

KNiCl_3	$hP30$	(185) $P6_3cm - dc^2ba$
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KNiCl_3 rt [1], perovskite 2H

Structural features: Distorted close-packed KCl_3 layers in h stacking; Ni in octahedral voids. Infinite columns of face-linked NiCl_6 octahedra (linear -Ni- chains).

Visser D. et al. (1980) [1]

Cl_3KNi

$a = 1.1795$, $c = 0.5926$ nm, $c/a = 0.502$, $V = 0.7140$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$12d$	1	0.1732	0.5056	0.1148		non-colinear Ni_2
Cl2	$6c$	$..m$	0.1598	0	0.2396		non-colinear Ni_2
K3	$6c$	$..m$	0.6647	0	0.1706		tricapped trigonal prism Cl_9
Ni4	$4b$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.377		8-vertex polyhedron Cl_6Ni_2
Ni5	$2a$	$3.m$	0	0	0.0		8-vertex polyhedron Cl_6Ni_2

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.047$, $T = 293$ K

Remarks: Phase stable at $T < 560$ K. Space groups (188) $P-6c2$ and (193) $P6_3/mcm$ were tested and rejected. Refinement of a disordered model in the same space group (superposition of two isopointal structures shifted along $[001]$) reduced the reliability factor to $R = 0.033$.

References: [1] Visser D., Verschoor G.C., Ijdo D.J.W. (1980), Acta Crystallogr. B 36, 28-34.