$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_6$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_8$	$x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_9$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{14}$	$x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{16}$	$-x_4 \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{17}$	$-x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{18}$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B}_{19}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{20}$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{21}$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B}_{22}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Cl II

$$\mathbf{B}_{23} = y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{24} = (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{25} = -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{26} = -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{27} = x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{28} = y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{29} = (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

$$\mathbf{B}_{30} = -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (12d) \quad \text{Cl II}$$

References

- [1] D. Visser, G. C. Verschoor, and D. J. W. IJdo, *The Structure of KNiCl₃ at Room Temperature*, Acta Crystallogr. Sect. B **36**, 28–34 (1980), doi:10.1107/S0567740880002385.

Found in

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

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