substance: boron compounds with group IV elements: boron carbide
property: lattice properties

Lattice vibrations and the bonding nature of boron carbide [96S1].

elastic moduli

boron carbides [91G1]

Sample	Young's modulus	Shear modulus	Poisson's ratio	Bulk modulus	Compressibility
[at.% C]	E [GPa]	G [GPa]	ν	B_0 [GPa]	κ [10^{-6} m^2/N]
20.0	472	200	0.18	247	4.05
18.2	463	197	0.17	237	4.22
15.4	462	197	0.17	236	4.24
13.3	446	189	0.18	231	4.33
11.5	352	150	0.17	178	5.62
10.0 (#1)	319	132	0.21	183	5.46
10.0 (#2)	348	150	0.16	170	5.87

hot-pressed and sintered boron carbide with free carbon [81S]

(the amount of free carbon can approximately be calculated by $C_{free} = 1.28\ C_{total} - 28$ [wt%]).

C_{total}	Bulk dens.	Young's modulus	Shear. modulus	Poisson's ratio	Flex. strenth	Fracture. toughness
[wt.% C]	d [g cm^{-3}]	E [GPa]	G [GPa]	ν	[MN m^{-2}]	[MPa m$^{1/2}$]
21.7	2.51	441	188	0.17	480(40)	3.6(3)
22.5	2.44	390	166	0.17	351(40)	3.3(2)
24.8	2.46	372	158	0.17	353(40)	3.2(2)

Young's modulus
(in GPa)

E	441	T = 300 K		85S
	450	T = 300 K	static	86G
	450	T = 300 K		91L
	434·	T = 300 K		71G
	480	T = 300 K	depends on density	82S
	448	T = 300 K		77M

Dependence of the Young's modulus on the C content in Fig. 1 [91G1, 91G3].

shear modulus

G	188 GPa			85S
	182	T = 300 K		71G
	200	T = 300 K	depends on density	82S
	186	T = 300 K		77M

Dynamic shear modulus in [91A2] (see internal friction Fig. 2).

Poisson´s ratio

ν	0.17			85S, 91L
	0.21	T = 300K		77M

bulk modulus

B_0	234		theoretical	92L, 93L
	245	T = 300 K	exp.	90T, 97L

Dependence of the compressibility on the C content in Fig. 3 [91G1].

The elastic modulus and fracture of boron carbide in [80H].

Effect of grinding conditions on the structure and physicomechanical properties of hot-pressed boron carbide [88K].

transverse sound velocity

v_t	$7.86 \cdot 10^5$ cm s^{-1}	T < 10 K	B_9C determined from resonance frequency of internal friction	97M

longitudinal sound velocity

v_l	13780 m s^{-1}	T = 300 K	71G 74M
	13800 m s^{-1}	T = 300 K	82S

shear sound velocity

v_s	8540 m s^{-1}	T = 300 K	71G
	8900 m s^{-1}	T = 300 K	82S

bulk velocity

v_b	9630 m s^{-1}	T = 300 K	71G

ultrasonic wave propagation velocity

v	$13.3 \cdot 10^5$ cm s^{-1}	T = 300 K	86G

Speed of sound variation depending on temperature in crystalline B_4C, $B_{13}C_2$, B_9C compared with amorphous B_9C and β-rhombohedral boron in Fig. 4 [98M].

Dependence of longitudinal sound velocity on the C content in Fig. 5 [91G1].

Dependence of the shear velocity on the C content in Fig. 6 [91G1].

lattice vibrations

Theoretical work on the lattice vibrations and the bonding nature of boron carbide in [96S2].

Calculation of the lattice vibrations with the valence force model in [97S]. Movement of the atoms for some specific vibrations in Fig. 7 [97S].

Discussion of the Badger rule on the relation between force constant and inter-atomic distance in molecules [34B, 35B], which holds according to [50W, 60P] for solids as well, for bonding in boron carbide in [91W].

IR-active optical phonon wavenumbers of boron carbide and their medium oscillator-strengths (uncertain values in brackets) [79B]

The complex dielectric constant can be described by

$$\varepsilon(\nu) = \varepsilon(\infty) + \sum_j \Delta\varepsilon_j/(1-(\nu/\nu_{j0})^2-i(\gamma/\nu_{j0})(\nu/\nu_{j0}))$$

$\varepsilon(\infty)$: optical dielectric constant (contribution of bound electrons)
$\Delta\varepsilon_j$: oscillator strength (contribution of the j-th oscillator)
ν: frequency (ν/c = wavenumbers (in cm^{-1}))
ν_j: resonance frequency of the sustained oscillators
γ: frequency independent damping constant

