

NdAl<sub>2.07</sub>B<sub>4</sub>O<sub>10.6</sub>*hP*19(189) *P*-62*m* – *ih*<sup>2</sup>*fba***NdAl<sub>2.07</sub>[B<sub>4</sub>O<sub>10</sub>]O<sub>0.6</sub>** [1]

Structural features: BO<sub>4</sub> tetrahedra share vertices to form infinite layers with 6-rings, which are interconnected via AlO<sub>5</sub> square pyramids on one side and NdO<sub>6</sub> trigonal prisms on the other side, to form a 3D-framework.

Pushcharovskii D.I. et al. (1978) [1]

Al<sub>2.07</sub>B<sub>4</sub>NdO<sub>10.60</sub>*a* = 0.4588, *c* = 0.9298 nm, *c/a* = 2.027, *V* = 0.1695 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>i</i>	.. <i>m</i>	0.582	0	0.339		non-colinear B <sub>2</sub>
O2	4 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.125		tetrahedron BAl <sub>3</sub>
B3	4 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.281		tetrahedron O <sub>4</sub>
Al4	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.388	0	0	0.69	square pyramid O <sub>5</sub>
Nd5	1 <i>b</i>	-62 <i>m</i>	0	0	<sup>1</sup> / <sub>2</sub>		trigonal prism O <sub>6</sub>
O6	1 <i>a</i>	-62 <i>m</i>	0	0	0	0.6	coplanar triangle Al <sub>3</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>Experimental: single crystal, diffractometer, X-rays, *R* = 0.074

References: [1] Pushcharovskii D.I., Karpov O.G., Leoniuk N.I., Belov N.V. (1978), Dokl. Akad. Nauk SSSR 241, 91-94.