New Compounds $RE(Zn,Al)_8$ and $Yb_4Zn_{20.3}Al_{12.7}$ and their Crystal Structures

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70th birthday

The crystal structures of several new compounds have been determined using X-ray analysis. The intermetallic compound $HoZn_5Al_3$ ($a = 8.586(3)$, $c = 16.538(5)$ Å, $R_F = 0.0413$, $R_W = 0.0521$) has its own structure type (space group $I4/mmm$), which has been found for the first time. The following compounds are isostructural with the previous one: $YZn_{5.52}Al_{2.48}$ ($a = 8.6183(1)$, $c = 16.5048(3)$ Å, $R_I = 0.078$, $R_P = 0.116$), $DyZn_{4.96}Al_{3.04}$ ($a = 8.5887(1)$, $c = 16.5002(3)$ Å, $R_I = 0.077$, $R_P = 0.114$), $ErZn_{5.37}Al_{2.63}$ ($a = 8.5525(2)$, $c = 16.3997(5)$ Å, $R_I = 0.081$, $R_P = 0.111$), $TmZn_{5.64}Al_{2.36}$ ($a = 8.70429(8)$, $c = 16.3943(4)$ Å, $R_I = 0.088$, $R_P = 0.095$), $LuZn_{5.58}Al_{2.42}$ ($a = 8.5616(1)$, $c = 16.3052(3)$ Å, $R_I = 0.081$, $R_P = 0.101$). The intermetallic compound $Yb_4Zn_{20.3}Al_{12.7}$ ($a = 8.6183(1)$, $c = 16.5048(3)$ Å, $R_I = 0.085$, $R_P = 0.112$) adopts the $Yb_8Cu_{17}Al_{49}$ – type structure (space group $I4/mmm$). The relationship between the $HoZn_5Al_3$-type and the $Yb_8Cu_{17}Al_{49}$-type structures is discussed.

Key words: Intermetallic Compound, Crystal Structure, Rare Earth Metal, X-Ray Diffraction

Introduction

The interaction of components in the *RE*-Zn-Al systems (*RE*-rare earth metal) has not been studied sufficiently. It is known that compounds with the $BaAl_4$ [1 – 3], KHg_2 [4], $CaIn_2$ [4], CsCl [4], and La_3Al_{11} [5] type structures form in these systems. During our investigations we discovered a number of new ternary compounds with $BaAl_4$ [6], La_3Al_{11} [6] and $BaHg_{11}$ [7] type structures. Taking into consideration that many compounds with complicated composition form in *RE*-T-Al systems (T – transition metal) [8 – 13], we carried out a systematic investigation of the *RE*-Zn-Al systems, of which the present work is the result.

Experimental Section

We used metal powders of the following purity (wt. %): Al – 99.99, Zn – 99.95, *RE* (Y, Dy, Ho, Er, Tm, Yb, Lu) – 99.5. The powders were mixed, pressed into pellets and sealed in evacuated quartz ampoules. Then they were slowly heated up to 800 K during 50 h. After cooling the ampoules were broken, the samples were ground into fine-dispersed powders and once again pressed into pellets. After that they were annealed in evacuated quartz ampoules at 670 K for 800 h. The samples were then quenched in cold water without breaking the ampoules.

Table 1. Crystal data of $HoZn_5Al_3$.

Empirical formula	$HoZn_5Al_3$
Space group	$I4/mmm$ (N 139)
Lattice constants [Å]	$a = 8.586(3)$, $c = 16.538(5)$
Cell volume [Å^3]	1219.2(1)
Formula units per cell	$Z = 8$
Formula mass	574
Number of atom sites	8
Number of free parameters	35
Number of atoms per cell	72.0
Calculated density [g/cm^3]	6.281(6)
Mode of refinement	$F(hkl)$
Radiation [Å]	Mo-K$_\alpha$, 0.71069
$2\theta_{max}$ and $\sin\theta_{max}/\lambda$	94.98, 1.04
Range in h,k,l	0 – 17, 0 – 17, 0 – 34
Weighing scheme	$1/[\sigma F^2 + 0.0033 {F_{obs}}^2]$
Extinction formalism	Sheldrick-1 0.000213
Number of measured reflections	2392
Numbers of unique reflections	1302
Restrictions	$F(hkl) > 4.00\mathrm{sig}(F)$
Goodness of fiting	1.000
Scale factor	0.923(4)
R_{sig}, R_{eq}, R_F, R_w	0.0297, 0.0595, 0.0413, 0.0521