(ν/c)	$\Delta\varepsilon$	$\Delta\varepsilon$		Prevailing
	Polycryst.	Single crystals		symmetry type
cm^{-1}	material	$E \parallel c$	$E \perp c$	
1580	0.15	0.45	0.12	A_{2u}
1090	0.35	0.25	0.5	E_u
(980)				
870	0.02	0.08	0.06	
873	0.01	0.04	0.02	
845	0.02	0.03	0.01	A_{2u}
700	0.07	0.05	0.04	
(660)				
582	0.06		0.20	E_u
(530)				
475				
390	0.6	0.35	0.60	E_u

For the dependence of (ν/c) and $\Delta\varepsilon$ on the C content of boron carbide, see Fig. 8.

numbers of IR and Raman active phonon modes for the different discussed structure models of boron carbide determined by group theory

$B_{12}X_3$ (chain)

A_{2u}	5	91W
E_u	7	
A_{1g}	5	
E_g	6	

$B_{12}X_4$ (B_4 plane, assumed by Yakel to replace X_3 in one quarter of the unit cells [75Y, 73Y, 86Y] (see Fig. 9), but this was not confirmed by other authors

A_{2u}	4	91W
E_u	7	
A_{1g}	4	
E_g	7	

parameters of the phonon dispersion oscillators of boron carbide

Example: $B_{4.3}C$ at 160 K [94K1]. Error margins: for oscillator strength $\Delta\varepsilon$ is 0.005, for damping constant γ is 1.6 cm^{-1}. Uncertain data in parentheses

ν/c [cm^{-1}]	$\Delta\varepsilon$	γ [cm^{-1}]	Symmetry type	
72.5				94K1
(130)				
(335)				
(362)				
(381)				
411.8	0.520	32.8	(E_u + A_{2u})	
605.6	0.016	(24.1)	E_u	
707.6	0.060	13.5	E_u	
767.4	(0.006)	(11.6)	(E_u)	
846.5	0.024	7.7	E_u	
873.5	0.025	15.4	A_{2u}	
954.5	0.023	(9)	A_{2u}	
(978)			(A_{2u})	
1006.5	(0.006)	(15.4)	(A_{2u})	
1097.2	0.290	46.3	E_u	
≈1580	0.155		A_{2u}	

For IR and Raman spectra, see optical properties

isotopic shift of the IR phonon frequencies

$\nu(^{10}B)/\nu(^{11}B)$	1.0444	T = 300 K	experimental	91W
	1.041		calculated $[m(^{10}B)/m(^{11}B)]^{-1/2}$	

resonance frequencies (ν/c in cm^{-1}), relative oscillator strengths (integrated area of the peaks) and half-widths of IR-active phonons in isotope enriched boron carbidesat 300 K

Uncertain values in parentheses. Examples of spectra ($B_{4.3}C$) in Fig. 10 [99W].

	$^{10}B_{4.3}C$			**$^{11}B_{4.3}C$**			**$^{10}B_{4.3}{}^{13}C$**		
No.	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$
1	---	---	---	---	---	---	---	---	---
2	421	48, 3	36, 2	399	36, 4	33, 8	423	34, 2	37, 6
3	510	0, 4	13, 5	487	0, 8	22, 9	(515)	---	---
4	625	1, 3	22, 4	601	1, 0	21, 5	624	1, 5	24, 6
5	668	---	---	668	---	---	668	---	---
6	727	6, 5	12, 4	702	3, 2	12, 6	719	5, 9	12, 7
7	(789)	---	---	---	---	---	(778)	---	---
8	866	3, 9	8, 2	841	1, 9	8, 2	858	3, 3	10, 8
9	900	1, 5	18, 3	863	1, 1	13, 0	898	1, 1	21, 9
10	992	0, 7	11, 1	946	0, 9	7, 1	992	1, 4	19, 5
11	(1023)	0, 3	---	(998)	0, 1	15, 2	(1018)	---	---
12	1120	58, 1	45, 7	1081	44, 6	49, 4	1111	46, 3	45, 1
13	---	---	---	1252	1, 1	37, 5	---	---	---
14	---	---	---	---	---	---	---	---	---
15	1624	32, 7	71, 5	1568	24, 3	67, 8	1609	27, 0	67, 9
16	---	---	---	1722	0, 9	21, 5	---	---	---
	$^{10}B_{6.5}C$			**$^{11}B_{6.5}C$**			**$^{10}B_{6.5}{}^{13}C$**		
No.	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$
1	(386)	---	---	(366)	---	---	(387)	---	---
2	427	34, 4	57, 1	407	31, 3	49, 3	429	36, 7	59, 9
3	537	1, 0	34, 2	(508)	---	---	(534)	---	---
4	626	2, 5	23, 5	600	1, 9	21, 6	625	2, 8	25, 3
5	668	---	---	668	---	---	668	---	---

