

La(OH₂)₉(CF₃SO₃)₃ [1]

Structural features: La(OH₂)₆(OH₂)₃ tricapped trigonal prisms surrounded by three F₃C-SO₃ units. See Fig. IV.78.

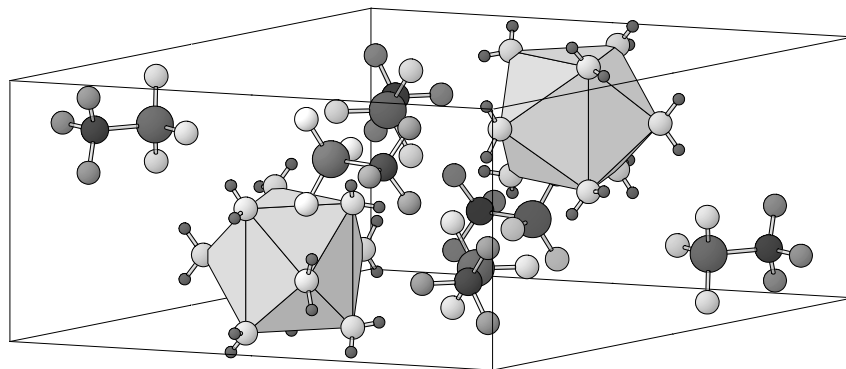


Fig. IV.78. **La(OH₂)₉(CF₃SO₃)₃**

Arrangement of La(OH₂)₆(OH₂)₃ tricapped trigonal prisms (O atoms medium, H atoms small) and CF₃SO₃ units (C atoms dark, F atoms medium, S atoms large, O atoms light). For clarity, atoms located in the cell but belonging to units with the C and S atoms in a neighboring cell are omitted.

Harrowfield J.M. et al. (1983) [1]

C₃F₉H₁₈LaO₁₈S₃

$a = 1.399$, $c = 0.7444$ nm, $c/a = 0.532$, $V = 1.2617$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.0178	0.399	0.0869		single atom S
F2	12i	1	0.0417	0.2035	0.1063		single atom C
O3	12i	1	0.5403	0.2053	0.0115		single atom La
C4	6h	$m..$	0.0082	0.2322	$\frac{1}{4}$		tetrahedron F ₃ S
S5	6h	$m..$	0.06126	0.3807	$\frac{1}{4}$		tetrahedron O ₃ C
O6	6h	$m..$	0.1791	0.4278	$\frac{1}{4}$		single atom S
F7	6h	$m..$	0.2799	0.1004	$\frac{1}{4}$		single atom C
O8	6h	$m..$	0.4888	0.3503	$\frac{1}{4}$		single atom La
La9	2d	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		tricapped trigonal prism O ₉
H10	12i	1	0.294	0.513	0.069		
H11	12i	1	0.45	0.349	0.153		
H12	12i	1	0.502	0.145	0.029		

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.043$, $T = 296$ K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Harrowfield J.M., Kepert D.L., Patrick J.M., White A.H. (1983), Aust. J. Chem. 36, 483-492.