substance: boron compounds with group V elements
property: properties of boron-nitrogen compounds

X-ray spectroscopic analysis of boron-nitride clusters deposited by ion-lating method [96K].

The structure and stability of B_n^+ clusters [96R].

B_6N

α-rhombohedral boron structure group

For synthesis at high pressures (5...7.5 GPa) see [97H, 97G].

lattice parameters
(in Å)

a	5.70			76C,
c	12.0			93S,
c/*a*	2.1			96L
a	5.682(15)	*T* = 300 K	refined data from [93S]	97H
c	12.117(58)			
c/*a*	2.132			
a	5.457(7)	*T* = 300 K	$B_6N_{0.92}$	97H
c	12.241(15)			
c/*a*	2.243			

For parallel electron-energy-loss spectrum (PEELS), see Fig. 1 [97G].

B and N K edges of B_6N (compared with the B and O K edges of B_6O) in Fig. 2 [97G].

$B_6N_{0.52}O_{0.51}$

For parallel electron-energy-loss spectrum (PEELS), see Fig. 1 [97G].

$B_{36}N_{24}$

Structure in Fig. 3 [94K].

interatomic distances in the cluster
(in Å)

d	1.972	B(1) – B(1)	determined by	94K
	2.016	B(2) – B(2)	molecular mechanics	
	1.670	B(1) – N		
	1.695	B(2) – N		

Calculated density of states in Fig. 4 [94K].

Comparison of the electronic structure with that of C_{60} in [94K].

energy gap

E_g	1.9 eV	calculated	94K

$B_{50}N_2$

Semiconductor (?); preparation [72P], crystalline structure [76W]

Structure: tetragonal

Space group: $P\bar{4}2m$

lattice parameters
(in Å)

a	8.615	*T* = 300 K	X-ray diffraction	86W
	8.562		calculated	92M
c	5.117	*T* = 300 K	X-ray diffraction	86W
	5.158		calculated	92M

References:

72P Ploog, K., Schmidt, H., Amberger, E., Will, G., Kossobutzki, K. H.: J. Less-Common Met. 29 (1972) 161.

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76W Will, G., Kossobutzki, K. H.: J. Less-Common Met. 47 (1976) 33.

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92M Morrison, I., Bylander, D.M., Kleinman, L.: Phys. Rev. B 45 (1992) 10872.

93S Saitoh, H., Mercurio, Yoshida, K., Yarbrough, W.A., : J. Mater. Res. 8 (1993) 8.

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96L Lundström, T., Andreev, Yu.G.: Mater. Sci. Eng. A209 (1996) 16.

96R Ricca, A., Bauschlicher Jr., C.W.: Chem. Phys. 208 (1996) 233.

97G Garvie, L.A.J., Buseck, P.R., Rez, P.: J. Solid State Chem. 133 (1997) 347 (Proc. 12th Int. Symp. Boron, Borides and Rel. Compounds, Baden, Austria, 1996).

97H Hubert, H., Garvie, L.A.J., Petuskey, W.T., McMillan, P.F.: J. Solid State Chem. 133 (1997) 356 (Proc. 12th Int. Symp. Boron, Borides and Rel. Compounds, Baden, Austria, 1996).

Fig. 1.

Boron carbide:O. Parallel electron energy-loss spectra (PEELS) of O-doped boron carbide compared with some other isostructural compounds ($B_6N_{0.92}$, $B_6O_{0.96}$, $B_6N_{0.52}O_{0.51}$, $B_6C_{0.91}(N,O)_{0.27}$ (background subtracted) [97G].

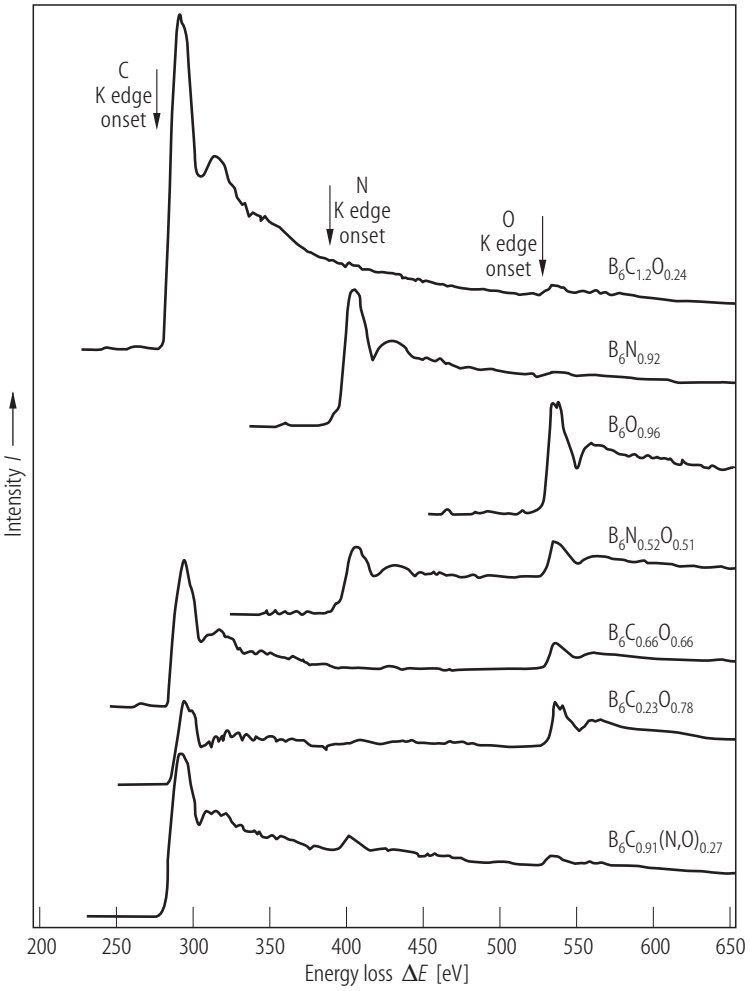

Fig. 2.

