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

general results

R_2MB_6 (R = rare earth, M = Ru, Os)

Magnetism and structural chemistry, magnetic behaviour between 1.5 and 1100 K [84H].

On boron-carbon chains, atomic distances and valence electron count in $La_{15}B_{14}C_{19}$; $Ce_{10}B_9C_{12}$; $Ce_5B_4C_5$; $La_{10}B_9C_6$; $Ce_5B_2C_6$; $Gd_5B_2C_5$; $Gd_{15}B_4C_{12}$ [97B].

$R_{5-x}Fe_{2+x}B_6$

Crystal structure of $R_{5-x}Co_{2+x}B_6$-type

Space group: $R\bar{3}m$

Preparation and structure determination in [86D].

unit cell parameters
(in nm)

Compound	*a*	*c*	
$Y_{5-x}Fe_{2+x}B_6$	0.5426(2)	2.328(2)	86D
$Ce_{5-x}Fe_{2+x}B_6$	0.5482(2)	2.443(1)	
$Pr_{5-x}Fe_{2+x}B_6$	0.5481(1)	2.433(1)	
$Nd_{5-x}Fe_{2+x}B_6$	0.5469(1)	2.402(2)	
$Sm_{5-x}Fe_{2+x}B_6$	0.5459(2))	2.368(1)	
$Eu_{5-x}Fe_{2+x}B_6$	0.5435(1)	2.33_6(1)	
$Gd_{5-x}Fe_{2+x}B_6$	0.5429(2)	2.330(2)	
$Tb_{5-x}Fe_{2+x}B_6$	0.5420(1)...0.5412(2)	2.323(1)...2.321(1)	
$Dy_{5-x}Fe_{2+x}B_6$	0.5427(1)	2.313(1)	
$Yb_{5-x}Fe_{2+x}B_6$	0.5427(2)	2.222(1)	

Variation of the unit cell parameters in Fig. 1a [86D].

$R_{5-x}Co_{2+x}B_6$

Crystal structure of $R_{5-x}CO_{2+x}B_6$-type

Space group: $R\bar{3}m$

Preparation and structure determination in [86D].

unit cell parameters
(in nm, 0≤x≤1)

Compound	*a*	*c*	
$Y_{5-x}Co_{2+x}B_6$	0.5422(2)	2.986(1)	86D
$La_{5-x}Co_{2+x}B_6$	0.5510(2)	2.460(2)	
$Ce_{5-x}Co_{2+x}B_6$	0.5478(2)	2.447(2)	
$Pr_{5-x}Co_{2+x}B_6$	0.5457(2)...0.5441(1)	2.472(1)...2.426(2)	
$Nd_{5-x}Co_{2+x}B_6$	0.5432(2)	2.405(2)	
$Sm_{5-x}Co_{2+x}B_6$	0.5420(2)	2.382(1)	
$Gd_{5-x}Co_{2+x}B_6$	0.5419(3)	2.340(1)	
$Tb_{5-x}Co_{2+x}B_6$	0.5401(1)...0.5400(1)	2.334(1)...2.320(1)	
$Dy_{5-x}Co_{2+x}B_6$	0.5400(1)	2.302(1)	
$Ho_{5-x}Co_{2+x}B_6$	0.5390(2)	2.280(2)	
$Er_{5-x}Co_{2+x}B_6$	0.5388(2)	2.257(2)	

Variation of the unit cell parameters in Fig. 1b [86D].

Atomic parameters, interatomic distances and coordination numbers in [86D].

density

d	7.43 g cm^{-3}	*T* = 300 K	exp., $Tb_{5-x}Co_{2+x}B_6$ (x = 0.85)	86D
	7.49 g cm^{-3}		calc., $Tb_{5-x}Co_{2+x}B_6$ (x = 0.85)	

ternary compounds based on La

$La_xEu_{1-x}B_6$

In $M^{II}_1{}_{-x}M^{III}_xB_6$ ternary compounds metals in the + II and the + III oxidation state are present simultaneously. So the development of their properties from semiconductor ($M^{II}B_6$) to metallic ($M^{III}B_6$) behavior can be observed [74M, 76M, 77E, 79A].