6	715	5, 6	12, 8	692	3, 5	15, 0	711	5, 7	12, 4
7	(774)	---	---	(739)	---	---	772	---	---
8	859	2, 5	14, 1	834	2, 4	17, 7	854	2, 5	15, 6
9	(890)	---	---	(853)	---	---	(885)	---	---
10	(962)	---	---	(923)	---	---	(960)	---	---
11	(995)	0, 8	17, 7	(947)	0, 9	25	(993)	0, 6	15, 6
12	1105	47, 5	45, 1	1074	40, 8	46, 6	1099	46, 5	49, 8
13	---	---	---	---	---	---	---	---	---
14	1458	4, 5	62, 4	1411	2, 6	62, 8	1440	4, 0	63, 9
15	1604	22, 7	55, 5	1558	19, 0	60, 7	1594	23, 8	61, 5
16	(1752)	---	---	1717	0, 2	---	---	---	---
	$^{10}B_{10}C$			**$^{11}B_{10}C$**			**$^{10}B_{10}{}^{13}C$**		
No.	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$	ν/c	A	$B_{1/2}$
1	(390)	---	---	(372)	---	---	(388)	---	---
2	431	35, 5	81, 5	410	26, 5	72, 6	432	31, 3	59, 2
3	(524)	---	---	514	1, 0	27, 7	(528)	---	---
4	624	2, 4	26, 8	600	2, 2	25, 0	620	2, 4	26, 9
5	668	---	---	668	---	---	668	---	---
6	710	4, 9	13, 8	684	3, 8	14, 4	706	4, 1	12, 3
7	(772)	---	---	(736)	---	---	(773)	---	---
8	856	2, 3	20, 8	829	3, 7	26, 4	850	3, 2	31, 6
9	(887)	---	---	(848)	---	---	(883)	---	---
10	955	---	---	914	---	---	950	---	---
11	996	0, 5	14, 0	(949)	0, 5	21, 8	990	0, 3	12, 5
12	1102	49, 0	49, 6	1065	43, 3	48, 5	1091	39, 6	53, 7
13	---	---	---	---	---	---	---	---	---
14	1448	5, 3	54, 0	1406	4, 4	55, 4	1436	3, 3	56, 5
15	1597	32, 0	51, 9	1550	19, 2	51, 6	1584	20.2	53, 3
16	---	---	---	---	---	---	---	---	---

Relative shift of the resonance frequencies of characteristic IR-active phonons close to the carbon-rich limit of the homogeneity range [86W, 87W].

Frequency shift of some phonons in boron carbide depending on the carbon content: IR active phonons in Fig. 11, Raman active phonons in Fig. 12 [94K1].

Vibrational analysis of meta-carboranes ($C_2B_{10}H_{12}$) in relation to carbon containing icosahedra in boron carbide in [86B].

Raman spectroscopy of boron carbides and related boron-containing materials [86S].

resonance wavenumbers of Raman active phonons

(ν/c in cm^{-1}, uncertain attributions in parantheses)

$^{nat}B_{4.3}C$	$^{10}B_{4.3}C$	Symmetry type	$B_{6.3}C$	$B_{7.91}C$	$B_{8.52}C$	$B_{10.37}C$	
270	275	A_{1g}	271(5)	270	265	(255)	94K1
320	326	A_{1g}	349(5)	326	333(5)	(316)	
420	430	A_{1g}	417	404	409		
449	-	E_g					
477	489	E_g					
532	551	E_g	(525)	537	521		
560	599	(E_g)					
591(5)	637	(E_g)		612(16)			
652	671	E_g					
725	748	E_g	718(5)	724	713		
797	821	A_{1g}	790(5)	799			
869	895	A_{1g}	859(5)	860	844		
928	958	A_{1g}	921	927	029		
990(5)	1009	A_{1g}					
1065	1108	A_{1g}	1059(8)	1075	1073	1041(16)	
1590(5)	1598(5)		(1590)	1581(20)	1585(20)	1585(20)	

(~1590 probably due to C-B-B or free C)

isotopic shifts of Raman frequencies

(in cm^{-1})

$\Delta\nu/c$	12	T = 300 K	$^{10}B/^{11}B$; 481 cm^{-1} band	91T1
	23		$^{10}B/^{11}B$; 534 cm^{-1} band	
	7		$^{12}C/^{13}C$; 481 cm^{-1} band	
	1		$^{12}C/^{13}C$; 534 cm^{-1} band	

force field constants

(in mdyn/Å)

k_{BC}	1.8(?)	intra-icosahedral, calculated	91B
$k_{\text{chain– chain}}$	5.4		
k_{CB} (chain)	5.38		91A1

calculated phonon modes

(in cm^{-1})

ν/c	446	A_{1g}	91A1
	504		
	1560	(A_{2u}) analogous to ν_3 vibration of XY_2 molecule	

