Crystal structure of diytterbium pentadecanickel nonaboride, $Yb_2Ni_{15}B_9$

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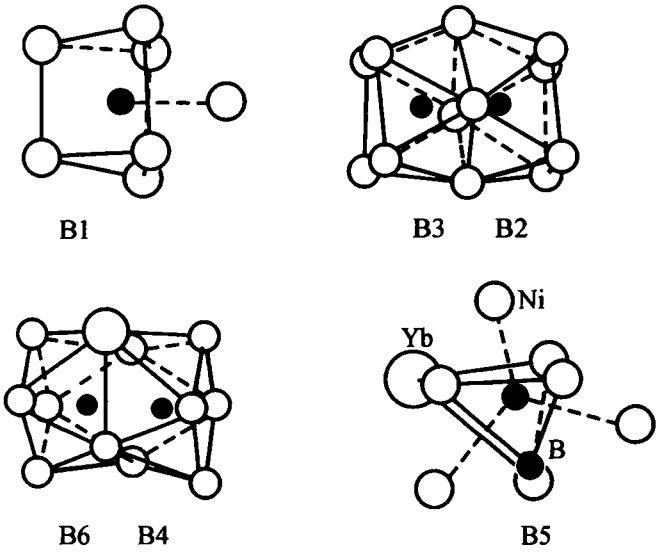

Abstract

$B_9Ni_{15}Yb_2$, orthorhombic, *Cmca* (no. 64), $a = 15.925(2)$ Å, $b = 11.590(1)$ Å, $c = 11.232(1)$ Å, $V = 2073.1$ Å^3, $Z = 8$, $R_{gt}(F) = 0.033$, $wR_{ref}(F^2) = 0.054$, $T = 293$ K.

Source of material

The title compound was obtained by systematic investigation of the Yb-Ni-B system. The samples were melted in the arc furnace (purified argon atmosphere) from compact Yb (99.5 wt. %) and powders of Ni (99.98 wt. %) and B (99.4 wt. %), which were previously mixed and pressed. Each alloy was wrapped in Mo-foil and annealed at 1070 K for 700 h in the evacuated quartz tube. Single needle-like crystals with metallic luster were extracted from the compact alloy with nominal composition $Yb_2Ni_{15}B_9$.

Discussion

The existence of $Yb_2Ni_{15}B_9$ (structure type $Ho_2Ni_{15}B_9$ [1]) was established in [2], but only unit cell parameters were determined, the atomic coordinates were not specified. The $Ln_2Ni_{15}B_9$ (*Ln* = Y, Tb, Dy, Er, Tm, Lu) borides belong also to $Ho_2Ni_{15}B_9$-structure type [2], but crystal structure was fully examined only for $Ho_2Ni_{15}B_9$. The single crystal investigation of $Yb_2Ni_{15}B_9$ showed lattice parameters in good agreement with the results of X-ray powder diffraction method [2]. Metal atoms in the $Yb_2Ni_{15}B_9$ structure are characterized by high coordination numbers (CN): the Yb atoms have CN = 20 and 18, the Ni atoms – 16, 14 and 13. Coordination spheres of the boron atoms are distorted Archimedean cubes which are connected with one another by square faces (B2–B3 and B4–B6). The B1 atoms center a trigonal prism composed of the metal atoms. The B5 atoms are also situated in a trigonal prism, in which one of the apices is occupied by a B5 atom. As a result, the boron atoms in $Yb_2Ni_{15}B_9$ are either isolated (B1) or form pairs (other boron atoms). Thus, according to the common tendency, the increase in boron content in a boride leads to substitution of isolated boron atoms (structure types $Ti_3Co_5B_2$, TiNiSi, $CeCo_3B_2$) by B_2 pairs (structure types $ZrCo_3B_2$, $CeCo_4B_4$, $NdCo_4B_4$), B_n chains (structure types W_3CoB_3, Mo_2IrB_2), B_n zigzag chains (structure types $NdCoB_2$, CrB, FeB) or layers (structure types AlB_2, $YCrB_4$, Y_2ReB_6) [3]. The minimal interatomic distances for Yb atoms are well correlated with the distances in the other boride structures. Specifically, *d*(Yb1—Ni3) and *d*(Yb1—B5) are 2.785(1) Å and 2.744(2) Å, respectively. The shortening of interatomic distances between Ni and B atoms (*d*(Ni5—B5) = 1.988(9) Å and *d*(Ni7—B1) = 1.972(3) Å) has the same order as in other boride structures. The distances between boron atoms in the pairs are: *d*(B2—B3) = 1.91(2) Å, *d*(B4—B6) = 1.97(1) Å, *d*(B5—B5) = 1.71(2) Å. Thus, they are in good agreement with the values of the boron atomic radii which are within the limits of 0.88 Å (for the CN 4) to 0.92 Å – 0.95 Å (for the CN 8) [3].

