

BaNd<sub>2</sub>Al<sub>2</sub>B<sub>12</sub>O<sub>25</sub>*hP46*(189) *P-62m* – i<sup>3</sup>h<sup>5</sup>fe<sup>2</sup>a**BaNd<sub>2</sub>Al<sub>2</sub>B<sub>12</sub>O<sub>25</sub>** [1]

Structural features: Layers of vertex-linked BO<sub>4</sub> tetrahedra, layers of edge- and vertex-linked AlO<sub>5</sub> square pyramids and layers containing single NdO<sub>6</sub> trigonal prisms share atoms to form infinite slabs (cation sequence B-Nd-B-Al-B-Nd-B), which alternate with double planar layers of vertex-linked BO<sub>3</sub> trigonal units (partial vacancies ignored) along [001]; Ba between the two kinds of slab.

Li D. et al. (1988) [1]

Al<sub>2</sub>B<sub>12</sub>BaNd<sub>2</sub>O<sub>25</sub>*a* = 0.4566, *c* = 2.492 nm, *c/a* = 5.458, *V* = 0.4499 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6i	..m	0.3706	0	0.4576	0.667	non-colinear B <sub>2</sub>
O2	6i	..m	0.4039	0	0.2503		non-colinear B <sub>2</sub>
O3	6i	..m	0.42	0	0.1282		non-colinear B <sub>2</sub>
O4	4h	3..	1/3	2/3	0.0472		tetrahedron BAl <sub>3</sub>
B5	4h	3..	1/3	2/3	0.1056		tetrahedron O <sub>4</sub>
B6	4h	3..	1/3	2/3	0.2708		tetrahedron O <sub>4</sub>
O7	4h	3..	1/3	2/3	0.3282		single atom B
B8	4h	3..	1/3	2/3	0.4542		non-coplanar triangle O <sub>3</sub>
Al9	3f	<i>m2m</i>	0.6126	0	0	0.667	square pyramid O <sub>5</sub>
Nd10	2e	3.m	0	0	0.1853		trigonal prism O <sub>6</sub>
Ba11	2e	3.m	0	0	0.3622	0.5	9-vertex polyhedron O <sub>9</sub>
O12	1a	-62m	0	0	0		coplanar triangle Al <sub>3</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.088

Remarks: In the abstracts of [1] the Hermann-Mauguin symbol for the space group is misprinted as *P6-2m* (English) and *P62m* (Chinese) instead of *P-62m*.

References: [1] Li D., Tu H., Xu Y., Kong H., He C. (1988), *Wuji Huaxue* 4, 23-29.