substance: boron compounds with group I elements
property: properties of boron-sodium compounds

NaB_6

Structure

There is some controversy, whether NaB_6 cristallizes in the CaB_6 structure or not. [63H, 74R, 75S, 77N].

Preparation and structure (cubic CaB_6 structure) [63H, 76N].

lattice parameters

a	4.16 Å	*T* = 300 K	X-ray diffraction	54B, 77N

Physical properties

Based on the CaB_6 structure the calculated band structure is basically similar in topology to that of CaB_6. But because of the lower number of electrons introduced by the monovalent metal the position of the Fermi level is expected at – 9.1 eV, i.e. within the valence band [76P1]. This contrasts with the high electrical resistance (see below) which indicates semiconducting behavior.

band structure: Fig. 1

***g*-factor**

g	2.0073(4)	*T* = 295 K	linewidth, *B* = 76 G	74R
Δg	$5(4)\cdot10^{-3}$	*T* = 295 K to 1.4 K	positive temperature independent *g*-shift $\Delta g = g - 2.0023$	

resistivity

ρ	10^6 Ω cm	*T* = 300 K	sintered sample	77N

stability limit

T	650°C		high vacuum	77N

density

d	2.12 g cm^{-3}	*T* = 300 K	pycnometric	63H, 67N

Na_3B_{20}

Recent results suggest that the compound NaB_6 should be described as Na_3B_{20}, which does not crystallize in the hexaboride structure [98A2, 98A1].

Structure: orthorhombic

Space group: Cmmm

Structure in Fig. 2 [98A2].

lattice parameters
(in Å)

a	1.86945(6)	*T* = 300 K	X-ray diffraction	98A2
b	0.57009(2)			
c	0.41506(1)			
B-B distance	1.76	*T* = 300 K	intra-polyhedral	98A2
B-B' distance	1.80		intra-polyhedral	
B-B distance	1.71		inter-polyhedral	

density

d	2.142 g cm^{-3}	*T* = 300 K	calculated	98A2

NaB_5C

Cubic CaB_6 structure

NaB_5C as an electron-precise compound is described in [98A3].

lattice parameters

a	4.09 Å	*T* = 300 K	X-ray diffraction	98A3
B/C-B/C dist.	1.706 Å			

density

d	2.11 g cm^{-3}			98A3

NaB_{15}

Structure

The elementary cell contains four formula groups. The structure can be described as a stacking of rather compact planes of quasi-spherical icosahedral clusters of boron atoms with a packing diameter of about 5.1 Å (see Fig. 3a). Otherwise it can be described as an alignment of icosahedron chains parallel to the *c*-axis, which are centered at (x = 0; y = 0) and (x = 1/2; y = 1/2) (see Fig. 3b). Two types of isolated boron atoms are present in the structure. The covalent skeleton formed by the boron atoms has two types of interstitial sites, one of them formed by 16, the other one by 12 boron atoms. The sodium atoms obtain these interstitial sites and can be assumed as at least partially ionized and to act as electron donors [70N, 76N, 77N].

lattice: orthorhombic; space group: D_{2h}^{28} – Imam.

lattice parameters

a	5.847 Å	70N,
b	8.415 Å	76N,
c	10.248 Å	77N,
		77M,
		77N

Physical properties

energy gap

E_g	0.32 eV	*T* > 300 K	electrical conductivity (see Fig. 4)	77N

Density of states calculation in Fig. 5 [86B].

impurity and defects

Because of the high volatility of sodium, deviations from stoichiometry are possible which lead to Na_xB_{15} phases ($0 \le x < 1$). Limit phase at 850ºC: $Na_{0.3}B_{15}$. Above 950ºC the last traces of sodium can be removed [76N, 77N].

conductivity

σ	$4 \cdot 10^{-4}\ \Omega^{-1}$ cm^{-1}	*T*= 300 K	polycrystalline sample, sintered at 650ºC, pressure 50 kbar; see Fig. 4	77N

densities

d	2.428 g cm^{-3}	calculated	77N
	2.44(2) g cm^{-3}	$NaB_{0.84}B_{14}$, experimental	76N
	2.398 g cm^{-3}	$NaB_{0.84}B_{14}$, calculated	

$NaB_{0.8}B_{14}$

Structure of NaB_{15} (structure type $MgAlB_{14}$)

lattice parameters
(in Å)

a	5.85	*T* = 300 K	X-ray diffraction	93W,
b	8.41			70N
c	10.27			

Comparison of the interatomic distances in $NaB_{0.8}B_{14}$ with $LiAlB_{14}$, $MgAlB_{14}$ and Mg_2B_{14} in [81H].