On anisotropy and effective charges in the vibration spectra of rhombohedral boron-rich solids (boron carbide included) see [94S]. According to this paper the number of polar vibrations is larger than predicted by group theory.

intraicosahedral force constant between boron atoms
(in mdyn/Å)

k_{BB}	0.4	T = 300 K	experimental	94K1
	0.7		calculated	91B, 94K2, 91A1
	1.1		calculated	96S2

force constant between the equatorial B(1) atom of the icosahedron and the end atom of the chain
(in mdyn/ Å)

k	2.2	T = 300 K	experimental	94K1
	2.3		calculated	91B, 91A1
	2.3		calculated	96S2

intericosahedral force constant between boron atoms
(in mdyn/Å)

k	2.4	T = 300 K	experimental	94K1
	2.4		calculated	91B, 91A1
	2.4		calculated	96S2

Dependence of the resonance frequency of the Raman active inter-icosahedral two-center B-B bond of the polar atoms in the icosahedra of boron carbide in Fig. 13 (experimental) [94K1, 94K2], theory [91B].

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Fig. 1.

Boron carbide. Young's modulus vs. carbon content; open circles: [91G1], full circles: [91G3].

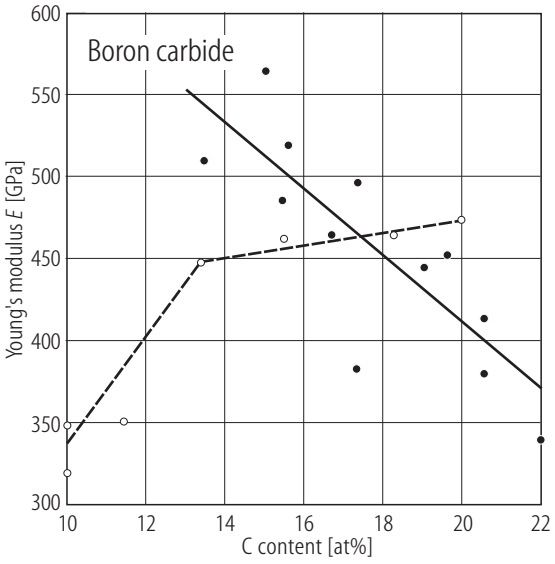

Fig. 2.

Boron carbide. (arc melted; composition not specified, probably approximately $B_{4.3}C$). High-temperature internal friction (*1*, *2*) and shear modulus (*1'*, *2'*). *(1)* initial arc melted specimen; *(2)* specimen after 1h annealing at 950 K in hydrogen atmosphere [91A2].

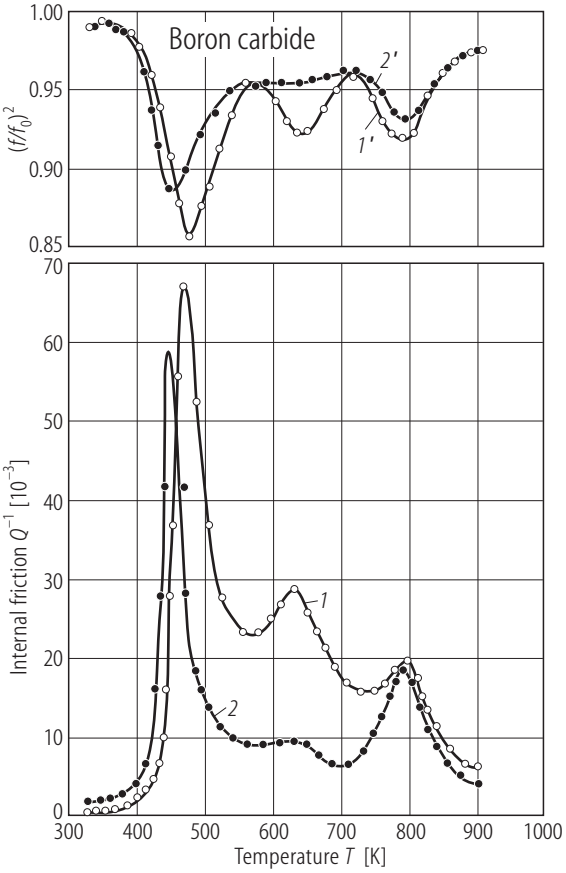

Fig. 3.

Boron carbide. Compressibility vs. carbon content [91G1].

