

$\text{Nd}_4\text{Mn}[\text{SiO}_4]_3\text{O}$	$hP60$	$(176) P6_3/m - i^3h^3fa$
--	--------	---------------------------

$\text{Nd}_4\text{Mn}(\text{SiO}_4)_3\text{O}$ [1], apatite family

Structural features: Infinite columns of base-linked $(\text{Mn},\text{Nd})\text{O}_6\text{O}_3$ tricapped trigonal prisms (split O sites) share atoms with SiO_4 tetrahedra to form a 3D-framework; additional O (trigonal coordination) in infinite columns of face-linked Nd_6 octahedra parallel to $[001]$.

Klüver E., Müller Buschbaum H. (1995) [1]

$\text{MnNd}_4\text{O}_{13}\text{Si}_3$

$a = 0.94986$, $c = 0.6944$ nm, $c/a = 0.731$, $V = 0.5426$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$12i$	1	0.0641	0.3068	0.0817	0.5	
O2	$12i$	1	0.1026	0.3702	0.0582	0.5	
O3	$12i$	1	0.1301	0.5971	0.2131	0.5	
Si4	$6h$	$m..$	0.0282	0.4039	$\frac{1}{4}$		
Nd5	$6h$	$m..$	0.2408	0.2293	$\frac{1}{4}$		
O6	$6h$	$m..$	0.496	0.1663	$\frac{1}{4}$		single atom Si
M7	$4f$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.0036		
O8	$2a$	$-6..$	0	0	$\frac{1}{4}$		coplanar triangle Nd_3

$\text{M7} = 0.5\text{Mn} + 0.5\text{Nd}$

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.031$

Remarks: Short interatomic distances for partly occupied site(s). Space groups (147) $P-3$ and (173) $P6_3$ were tested and rejected ($R = 0.116$ and 0.050 , respectively).

References: [1] Klüver E., Müller Buschbaum H. (1995), Z. Naturforsch. B 50, 61-65.