$NaPt_3B_{1+x}$

Preparation and structure [87M].

$Na_3Pt_9B_5$

Preparation and structure [87M].

$Na_xBa_{1-x}B_6$

semiconductor (?); preparation [77N, 52B]; crystalline structure CaB_6-type [77N, 54B]

$Na_xTh_{1-x}B_6$

semiconductor (?); preparation [77N, 52B]; crystalline structure CaB_6-type [77N, 54B]

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Fig. 1.

NaB_6. Calculated hand structure [76P2].

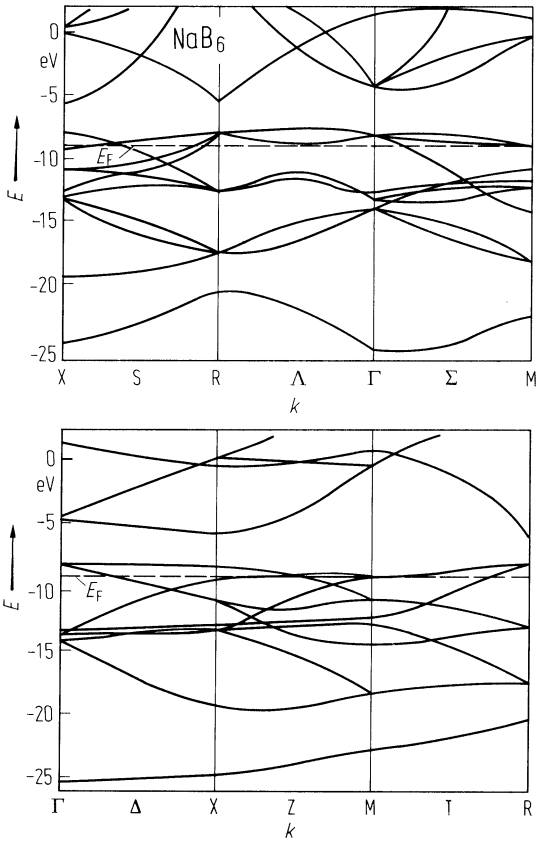

Fig. 2.

Na_3B_{20}. Crystal structure. **(a)** Projection on the *ab*-plane, unit cell marked; **(b)** section of the structure in the [001] direction. All the boron atoms are shown, whose distance from the Na atom is smaller than 0.340 Å [98A2].

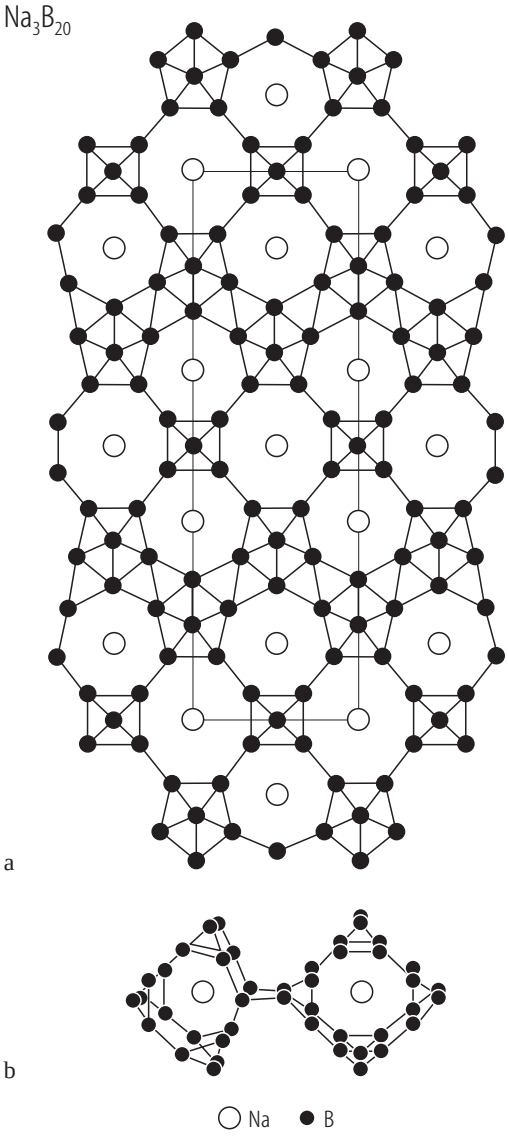

Fig. 3.

