substance: boron compounds with group VI elements
property: properties of boron-oxygen compounds: B_2O

Preparation [77G], crystalline structure [77G, 65H]

The compound has been proposed to be an isoelectronic analog to carbon. By high-pressure, high-temperature synthesis graphite-like and diamond-like phases have been obtained. Synthesis from B and B_2O_3 powders compressed at 50...75 kbar and then heated to 1200...1800 °C [65H]. Preparation based on an oxidation of BP by Cr_2O_3, then compressed to 40 kbar and heated to 1000...1300 °C [85E, 87E]. According to theoretical calculations based on the density-functional total-energy method the graphite-like structure is unstable [95G].

Structure in Fig. 1 [85E, 87E, 95G].

lattice parameters
(in Å)

a	7.98	*T* = 300 K	X-ray diffraction	65H
c	9.09			
a	2.879	*T* = 300 K	X-ray diffraction	85E,
c	7.052			87E
a	2.879		theor.; density-functional total energy	95G
c	7.052		method	

atomic distances in [111] direction
(in Å)

B-B (buckle)	0.5876	calculated	cell: ideal/basis: ideal	95G
	0.3182	calculated	cell: ideal/basis: relaxed	
B-O (buckle)	0.5876	calculated	cell: ideal/basis: ideal	
	0.5260	calculated	cell: ideal/basis: relaxed	
BB-BO (spacing)	1.7630	calculated	cell: ideal/basis: ideal	
	1.9959	calculated	cell: ideal/basis: relaxed	
BO-BO (spacing)	1.7630	calculated	cell: ideal/basis: ideal	
	1.6895	calculated	cell: ideal/basis: relaxed	

theoretically determined different diamond-like 100 structure.

Structure: body-centered tetragonal

Space group: $I\bar{4}m2$

lattice parameters

a	2.845 Å	theoretical	95G
c	10.934 Å		

Electronic properties

Reddish-brown color [65H] and brown color [85E, 87E], respectively of the experimentally obtained compounds indicate semiconducting behavior.

Calculated electronic band structure for the theoretical 100 structure in Fig. 2 [95G].

density

d	2.24 g cm^{-3}	exp.	65H
	2.48 g cm^{-3}	exp.	85E, 87E

bulk modulus

Since the internal coordinates do not significantly relax from their ideal values, the bulk modulus is assumed to be similar to that of SiC, i.e. 2.1 Mbar [95G].

References:

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77G Gal'chenko, G. L., Lavut, E. G., Lavut, E. A., Vidavsky, L. M.: see [77B], p. 331.

85E Endo, T.: Japan Kokai Tokkyo Koho, Patent No. 60-21912 (1985).

87E Endo, T., Sato, T., Shimada, M.: J. Mater. Sci. Lett. 6 (1987) 683.

95G Grumbach, M.P., Sankey, O.F., McMillan, P.F.: Phys. Rev . B 52 (1995) 15807.

Fig. 1.

B_2O.Crystal structure [85E, 87E, 95G].

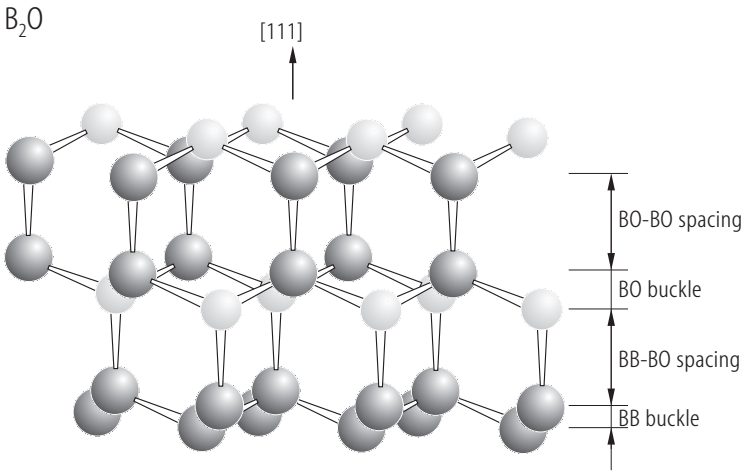

Fig. 2.

B_2O. Calculated electronic band structure of the theoretically obtained 100 structure [95G].