$KNiCl_3$	*hP*60	(185) $P6_3cm$ – $d^2c^4b^2a^2$

$KNiCl_3$ rt [1], perovskite 2H
Structural features: Distorted close-packed KCl_3 layers in h stacking; Ni in octahedral voids (high degree of disorder). Derivative of $BaNiO_3$.

Visser D. et al. (1980) [1]
Cl_3KNi
a = 1.1795, c = 0.5926 nm, c/a = 0.502, V = 0.7140 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12*d*	1	0.1729	0.5058	0.1296	0.332	
Cl2	12*d*	1	0.1746	0.505	0.2065	0.668	
Cl3	6*c*	..*m*	0.1599	0	0.2919	0.332	
Cl4	6*c*	..*m*	0.1602	0	0.2374	0.668	
K5	6*c*	..*m*	0.6636	0	0.2284	0.332	
K6	6*c*	..*m*	0.6662	0	0.1502	0.668	
Ni7	4*b*	3..	$^1/_3$	$^2/_3$	0.3903	0.332	
Ni8	4*b*	3..	$^1/_3$	$^2/_3$	0.4641	0.668	
Ni9	2*a*	3.*m*	0	0	0.0	0.668	
Ni10	2*a*	3.*m*	0	0	0.0478	0.332	

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.9522
Experimental: single crystal, diffractometer, X-rays, wR = 0.033, T = 293 K

Remarks: Phase stable at T < 560 K. Short interatomic distances for partly occupied site(s). Twinning model; refinement of the corresponding ordered model in the same space group gave R = 0.047. Space groups (158) *P*3*c*1, (165) *P*-3*c*1, (188) *P*-6*c*2 and (193) $P6_3/mcm$ (R > 0.50 for the latter two) were tested and rejected.

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