Phase analysis was carried out using X-ray powder diffraction patterns obtained by the Debye-Scherrer tech-

Table 2. Structural data of the $HoZn_5Al_3$.

Atoms	Wyckoff position	Coordinates x	y	z	B_{eq}, Å^2
Ho1	4*c*	0	1/2	0	0.68(1)
Ho2	4*e*	0	0	0.72021(3)	0.35(1)
T1(2.40(8)Zn+5.60(8)Al)	8*f*	1/4	1/4	1/4	0.72(2)
T2(8Zn)	8*h*	0.1520(1)	x	0	0.88(1)
T3(1.71(9)Zn+14.29(9)Al)	16*n*	0	0.2315(2)	0.1392(1)	0.77(3)
T4(16Zn)	16*n*	0	0.3499(1)	0.3245(1)	0.91(1)
T5(12.21(9)Zn+3.79(9)Al)	16*m*	0.1641(2)	x	0.4196(1)	1.36(1)

Table 3. Anisotropic displacement parameters (Å^2) for $HoZn_5Al_3$.

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ho1	1.04(2)	0.57(1)	0.45(1)	0	0	0
Ho2	0.34(1)	0.34(1)	0.37(1)	0	0	0
T1	0.66(3)	0.66(3)	0.83(5)	0.07(4)	0.07(3)	0.07(3)
T2	0.93(2)	0.93(2)	0.76(3)	0.07(2)	0	0
T3	0.74(4)	0.74(5)	0.82(4)	0	0	0.13(4)
T4	0.63(2)	0.68(2)	1.40(2)	0	0	−0.15(2)
T5	1.41(2)	1.41(2)	1.25(3)	0.40(3)	−0.57(2)	−0.57(2)

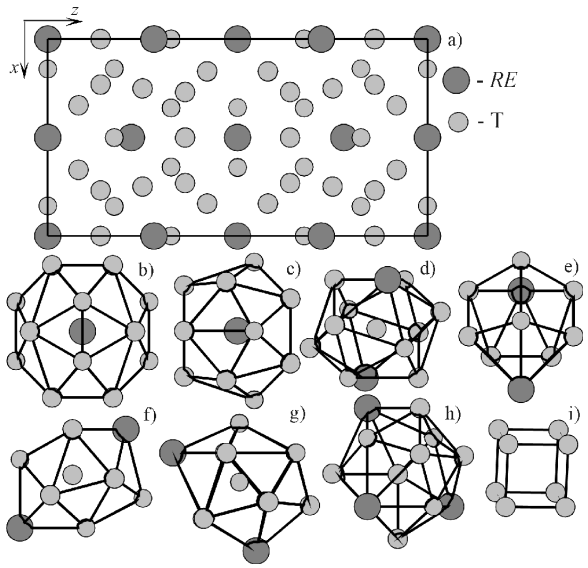

Fig. 1. An *xz* projection of the $HoZn_5Al_3$ structure (a) and the coordination polyhedra of the atoms: [**Ho1**20T] (b), [**Ho2**16T] (c), [**T1**10T2Ho] (d), [**T2**8T2Ho] (e), [**T3**11T2Ho] (f), [**T4**10T2Ho] (g), [**T5**9T3Ho] (h), vacant distorted cubes [8T] (i).

