$KNiCl_3$ Structure: A3BC_hP30_185_cd_c_ab-001

This structure originally had the label `A3BC_hP30_185_cd_c_ab`. Calls to that address will be redirected here.

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https://aflow.org/p/PKFR

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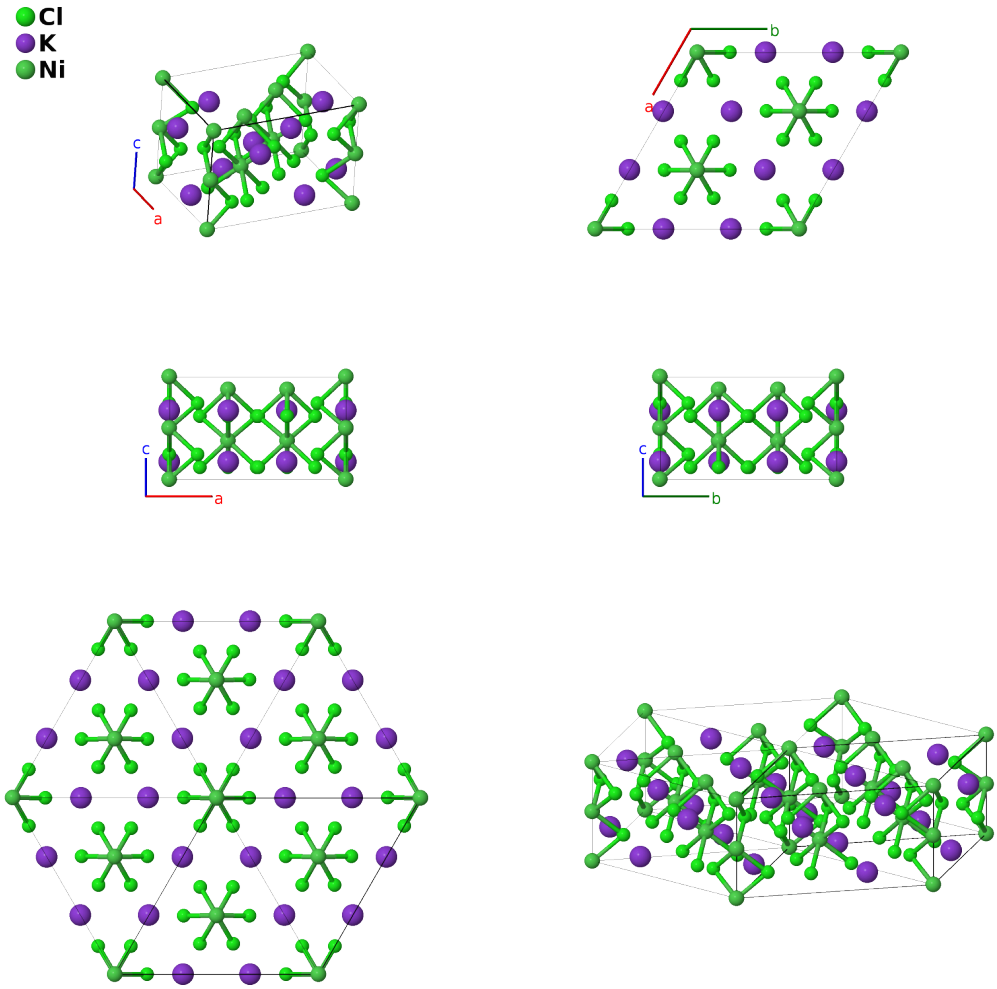


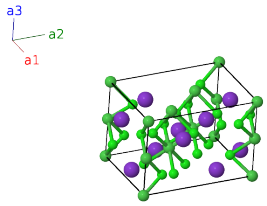
Prototype	Cl_3KNi
AFLOW prototype label	A3BC_hP30_185_cd_c_ab-001
ICSD	10508
Pearson symbol	hP30
Space group number	185
Space group symbol	$P6_3cm$

AFLOW prototype command `aflow --proto=A3BC_hP30_185_cd_c_ab-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

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

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ni 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)	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
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	Ni II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Cl I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	K I
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5+y_5\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{20}}$	=	$-y_5\,\mathbf{a}_1+\left(x_5-y_5\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5-2y_5\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{21}}$	=	$-\left(x_5-y_5\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5-y_5\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{22}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5+y_5\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{23}}$	=	$y_5\,\mathbf{a}_1-\left(x_5-y_5\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5+2y_5\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{24}}$	=	$\left(x_5-y_5\right)\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5-y_5\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II

$\mathbf{B_{25}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{26}}$	=	$-\,(x_5 - y_5)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{27}}$	=	$x_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{28}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{29}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II
$\mathbf{B_{30}}$	=	$-x_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	Cl II

References

[1] D. Visser, G. C. Verschoor, and D. J. W. IJdo, *The Structure of $KNiCl_3$ 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.