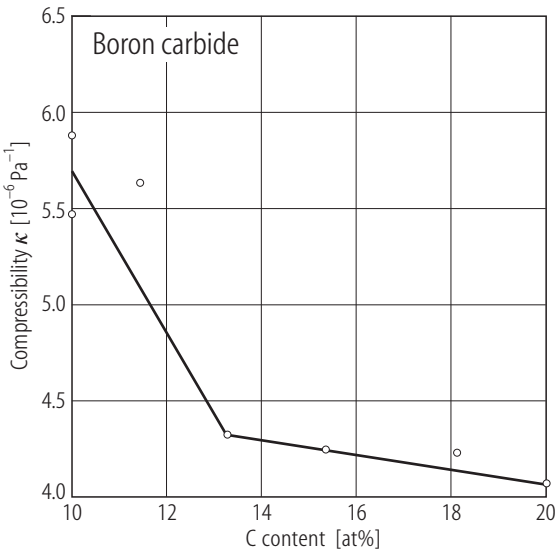

Fig. 4.

Boron carbide. Speed of sound variation vs. temperature. Full triangles, cryst. B_4C, open squares, cryst $B_{13}C_2$, full circles, cryst B_9C compared with (open circles) amorphous B_9C and (open triangles) β-rhombohedral boron; (———) tunneling model fit [98M].

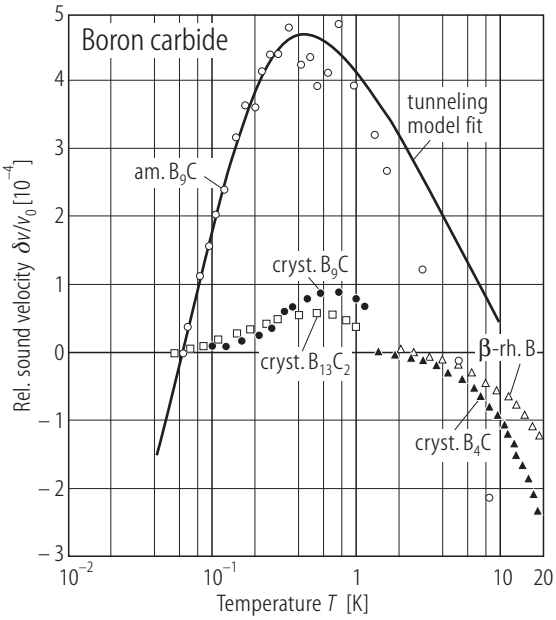

Fig. 5.

Boron carbide. Longitudinal sound velocity vs. carbon content [91G1]. Different symbols correspond to different sample directions (open circles 1, triangles down 2, triangles up 3).

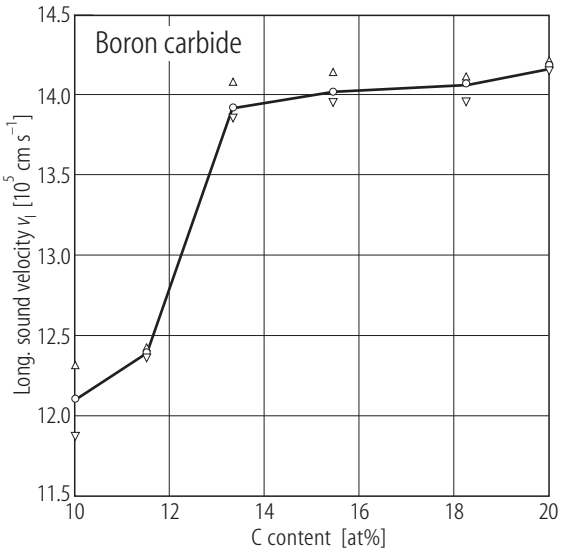

Fig. 6.

Boron carbide. Shear velocity vs. carbon content [91G1]. Sample direction 3 (cp. Fig. 5).

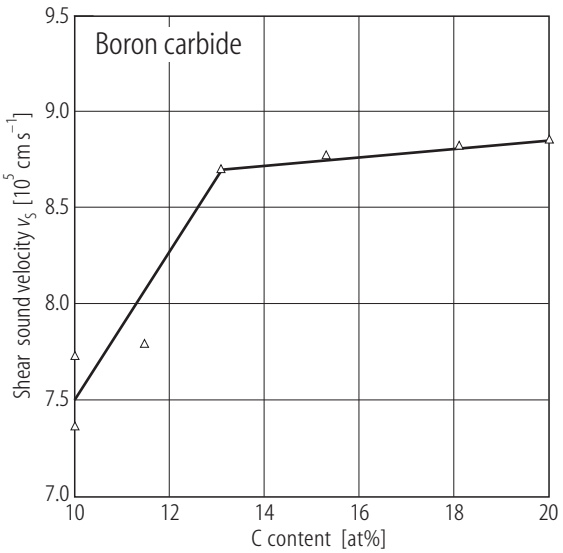

Fig. 7.

Boron carbide. Movement of the atoms for some specific vibrations [97S]. Numerical values calculated for the hypothetical idealized composition $B_{13}C_2$.