nique with nonfiltered Cr-K radiation in cameras of 57.3 mm in diameter. The lattice and crystal structure parameters were refined by full-matrix least squares using powder diffraction patterns recorded on a DRON-3M diffractometer (Cu-K$_\alpha$ radiation) using the $\theta - 2\theta$ scan technique with steps of 0.02 2θ ($2\theta_{max} = 120°$) and an exposition time of 40 s at every point with Cu-K$_\alpha$ radiation, using Ni as β-filter. The preliminary single crystal investigations were carried out using the Laue method and a rotation analysis (cameras RKV-86, Mo-K, Cu-K radiation). Experimental intensities were obtained on a four-circle single crystal DARCH-1 diffractometer (Mo-K$_\alpha$ radiation). All calculations were performed using the CSD software [14].

Table 4. Lattice constants and volumes of $RE(Zn,Al)_8$ compounds.

Compound*	*a*, Å	*c*, Å	V, Å^3
$YZn_{5.52}Al_{2.48}$	8.6180(1)	16.5064(2)	1225.93(4)
$DyZn_{4.96}Al_{3.04}$	8.5888(1)	16.6011(2)	1224.62(4)
$HoZn_{5.55}Al_{2.45}$	8.5814(1)	16.5263(2)	1217.00(4)
$ErZn_{5.37}Al_{2.63}$	8.5825(2)	16.3997(5)	1207.99(9)
$TmZn_{5.64}Al_{2.36}$	8.5674(2)	16.3943(4)	1203.36(7)
$Yb_4Zn_{20.3}Al_{12.7}$	8.7043(1)	16.4031(2)	1242.77(4)
$LuZn_{5.58}Al_{2.42}$	8.5616(1)	16.3052(3)	1195.19(6)

* The lattice constants and compositions have been determined for the polycrystalline samples by the Rietveld method.

Results

We took a single crystal with irregular shape from the sample with the composition $Ho_{11}Zn_{40}Al_{41}$. The conditions of the investigation are shown in Table 1. The structure model has been determined by direct methods (MULTAN software) with a final examination of the electron density distribution map by Fourier synthesis. The refinement of the atomic coordinates and their anisotropic displacement parameters was carried out using full-matrix least squares with absorption and extinction correction. Residual electron density calculations revealed no significant additional maxima. The atomic coordinates, atomic distribution and displacement parameters are shown in Tables 2 and 3, and the interatomic distances are shown in Table 6.

The *xz* projection of the crystal structure of $HoZn_5Al_3$ and the coordination polyhedra of all atoms are shown in Fig. 1. This structure is characterized by a partly ordered distribution of the Zn and Al atoms. The positions with the Zn atoms have a smaller coordination number (CN) (10 – 12) and the positions with a lager CN (12, 13) are occupied by a statistical mixture of Zn and Al atoms. The existence of distorted vacant

Table 5. Structural data of the RE(Zn,Al)$_8$ compounds (sg $I4/mmm$).

