

Nd[BrO ₃] ₃ [H ₂ O] ₉	<i>hP44</i>	(186) <i>P6₃mc</i> – dc ⁵ b
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Nd(BrO₃)₃·9H₂O [1], Strukturbericht notation G2₂

Structural features: Nd(OH₂)₆(OH₂)₃ tricapped trigonal prisms in a Mg-type (h.c.p.) arrangement; :BrO₃ ψ-tetrahedra between the units.

Helmholz L. (1939) [1]

Br₃H₁₈NdO₁₈

a = 1.173, *c* = 0.676 nm, *c/a* = 0.576, *V* = 0.8055 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.365	0.065	0.0		single atom Br
(OH ₂)2	6 <i>c</i>	. <i>m</i> .	0.215	0.785	0.0		single atom Nd
(OH ₂)3	6 <i>c</i>	. <i>m</i> .	0.425	0.575	0.24		single atom Nd
(OH ₂)4	6 <i>c</i>	. <i>m</i> .	0.575	0.425	0.26		single atom Nd
Br5	6 <i>c</i>	. <i>m</i> .	0.87	0.13	0.02		single atom O
O6	6 <i>c</i>	. <i>m</i> .	0.895	0.105	0.22		single atom Br
Nd7	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.0		tricapped trigonal prism (OH ₂) ₉

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.25

Experimental: single crystal, oscillation photographs, X-rays

Remarks: Short interatomic distances: d(Br5-O6) = 0.144 nm. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Helmholz L. (1939), J. Am. Chem. Soc. 61, 1544-1550.