

$\text{Na}_{0.5}\text{NdCl}_3$	$hP10$	(176) $P6_3/m - hca$
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NaNd₂Cl₆ [1]; $\text{Na}_{0.9}(\text{Ca}_{0.9}\text{R}_{1.1})\text{F}_6$ [2], gagarinite-(Y)

Structural features: Infinite columns of base-linked NdCl_6Cl_3 tricapped trigonal prisms share atoms to form a 3D-framework; Na in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of UCl_3 .

Schleid T., Meyer G. (1987) [1]

$\text{Cl}_3\text{Na}_{0.50}\text{Nd}$

$a = 0.7626$, $c = 0.4388$ nm, $c/a = 0.575$, $V = 0.2210$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	6h	$m..$	0.3864	0.0821	$\frac{1}{4}$		single atom Na
Nd2	2c	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cl ₉
Na3	2a	$-6..$	0	0	$\frac{1}{4}$	0.5	trigonal bipyramid Na ₂ Cl ₃

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.060

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Schleid T., Meyer G. (1987), Inorg. Chim. Acta 140, 113-116. [2] Hughes J.M., Drexler J.W. (1994), Can. Mineral. 32, 563-565.