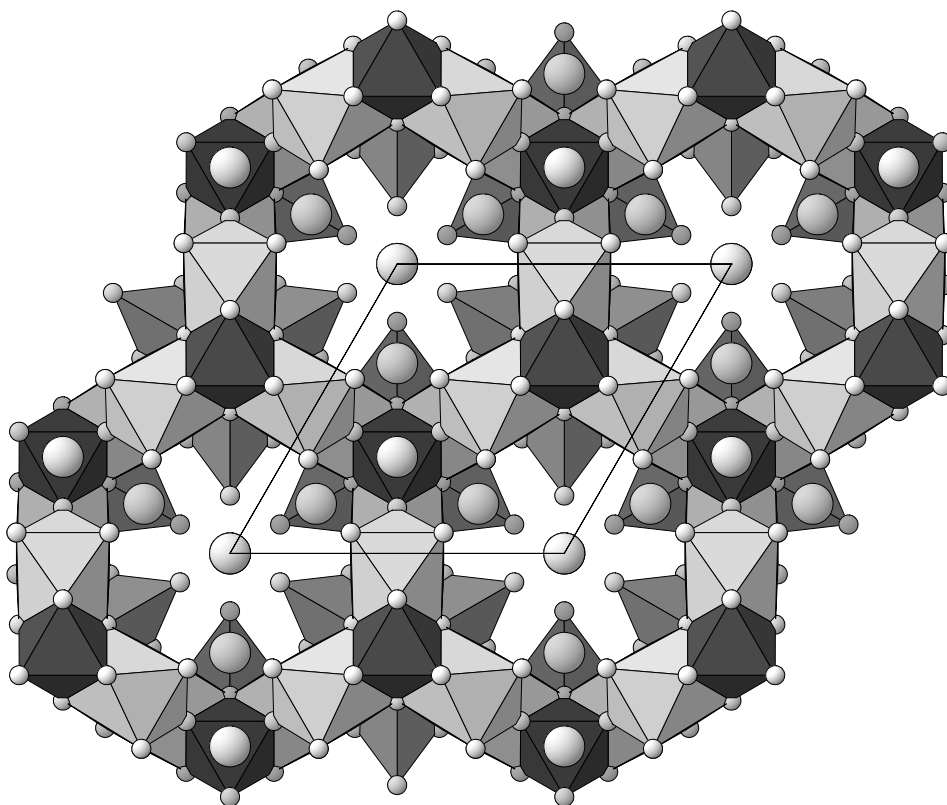


**Ba<sub>6</sub>Nd<sub>2</sub>Al<sub>4</sub>O<sub>15</sub>** [1]

Structural features: Infinite columns of base-linked (Nd,Ba)O<sub>6</sub>O<sub>2</sub> bicapped trigonal prisms ((Nd,Ba)O<sub>8</sub> square antiprisms) are interconnected via common atoms, AlO<sub>6</sub> octahedra and AlO<sub>4</sub> tetrahedra to form a 3D-framework; Ba in octahedral (infinite columns of face-sharing BaO<sub>6</sub> octahedra), cuboctahedral and 10-coordinated voids. See Fig. IV.31.

Fig. IV.31. **Ba<sub>6</sub>Nd<sub>2</sub>Al<sub>4</sub>O<sub>15</sub>**

Arrangement of (Nd,Ba)O<sub>8</sub> square antiprisms (light), AlO<sub>4</sub> tetrahedra (medium), AlO<sub>6</sub> octahedra (dark) (O atoms small) and additional Ba atoms (large) viewed along [001].

Rüter I., Müller Buschbaum H. (1989) [1]

Al<sub>4</sub>Ba<sub>6</sub>Nd<sub>2</sub>O<sub>15</sub>

$a = 1.15696$ ,  $c = 0.69662$  nm,  $c/a = 0.602$ ,  $V = 0.8075$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12d	1	0.3973	0.0722	0.047		single atom Al
Ba2	6c	.m.	0.17156	0.82844	0.18163		9-vertex polyhedron O <sub>9</sub>
O3	6c	.m.	0.4206	0.5794	0.184		single atom Al
M4	6c	.m.	0.52099	0.47901	0.35897		8-vertex polyhedron O <sub>8</sub>
O5	6c	.m.	0.7542	0.2458	0.3512		single atom Al
Al6	6c	.m.	0.819	0.181	0.1784		tetrahedron O <sub>4</sub>
O7	6c	.m.	0.9001	0.0999	0.2686		single atom Al
Al8	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0344		octahedron O <sub>6</sub>

Ba9	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.48613	non-coplanar triangle O <sub>3</sub>
Ba10	<i>2a</i>	<i>3m.</i>	0	0	0.0	octahedron O <sub>6</sub>

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M4 = 0.667Nd + 0.333Ba

Experimental: single crystal, diffractometer, X-rays, wR = 0.029

References: [1] Rüter I., Müller Buschbaum H. (1989), Monatsh. Chem. 120, 1069-1074.