

YBO <sub>3</sub>	<i>hP</i> 18	(176) <i>P</i> 6 <sub>3</sub> / <i>m</i> – h <sup>2</sup> fb
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**YBO<sub>3</sub>** [1]; Y<sub>2</sub>AlSiO<sub>5</sub>N [3]

Structural features: 3-rings of vertex-linked BO<sub>4</sub> tetrahedra arranged in layers (partial disorder) share atoms with distorted YO<sub>8</sub> cubes (split O site) to form a 3D-framework.

Chadeyron G. et al. (1997) [1]

BO<sub>3</sub>Y

*a* = 0.3776, *c* = 0.8806 nm, *c/a* = 2.332, *V* = 0.1087 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
B1	6 <i>h</i>	<i>m</i> ..	0.151	0.565	<sup>1</sup> / <sub>4</sub>	0.333	
O2	6 <i>h</i>	<i>m</i> ..	0.226	0.107	<sup>1</sup> / <sub>4</sub>	0.333	non-colinear O <sub>2</sub>
O3	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1103		
Y4	2 <i>b</i>	-3..	0	0	0		icosahedron O <sub>12</sub>

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, *R* = 0.035, *T* = 293 K

Remarks: Short interatomic distances for partly occupied site(s). Superseded a structure proposal with B in trigonal coordination in [2]. 4-fold coordination of B was confirmed by IR and NMR spectroscopy, the presence of two different environments of Y by Eu<sup>3+</sup> luminescence studies. The similar model proposed for so-called B-(AlNOSiY) in [3] was rejected in favor of an alternative model with N in Wyckoff position 2*b* (*R*<sub>B</sub> = 0.036).

References: [1] Chadeyron G., El Ghazzi M., Mahiou R., Arbus A., Cousseins J.C. (1997), J. Solid State Chem. 128, 261-266. [2] Newnham R.E., Redman M.J., Santoro R.P. (1963), J. Am. Ceram. Soc. 46, 253-256. [3] Gonon M.F., Descamps D.C., Cambier F., Thompson D.P. (2000), Mater. Sci. Forum 325/326, 325-333.