A composition-induced metal-insulator transition occurs at $0 < x < 0.01$ [76M].

For work function, see [78B]; electrical resistivity: Fig. 2; thermoelectric power: Fig. 3.

For further ternary compounds, see [74S, 79K, 79M, 74H, 77S, 78B].

$La_{1-x}Ce_xB_6$

Studies of the crystal structure of $Ce_{1-x}La_x{}^{11}B_6$ solid solutions by high-resolution powder neutron diffraction [91T].

lattice parameters of $Ce_{1-x}La_x{}^{11}B_6$
(in Å)

a	4.14334(3)	*T* = 300 K	x = 0.25, neutron diffraction	91T
	4.14663(3)		x = 0.5, neutron diffraction	
	4.1443(3)		x = 0.28, X-ray diffraction	89B
	4.1470(3)		x = 0.4, X-ray diffraction	

Lattice parameter of $Sm_xLa_{1-x}B_6$ and $Sm_xCa_{1-x}B_6$ depending on temperature Fig. 4 [88A, 91A].

Preparation of single crystals in [91O1, 91O2].

Dependence of the boundary density on the CeB_6 content in [91O2, 93O].

Solid solution hardening and atomic displacement parameters [96K2].

For preparation by the traveling solvent floating zone method of (La, Ce)B_6, growth conditions of boundary-free crystals, dependence of density and hardness on composition and temperature, see [94O].

$La_{1-x}Pr_xB_6$

Preparation of single crystals in [91O3, 91O1].

Dependence of the boundary density on the PrB_6 content in [91O3].

$La_{1-x}Nd_xB_6$

Preparation of single crystals in [91O1].

ternary compounds based on Ce

$CeCr_2B_6$

Preparation and structure refinement in [96K1].

ternary compounds based on Sm

Composition dependence of the lattice constants in $Sm_{1-x}Eu_xB_6$, $Sm_{1-x}La_xB_6$, $Sm_{1-x}Gd_xB_6$ in Fig. 5 [87P].

Samarium effective valence in $Sm_{1-x}M_xB_6$ in Fig. 6 [87P].

Optical absorption and effective valency of Sm ions in $Sm_{1-x}M_xB_6$ solid solutions [81F].

ternary compounds based on Yb

Yb_2AlB_6

Structure: orthorhombic Y_2ReB_6-type

Space group: Pbam

lattice parameters
(in Å)

a	9.127(5)	*T* = 300 K	X-ray diffraction	91D
b	11.46(1)			
c	3.584(4)			

ternary compounds based on Lu

Lu_2AlB_6

Structure: orthorhombic

Space group: Pbam

lattice parameters
(in nm)

a	0.8987(1)	*T* = 300 K	X-ray diffraction	96O
b	1.1334(1)			
c	0.3633(1)			

resistivity

ρ	31(3) μΩ cm	T = 300 K		96O

microhardness

H_V	18.9(7) GPa	T = 300 K	load 100 g	96O

$LuAlB_6$

Structure orthorhombic

lattice parameters
(in nm)

a	0.5898(1)	T = 300 K	X-ray diffraction	96O
b	1.1420(1)			
c	0.3485(1)			

Lu-Co-B compounds

The ternary Lu-Co-B system [88D].

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Fig. 1.

$R_{5-x}M_{2+x}B_6$ hexaborides. Variation of the unit cell parameters of **(a)** $R_{5-x}Fe_{2+x}B_6$ and **(b)** $R_{5-x}Co_{2+x}B_6$ [86D].

