

Nd[CO ₃][OH]	hP108	(174) <i>P</i> -6 – 1 ¹¹ k ⁶ j ⁶ ihg
--------------------------	-------	---

NdCO₃(OH) [1]

Structural features: Nd(O₆[OH]₂)[OH] monocapped square antiprisms are interconnected via common atoms and CO₃ trigonal units to form a 3D-framework.

Christensen A.N. (1973) [1]

CHNd_{0.93}O₄

a = 1.232, *c* = 0.988 nm, *c/a* = 0.802, *V* = 1.2987 nm³, *Z* = 18

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH)1	6 <i>l</i>	1	0.00567	0.35233	0.321		non-coplanar triangle Nd ₃
O2	6 <i>l</i>	1	0.07067	0.24933	0.115		single atom C
O3	6 <i>l</i>	1	0.08867	0.59833	0.385		single atom C
O4	6 <i>l</i>	1	0.09467	0.51133	0.115		single atom C
O5	6 <i>l</i>	1	0.14767	0.23333	0.385		single atom C
Nd6	6 <i>l</i>	1	0.21817	0.43933	0.2537		tricapped trigonal prism (OH) ₃ O ₆
Nd7	6 <i>l</i>	1	0.23037	0.10623	0.2638	0.83	tricapped trigonal prism O ₆ (OH) ₃
(OH)8	6 <i>l</i>	1	0.32067	0.32133	0.18		non-coplanar triangle Nd ₃
O9	6 <i>l</i>	1	0.41867	0.25433	0.385		single atom C
O10	6 <i>l</i>	1	0.43567	0.17533	0.115		single atom C
Nd11	6 <i>l</i>	1	0.56087	0.10493	0.2375	0.95	tricapped trigonal prism O ₆ (OH) ₃
C12	3 <i>k</i>	<i>m</i> ..	0.08667	0.19733	¹ / ₂		non-coplanar triangle O ₃
O13	3 <i>k</i>	<i>m</i> ..	0.16767	0.03633	¹ / ₂		single atom C
O14	3 <i>k</i>	<i>m</i> ..	0.23367	0.47233	¹ / ₂		single atom C
C15	3 <i>k</i>	<i>m</i> ..	0.34467	0.48133	¹ / ₂		non-coplanar triangle O ₃
C16	3 <i>k</i>	<i>m</i> ..	0.47067	0.30833	¹ / ₂		non-coplanar triangle O ₃
O17	3 <i>k</i>	<i>m</i> ..	0.57967	0.15033	¹ / ₂		single atom C
C18	3 <i>j</i>	<i>m</i> ..	0.01867	0.19533	0		non-coplanar triangle O ₃
C19	3 <i>j</i>	<i>m</i> ..	0.12667	0.48233	0		non-coplanar triangle O ₃
O20	3 <i>j</i>	<i>m</i> ..	0.17767	0.08833	0		single atom C
O21	3 <i>j</i>	<i>m</i> ..	0.19567	0.42833	0		single atom C
C22	3 <i>j</i>	<i>m</i> ..	0.48167	0.16233	0		non-coplanar triangle O ₃
O23	3 <i>j</i>	<i>m</i> ..	0.57667	0.14233	0		single atom C
(OH)24	2 <i>i</i>	3..	² / ₃	¹ / ₃	0.272		non-coplanar triangle Nd ₃
(OH)25	2 <i>h</i>	3..	¹ / ₃	² / ₃	0.23		non-coplanar triangle Nd ₃
(OH)26	2 <i>g</i>	3..	0	0	0.23		non-coplanar triangle Nd ₃

Transformation from published data: origin shift ¹/₃ ²/₃ 0

Experimental: single crystal, diffractometer, X-rays, R = 0.082

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

References: [1] Christensen A.N. (1973), Acta Chem. Scand. 27, 2973-2982.