

$\text{Na}_{0.5}\text{SmCl}_3$ $hP12$ $(176) P6_3/m - hcba$ **NaSm₂Cl₆** [1]

Structural features: Infinite columns of base-linked SmCl₆Cl₃ 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 UCl₃.

Lissner F. et al. (1994) [1]

 $\text{Cl}_3\text{Na}_{0.50}\text{Sm}$ $a = 0.75614$, $c = 0.43326$ nm, $c/a = 0.573$, $V = 0.2145$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$6h$	$m..$	0.387	0.0872	$\frac{1}{4}$		
Sm2	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cl ₉
Na3	$2b$	$-3..$	0	0	0	0.344	
Na4	$2a$	$-6..$	0	0	$\frac{1}{4}$	0.156	

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.017

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

References: [1] Lissner F., Krämer K., Schleid T., Meyer G., Hu Z., Kaindl G. (1994), Z. Anorg. Allg. Chem. 620, 444-450.