

La₃Nd₁₁[SiO₄]₉O₃*hP*126(176) *P*6₃/*m* – i⁷h⁴f³ea**La₃Nd₁₁(SiO₄)₉O₃** [1], apatite family

Structural features: Infinite columns of base-linked NdO₆ and LaO₆ trigonal prisms (partial vacancies for the latter) share vertices with SiO₄ tetrahedra to form a 3D-framework; additional O (trigonal coordination) in infinite columns of face-linked Nd₆ octahedra in channels parallel to [001].

Malinovskii Y.A. et al. (1990) [1]

La₃Nd₁₁O₃₉Si₉*a* = 0.9638, *c* = 2.135 nm, *c/a* = 2.215, *V* = 1.7175 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.165	0.483	0.0875		single atom Si
Nd2	12 <i>i</i>	1	0.2367	0.2509	0.0813		pentagonal bipyramid O ₇
O3	12 <i>i</i>	1	0.258	0.347	0.1883		single atom Si
O4	12 <i>i</i>	1	0.312	0.069	0.0283		single atom Si
O5	12 <i>i</i>	1	0.365	0.105	0.1475		single atom Si
Si6	12 <i>i</i>	1	0.3991	0.0279	0.0834		tetrahedron O ₄
O7	12 <i>i</i>	1	0.593	0.122	0.0774		single atom Si
O8	6 <i>h</i>	<i>m</i> ..	0.127	0.529	¹ / ₄		single atom Si
Nd9	6 <i>h</i>	<i>m</i> ..	0.2502	0.0152	¹ / ₄		pentagonal bipyramid O ₇
Si10	6 <i>h</i>	<i>m</i> ..	0.3728	0.403	¹ / ₄		tetrahedron O ₄
O11	6 <i>h</i>	<i>m</i> ..	0.494	0.331	¹ / ₄		single atom Si
La12	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0012	0.5	octahedron O ₆
La13	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.165		tricapped trigonal prism O ₉
Nd14	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.6617		tricapped trigonal prism O ₉
O15	4 <i>e</i>	3..	0	0	0.1054		non-coplanar triangle Nd ₃
O16	2 <i>a</i>	-6..	0	0	¹ / ₄		coplanar triangle Nd ₃

Transformation from published data: origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.041

Remarks: In the abstract of [1] the Hermann-Mauguin symbol for the space group is misprinted as *P*6₃*m* instead of *P*6₃/*m* (given elsewhere).

References: [1] Malinovskii Y.A., Genkina E.A., Dimitrova O.V. (1990), Sov. Phys. Crystallogr. 35, 184-186 (Kristallografiya 35, 328-331).