

$\text{Ce}_4\text{S}_3(\text{S}_{0.33}\text{Cl}_{0.67})_3\text{O}$ *hP22*(186) $P6_3mc - c^3b^2$ **Ce₄OS₄Cl₂** [1]; Na₅SrNbP₄ [2]; La₄NS₃Cl₃ [3]Structural features: OCe₄ tetrahedra in a Mg-type (h.c.p.) arrangement in a matrix of S and Cl atoms. Ordering variant of Ba₄Cl₆O, Ce₄[S₃(Cl,S)₃]O.

Schleid T. (1991) [1]

Ce₄Cl₂OS₄ $a = 0.92549$, $c = 0.69413$ nm, $c/a = 0.750$, $V = 0.5149$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>c</i>	. <i>m</i> .	0.1324	0.8676	0.2774		non-coplanar triangle Ce ₃
S2	6 <i>c</i>	. <i>m</i> .	0.5302	0.4698	0.1076		non-coplanar triangle Ce ₃
Ce3	6 <i>c</i>	. <i>m</i> .	0.80505	0.19495	0.3858		square antiprism OCl ₃ S ₄
O4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		tetrahedron Ce ₄
Ce5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3453		tetrahedron OS ₃

M1 = 0.667Cl + 0.333S

Transformation from published data: origin shift 0 0 0.3642

Experimental: single crystal, diffractometer, X-rays, wR = 0.019

Remarks: A fully ordered structure is reported for La₄NS₃Cl₃.

References: [1] Schleid T. (1991), Eur. J. Solid State Inorg. Chem. 28, 737-748. [2] Lin J., Hönlé W., Von Schnering H.G. (1992), J. Alloys Compd. 183, 403-412. [3] Lissner F., Schleid T. (1994), Z. Anorg. Allg. Chem. 620, 1998-2002.