substance: boron compounds with lanthanides
property: properties of lanthanide hexaborides: NdB_6

Structure, chemical bond

lattice parameter

a	4.1258 Å	*T* = 300 K	obtained from diagram (neutron powder diffraction)	94M
	4.1269(1) Å		single crystal X-ray diffraction	95B

Temperature dependences of the lattice parameter and of the equivalent temperature factors of Nd and B in $Nd^{11}B$ in Fig. 1 [94M, 94T].

interatomic distances
(in Å)

d	1.7574(12)	B – B	95B
	1.6415(17)	B – B'	
	3.0314(3)	B – Me	

Force constants [90Y]

Preparation in [85G, 91T, 93T].

Electronic properties

Metallic [84A].

Lattice properties

For vibrational frequencies [88T, 90Y, 93Y]

Thermal vibrations and static displacement of atoms in neodymium and samarium hexaboride crystals [94T].

Thermal expansion coefficient: $\alpha\,[10^{-6}K^{-1}] = 4.1232\,(1+6.37\cdot10^{-6}\,T + 1.76\cdot10^{-9}\,T^2)$, *T* in K [73D].

Temperature dependence (20...300 K) of the lattice constant and the temperature factors of the Nd atom in [94M].

Optical properties

IR diffuse reflection and Raman spectra (La, Nd, Gd, Tb, Dy, Yb)B_6 in Figs.2 and 3 [88T, 93Y].

Further properties

entropy

S	103.45(21) J mol^{-1} K^{-1}	86B

melting point

T_m	2610 °C	96G

microhardness
(in kg mm^{-2})

H_K	2020	*T* = 300 K	cube, average value; load 50 g	96G
	1870		cube, average value; load 200 g	
	1700		rhombododecahedron, average value, load 50 g	

High temperature hardness of single crystals of LaB_6, CeB_6, PrB_6, NdB_6 and SmB_6 [99O].

Debye temperature

Θ_D	549 K	*T* < 300 K	$Nd^{11}B_6$ average (for *T*-dep. see ref.)	94T

For Einstein temperatures of metal hexaborides see Fig. 4.

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Fig. 1.

NdB_6. **(a)** Temperature dependence of the lattice parameter of $Nd^{11}B_6$. **(b)** Temperature dependence of the equivalent temperature factors of Nd (full circles) and B (open circles, experimental points; triangles, with correction for the contribution from the static displacements), solid lines, Einstein calculation for Nd and Debye calculation for B respectively [94M].

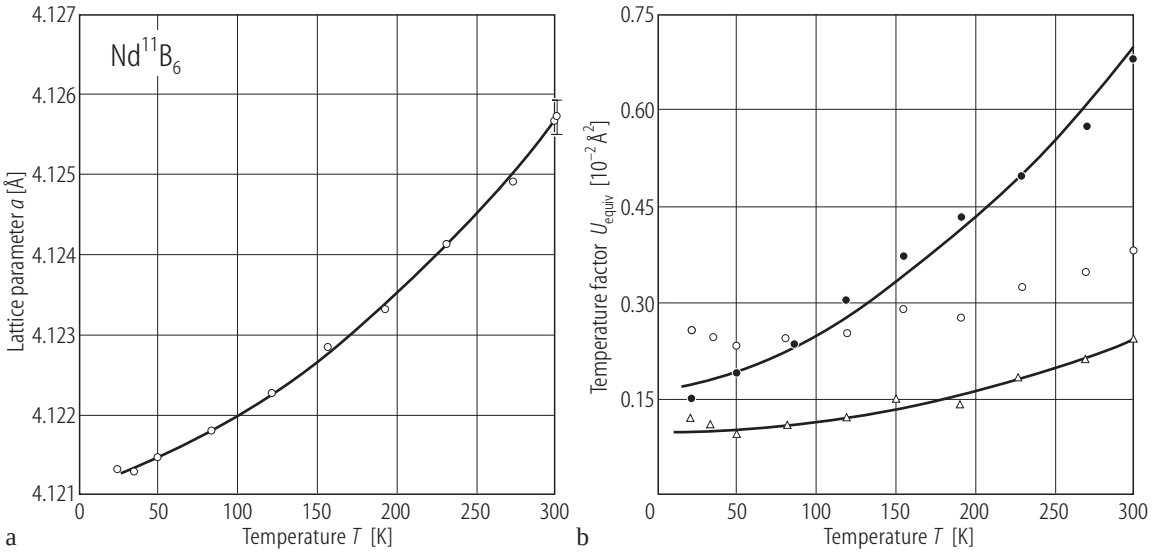

Fig. 2.

Metal hexaborides. IR diffuse reflectance spectra of representative MB_6 compounds with two-valent Ca, Sr and Yb, and three-valent Nd, Gd, La, Tb and Dy metal atoms [88T, 93Y].