NaB_{15}. Projection of the crystal structure (a) on the *yz* plane, (b) on the *xy* plane (only atoms with $1/4 \leq x \leq 1/4$ are represented) [76N, 77N]. The numbers denote crystallographically different atomic positions in the lattice.

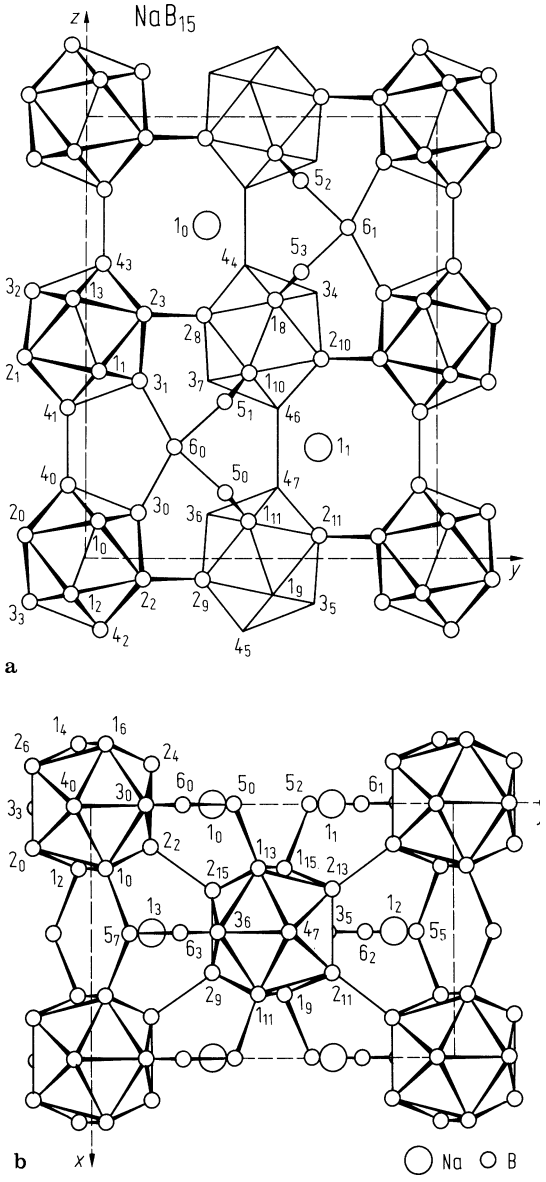

Fig. 4.

NaB_{15}. Electrical conductivity vs. reciprocal temperature for polycrystalline sample [77N].

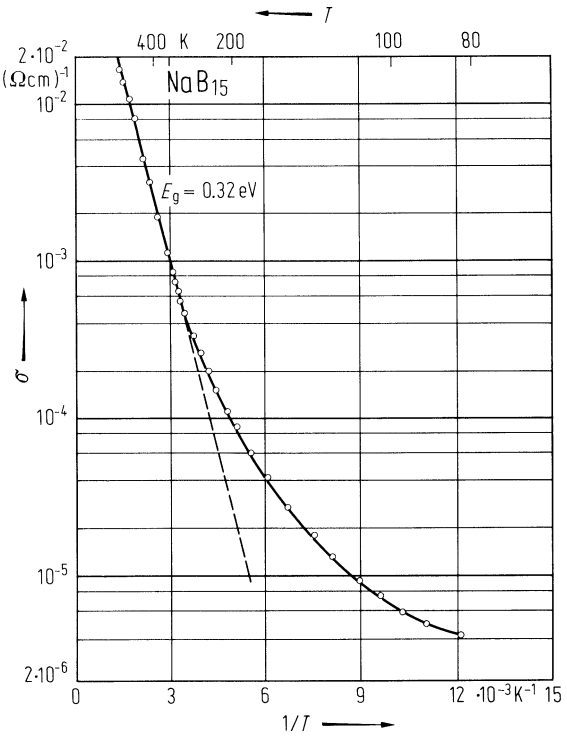

Fig. 5.

NaB_{15}. Calculated density of states [86B].