

Na<sub>1.3</sub>Nd<sub>0.9</sub>Al<sub>23</sub>O<sub>36.5</sub>

hP71

(187) *P*-6*m*2 – n<sup>6</sup>k<sup>3</sup>j<sup>2</sup>i<sup>3</sup>h<sup>3</sup>g<sup>4</sup>**Na<sub>1.3</sub>Nd<sub>0.9</sub>Al<sub>23</sub>O<sub>36.5</sub>** [1]

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) alternate with NaO layers (split O site, Na near BR positions) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Nd atoms (split site), along [001]. Magnetoplumbite- and β alumina-type slabs.

Kahn A., Thery J. (1986) [1]

Al<sub>23</sub>Na<sub>1.32</sub>Nd<sub>0.90</sub>O<sub>36.20</sub>*a* = 0.557, *c* = 2.2257 nm, *c/a* = 3.996, *V* = 0.5980 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>n</i>	. <i>m</i> .	0.1557	0.8443	0.1936		tetrahedron Al <sub>4</sub>
Al2	6 <i>n</i>	. <i>m</i> .	0.1686	0.8314	0.353		octahedron O <sub>6</sub>
O3	6 <i>n</i>	. <i>m</i> .	0.4986	0.5014	0.3947		non-coplanar triangle Al <sub>3</sub>
O4	6 <i>n</i>	. <i>m</i> .	0.505	0.495	0.0971		non-coplanar triangle Al <sub>3</sub>
Al5	6 <i>n</i>	. <i>m</i> .	0.8315	0.1685	0.139		octahedron O <sub>6</sub>
O6	6 <i>n</i>	. <i>m</i> .	0.8436	0.1564	0.2957		tetrahedron Al <sub>4</sub>
Na7	3 <i>k</i>	<i>mm</i> 2	0.0506	0.9494	<sup>1</sup> / <sub>2</sub>	0.18	
Na8	3 <i>k</i>	<i>mm</i> 2	0.1931	0.8069	<sup>1</sup> / <sub>2</sub>	0.26	
O9	3 <i>k</i>	<i>mm</i> 2	0.712	0.288	<sup>1</sup> / <sub>2</sub>	0.4	
O10	3 <i>j</i>	<i>mm</i> 2	0.1803	0.8197	0		
Nd11	3 <i>j</i>	<i>mm</i> 2	0.6803	0.3197	0	0.3	
O12	2 <i>i</i>	3 <i>m</i> .	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0.1907		tetrahedron Al <sub>4</sub>
Al13	2 <i>i</i>	3 <i>m</i> .	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0.2716		tetrahedron O <sub>4</sub>
Al14	2 <i>i</i>	3 <i>m</i> .	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0.4245		
Al15	2 <i>h</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0595		octahedron O <sub>6</sub>
Al16	2 <i>h</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2203		tetrahedron O <sub>4</sub>
O17	2 <i>h</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2999		tetrahedron Al <sub>4</sub>
Al18	2 <i>g</i>	3 <i>m</i> .	0	0	0.0086	0.5	
O19	2 <i>g</i>	3 <i>m</i> .	0	0	0.0986		tetrahedron Al <sub>4</sub>
Al20	2 <i>g</i>	3 <i>m</i> .	0	0	0.2467		octahedron O <sub>6</sub>
O21	2 <i>g</i>	3 <i>m</i> .	0	0	0.3896		non-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 = 0.049, T = 297 K

Remarks: Short interatomic distances for partly occupied site(s). Space group (194) *P*6<sub>3</sub>/*mmc* was tested and rejected.

References: [1] Kahn A., Thery J. (1986), J. Solid State Chem. 64, 102-107.