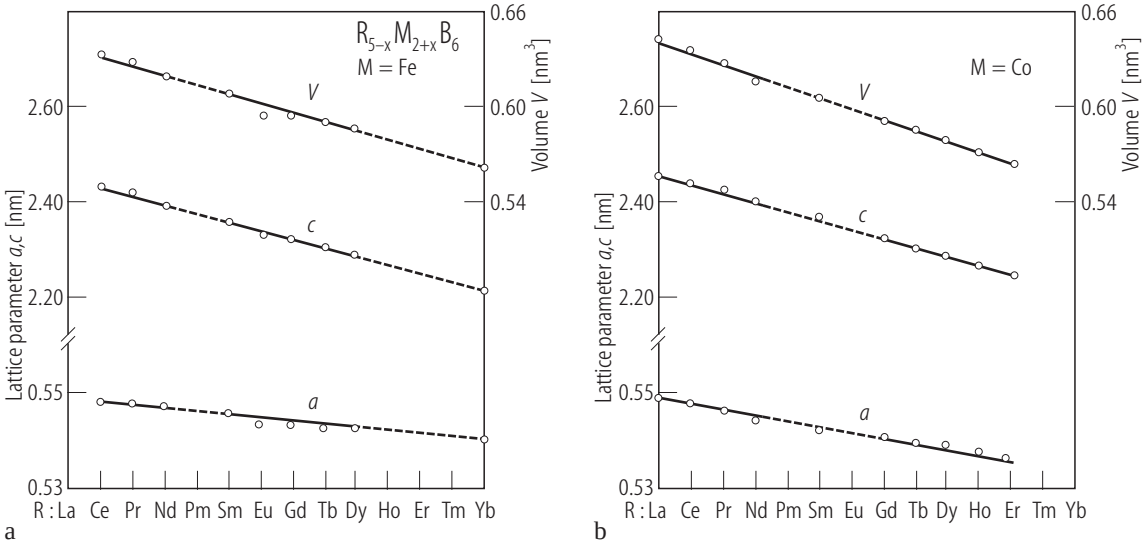

Fig. 2.

$La_xEu_{1-x}B_6$. Resistivity vs. temperature [77E, 74M].

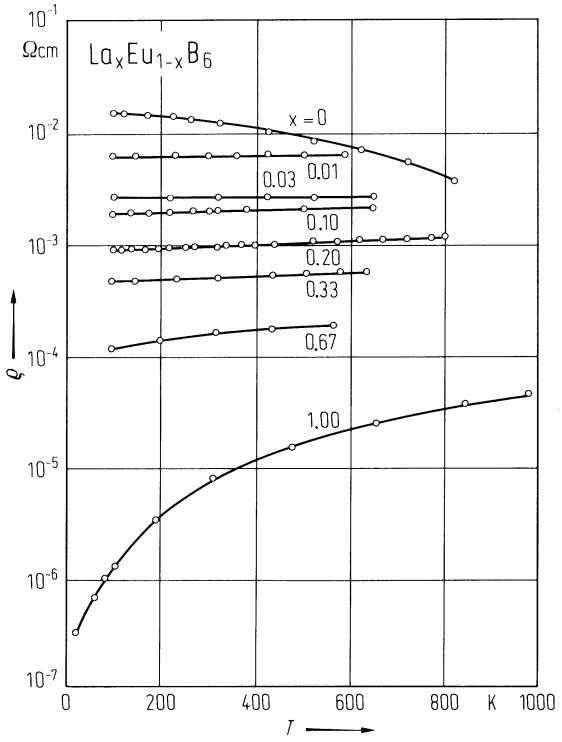

Fig. 3.

$La_xEu_{1-x}B_6$. Thermoelectric power vs. temperature [77E, 74M].

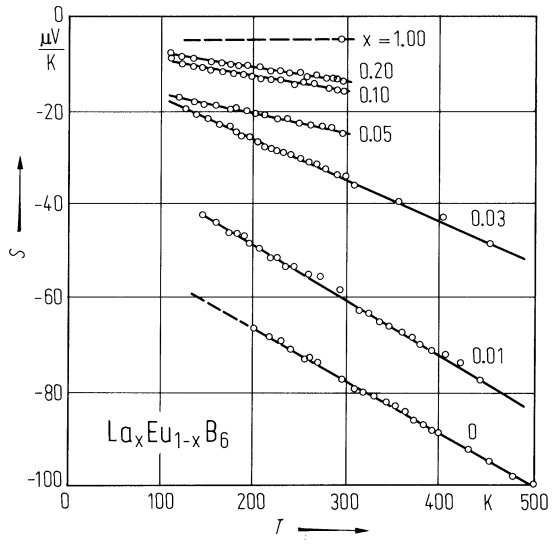

Fig. 4.