Table 1. Data collection and handling.

Crystal:	metallic luster needle, size 0.03 × 0.04 × 0.2 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	443.04 cm^{-1}
Diffractometer, scan mode:	STOE IPDS I, 225 exposures, $\Delta\omega = 0.8$
$2\theta_{max}$:	63.88°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11956, 1838
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1516
$N(param)_{refined}$:	106
Programs:	SHELXS-97 [4], SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
B(1)	8*d*	0.1352(7)	0	0	0.006(2)
B(2)	8*f*	0	0.046(1)	0.172(1)	0.005(2)
B(3)	8*f*	0	0.441(1)	0.198(1)	0.005(2)
B(4)	16*g*	0.1302(4)	0.2489(7)	0.2452(8)	0.007(1)
B(5)	16*g*	0.1497(5)	0.0541(7)	0.4486(8)	0.010(1)
B(6)	16*g*	0.2010(5)	0.2486(7)	0.1011(8)	0.008(1)

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Yb(1)	8*e*	¼	0.05912(4)	¼	0.0040(2)	0.0045(2)	0.0048(2)	0	0.0009(1)	0
Yb(2)	8*f*	0	0.23902(4)	0.45868(4)	0.0048(2)	0.0056(2)	0.0026(2)	0	0	–0.0006(2)
Ni(1)	4*b*	0	0	½	0.0117(8)	0.0067(8)	0.0031(8)	0	0	–0.0011(7)
Ni(2)	4*a*	0	0	0	0.0036(7)	0.0055(8)	0.0005(8)	0	0	–0.0007(6)
Ni(3)	8*f*	0	0.2633(1)	0.2120(1)	0.0036(4)	0.0055(5)	0.0032(5)	0	0	0.0006(5)
Ni(4)	8*e*	¼	0.3188(1)	¼	0.0068(5)	0.0056(5)	0.0021(5)	0	0.0008(5)	0
Ni(5)	16*g*	0.09688(5)	0.41174(8)	0.33989(8)	0.0062(3)	0.0045(3)	0.0021(4)	0.0013(3)	–0.0005(3)	–0.0001(3)
Ni(6)	16*g*	0.10668(5)	0.13667(8)	0.09638(8)	0.0065(3)	0.0070(4)	0.0019(4)	0.0012(3)	0.0004(3)	–0.0003(3)
Ni(7)	16*g*	0.11602(5)	0.38670(7)	0.11731(8)	0.0049(3)	0.0045(4)	0.0027(4)	0.0008(3)	0.0002(3)	–0.0003(3)
Ni(8)	16*g*	0.16977(5)	0.22263(7)	0.41610(9)	0.0053(3)	0.0040(4)	0.0027(3)	–0.0008(3)	–0.0004(3)	0.0007(3)
Ni(9)	16*g*	0.07931(5)	0.08802(8)	0.30669(8)	0.0036(3)	0.0044(4)	0.0018(4)	–0.0007(3)	–0.0009(3)	–0.0005(3)
Ni(10)	16*g*	0.26331(5)	0.39985(8)	0.03203(9)	0.0046(3)	0.0055(4)	0.0058(4)	–0.0022(3)	–0.0009(3)	0.0023(3)

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