B_6N, B_6O. B and O K edges of B_6O compared with B and N K edges of B_6N aligned on a relative energy scale. The estimated onset of the conduction band is at 0 eV [97G].

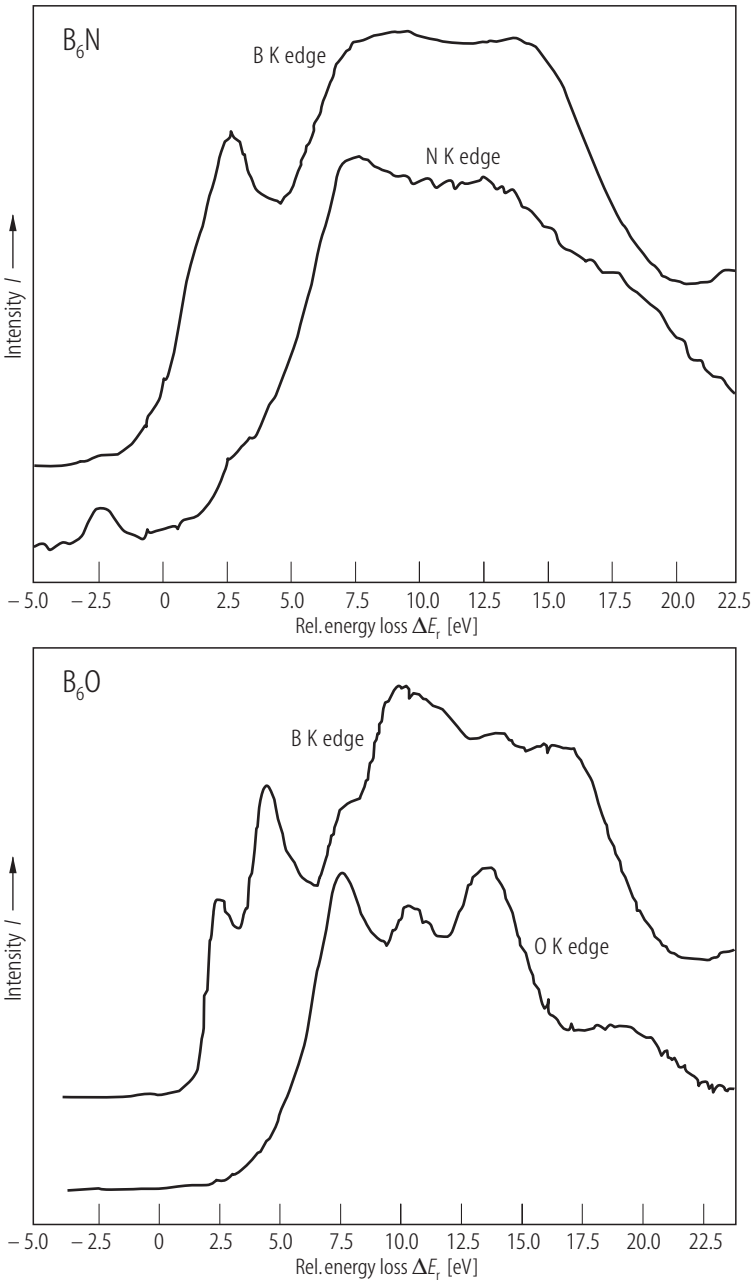

Fig. 3.

$B_{36}N_{24}$. Molecular structure [94K].

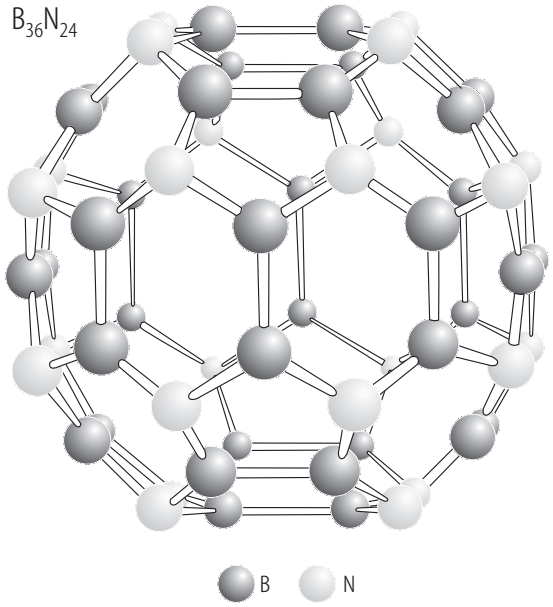

Fig. 4.

$B_{36}N_{24}$. Calculated total electron density of states (full line) and **(a)** N 2p partial and local density of states (dashed line) and **(b)** type 1 (dashed line) and type 2 (broken line) B 2p partial and local electron density of states [94K].