Metal hexaborides. Temperature dependence of the lattice parameters of CaB_6, $Sm_{0.05}Ca_{0.95}B_6$, $Sm_{0.4}Ca_{0.6}B_6$, SmB_6, $Sm_{0.5}La_{0.5}B_6$, LaB_6 determined by neutron scattering in [88A, 91A].

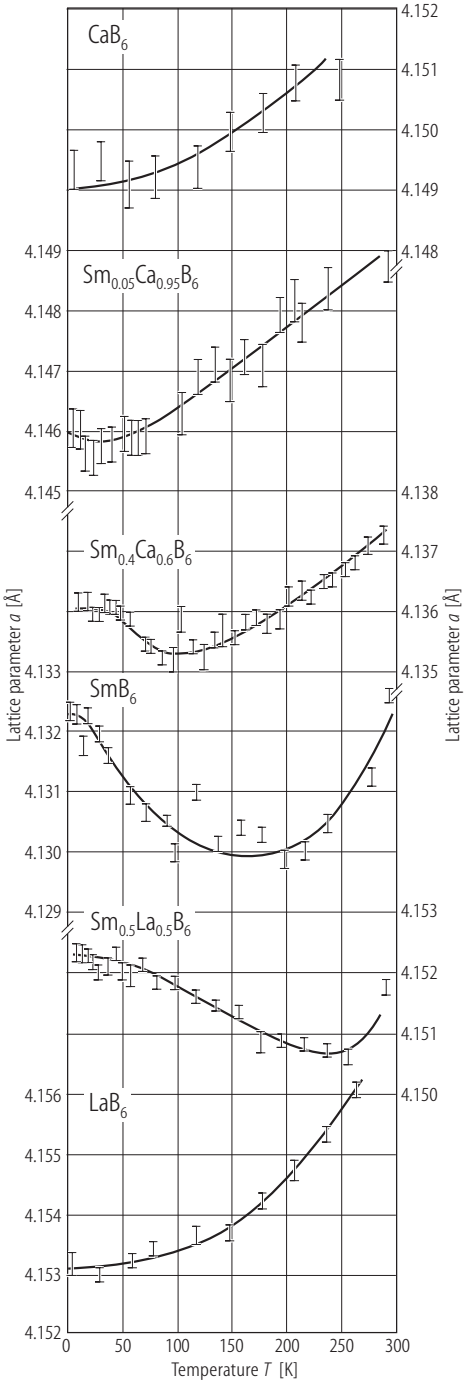

Fig. 5.

SmB_6 (:La, Eu, Gd). Lattice constants of $Sm_{1-x}La_xB_6$, $Sm_{1-x}Eu_xB_6$, $Sm_{1-x}Gd_xB_6$, vs. degree of substitution x [87P].

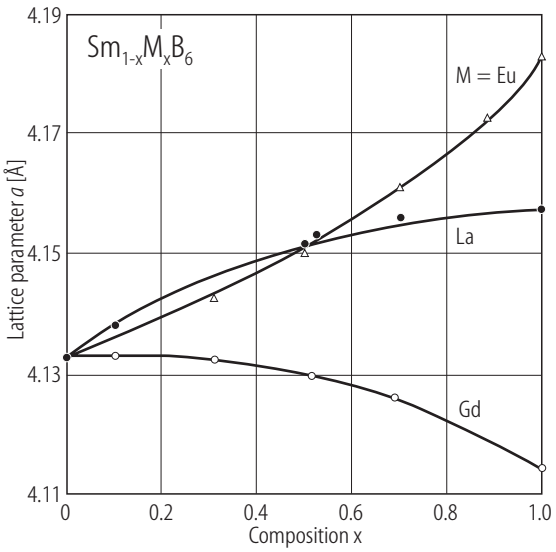

Fig. 6.

SmB_6. Effective valence of the Sm atoms vs. content of Eu, La, Yb, Dy, Ba, Gd atoms substituting for Sm [81F, 87P]. Note: in figure full circle should be for M = Ca instead of Eu.