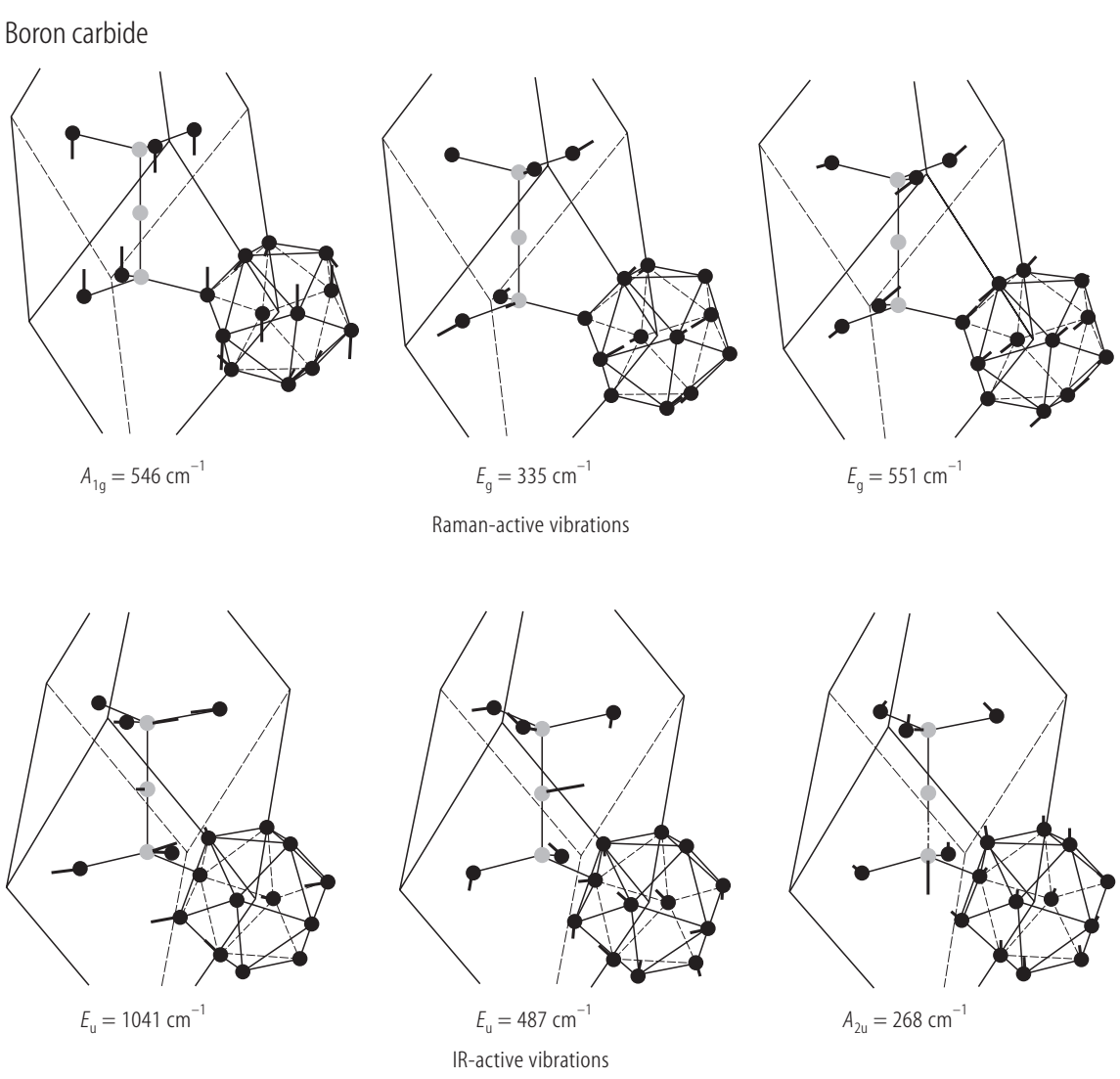

Fig. 8.

Boron carbide. a) Relative shift of the resonance wavenumber of IR-active phonons at RT (1080 cm^{-1} phonon: split icosahedral mode; 1580 cm^{-1} phonon: vibration of the C–B–C chain) vs. carbon content [82W] (cp. also [81B1, 81B2]). b) Oscillor strength of the phonons vs. carbon content [82W].