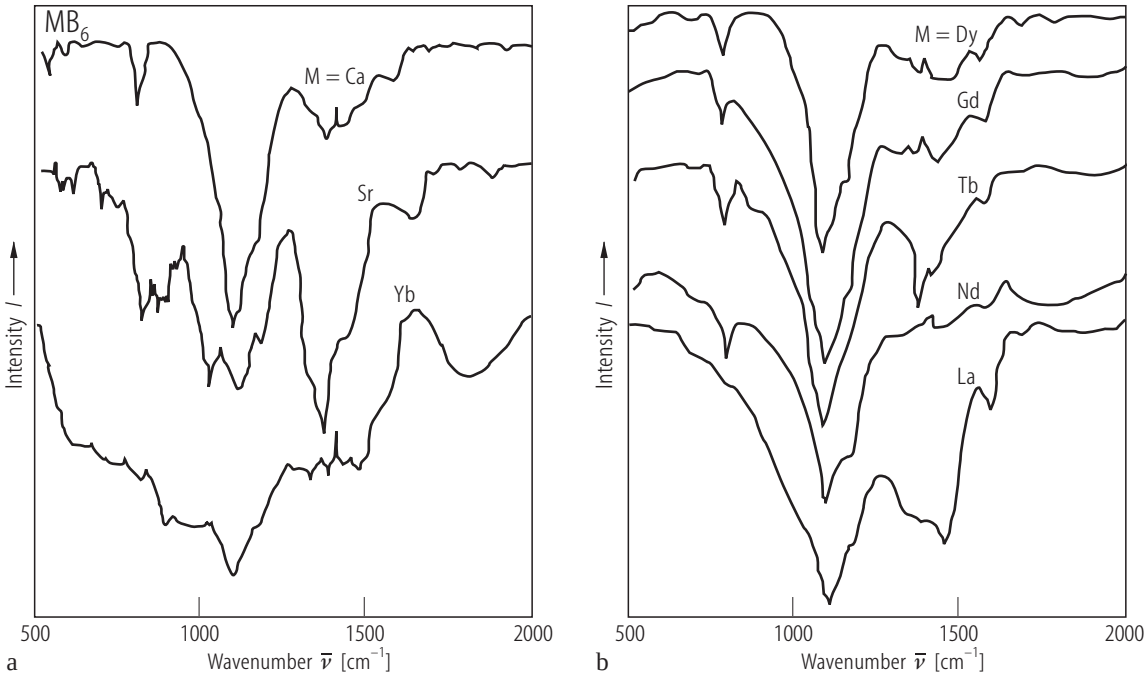

Fig. 3.

Metal hexaborides. Raman spectra, relative intensity vs. Raman shift for hexaborides with twofold and threefold ionized metal atoms [88T, 93Y].

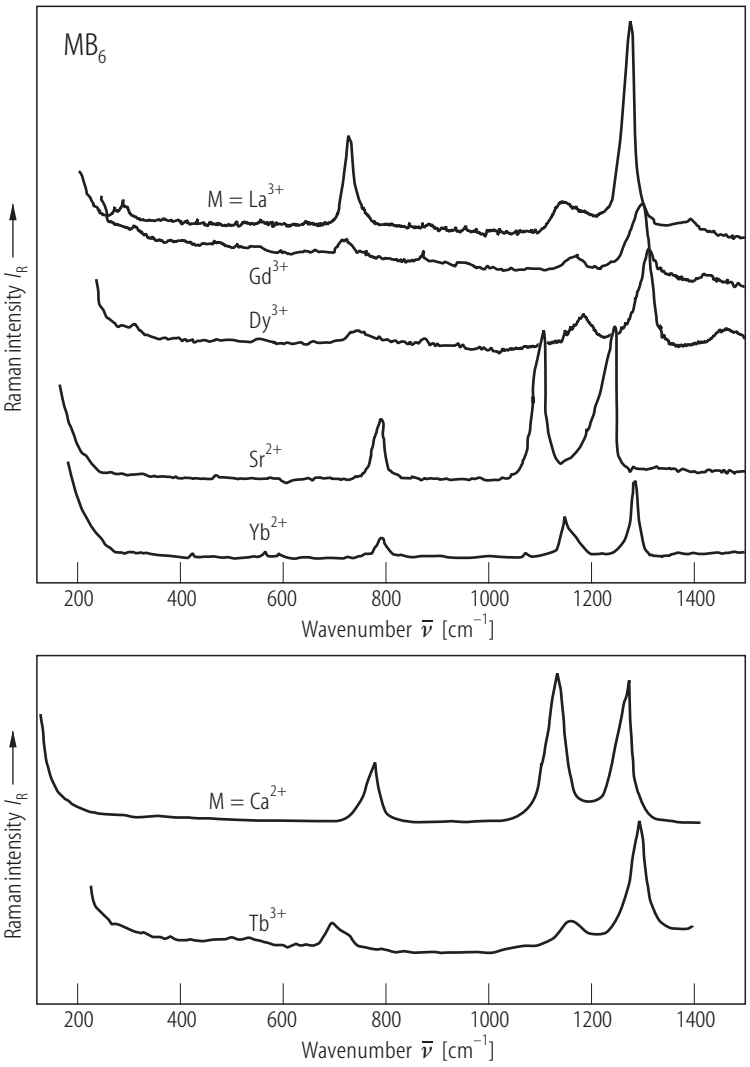

Fig. 4.

Metal hexaborides. Characteristic Einstein temperatures of the Ln atoms vs. atomic number of the Ln element; full circles [94K]; triangles [99T].