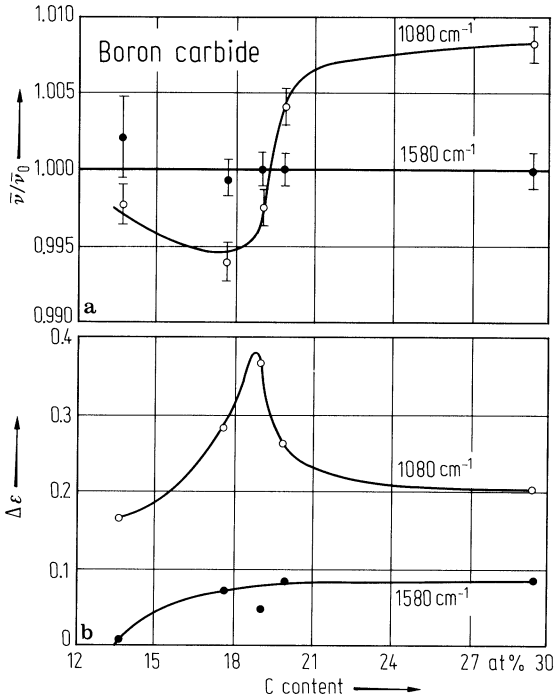

Fig. 9.

Boron carbide. a) C–B–C chain in the unit cell and the equatorial icosahedral B atoms to which it bonds. b) Planar B_4 group and the icosahedral atoms to which it bonds in one of six possible locations for the pair of B(6) atoms. c) Icosahedron with the atom positions to which the C–B–C chain (Fig. a) or the planar B_4 group (Fig. b) bonds [75Y].

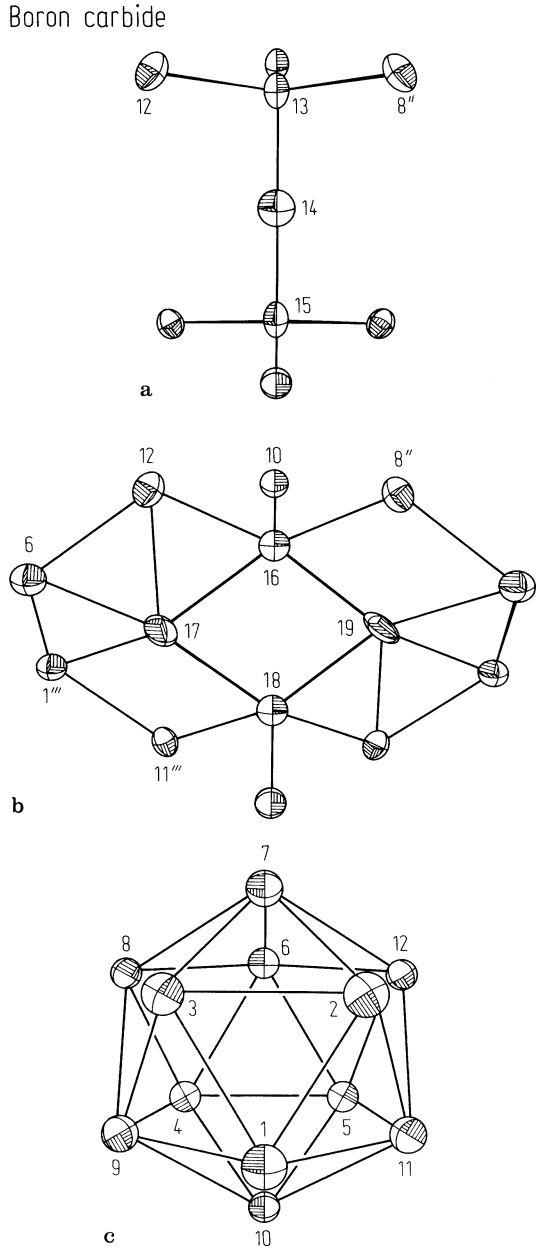

Fig. 10.

Boron carbide ($B_{\sim 4.3}C$). Spectra of the IR-active phonons of isotope-enriched boron carbide: $^{10}B_{4.3}C$, $^{11}B_{4.3}C$, $^{10}B_{4.3}{}^{13}C$; enrichment: 98.4 at.% ^{10}B, 99.4(2) at.% ^{11}B and 80.1(2) at.% ^{13}C, respectively. Impurities are Fe (0.6 mass %) and Mg, Si, Al, Ca, Cu (in total 1.3 wt.%). **(a)** Reflectivity; **(b)** absorption index [99W]. For the corresponding spectra of $B_{6.5}C$ and $B_{10}C$ see ref.

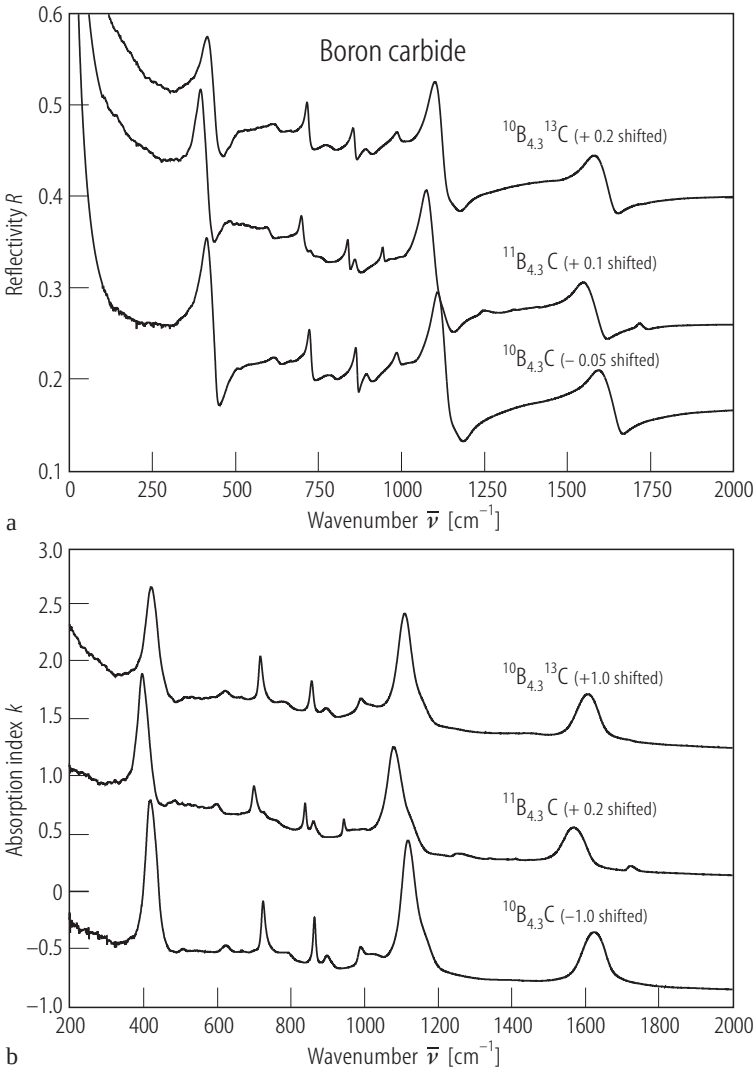

Fig. 11.

Boron carbide. Shift of the resonance frequencies of the prominent IR active phonons vs. C content [94K1].

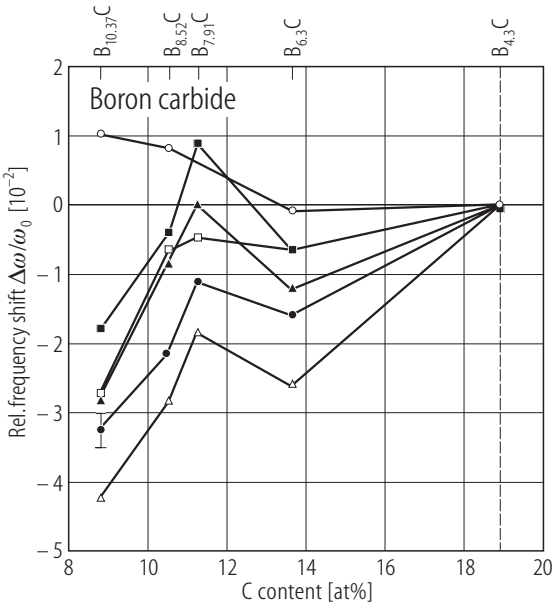

Fig. 12.

Boron carbide. Shift of the resonance frequencies of the prominent Raman active phonons vs. C content [94K1].

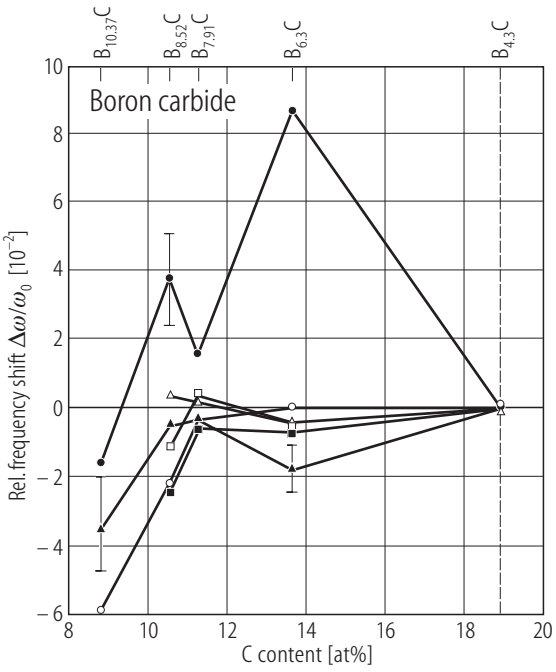

Fig. 13.

Boron carbide. Resonance frequency of the Raman active inter-icosahedral two-center B-B bond of the polar atoms in the icosahedra of boron carbide vs. C content. (Open circles) experimental [94K14, 94K16]; (full circles) calculated [91B].