Atoms	Wyckoff position	Coordinates x	y	z	B_{iso}, Å^2
$YZn_{5.62}Al_{2.38}$ ($R_I = 0.078$, $R_P = 0.116$)					
Y1	4*c*	0	1/2	0	0.89(4)
Y2	4*e*	0	0	0.7198(1)	1.07(4)
T1(3.5(1)Zn+4.5(1)Al)	8*f*	1/4	1/4	1/4	0.53(6)
T2(Zn)	8*h*	0.1510(2)	x	0	1.19(5)
T3(3.6(1)Zn+12.4(1)Al)	16*n*	0	0.2286(4)	0.1406(2)	1.11(6)
T4(Zn)	16*n*	0	0.3503(2)	0.3243(1)	0.81(3)
T5(13.8(1)Zn+2.2(1)Al)	16*m*	0.1685(2)	x	0.4185(1)	1.34(4)
$DyZn_{4.96}Al_{3.04}$ ($R_I = 0.077$, $R_P = 0.114$)					
Dy1	4*c*	0	1/2	0	0.74(4)
Dy2	4*e*	0	0	0.7220(1)	0.44(5)
T1(2.4(1)Zn+5.6(1)Al)	8*f*	1/4	1/4	1/4	0.91(9)
T2(7.5(1)Zn+0.5(1)Al)	8*h*	0.1518(3)	x	0	0.91(8)
T3(2.5(1)Zn+13.5(1)Al)	16*n*	0	0.2315(6)	0.1395(3)	1.09(9)
T4(Zn)	16*n*	0	0.3498(2)	0.3254(1)	1.08(5)
T5(11.3(1)Zn+4.7(1)Al)	16*m*	0.1647(2)	x	0.4197(2)	1.18(6)
$ErZn_{5.37}Al_{2.63}$ ($R_I = 0.081$, $R_P = 0.111$)					
Er1	4*c*	0	1/2	0	1.08(7)
Er2	4*e*	0	0	0.7207(2)	0.84(7)
T1(3.3(1)Zn+4.7(1)Al)	8*f*	1/4	1/4	1/4	0.56(9)
T2(Zn)	8*h*	0.1503(4)	x	0	1.33(9)
T3(3.4(2)Zn+12.6(2)Al)	16*n*	0	0.2299(9)	0.1388(5)	1.53(9)
T4(Zn)	16*n*	0	0.3491(4)	0.3242(2)	1.19(8)
T5(12.3(2)Zn+3.7(2)Al)	16*m*	0.1648(4)	x	0.4190(3)	1.32(9)
$TmZn_{5.64}Al_{2.36}$ ($R_I = 0.088$, $R_P = 0.095$)					
Tm1	4*c*	0	1/2	0	0.88(5)
Tm2	4*e*	0	0	0.7211(1)	0.68(5)
T1(3.9(1)Zn+4.1(1)Al)	8*f*	1/4	1/4	1/4	0.76(9)
T2(Zn)	8*h*	0.1510(3)	x	0	1.25(8)
T3(4.7(1)Zn+11.3(1)Al)	16*n*	0	0.2317(6)	0.1399(3)	1.41(9)
T4(Zn)	16*n*	0	0.3504(3)	0.3244(1)	0.61(6)
T5(12.5(1)Zn+3.5(1)Al)	16*m*	0.1659(2)	x	0.4190(2)	1.09(7)
$Yb_4Zn_{20.3}Al_{12.7}$ ($R_I = 0.087$, $R_P = 0.118$)					
Yb1	4*c*	0	1/2	0	0.52(3)
Yb2	4*e*	0	0	0.7147(1)	0.36(3)
T1(3.0(1)Zn+5.0(1)Al)	8*f*	1/4	1/4	1/4	0.57(9)
T2(6.7(1)Zn+1.3(1)Al)	8*h*	0.1486(3)	x	0	0.68(7)
T3(3.1(1)Zn+12.9(1)Al)	16*n*	0	0.2314(6)	0.1410(3)	1.37(8)
T4(15.4(1)Zn+0.6(1)Al)	16*n*	0	0.3512(3)	0.3220(1)	0.45(4)
T5(11.3(1)+4.7(1)Al)	16*m*	0.1744(2)	x	0.4159(2)	1.04(4)
T6(1.12(2)Zn+0.88(2)Al)	2*b*	0	1/2	0	1.2(2)
$LuZn_{5.58}Al_{2.42}$ ($R_I = 0.081$, $R_P = 0.101$)					
Lu1	4*c*	0	1/2	0	0.67(4)
Lu2	4*e*	0	0	0.7205(1)	0.66(4)
T1(4.4(1)Zn+3.6(1)Al)	8*f*	1/4	1/4	1/4	0.62(9)
T2(7.1(1)Zn+0.9(1)Al)	8*h*	0.1516(3)	x	0	0.74(8)
T3(4.9(1)Zn+11.1(1)Al)	16*n*	0	0.2298(5)	0.1411(3)	0.83(8)
T4(15.4(1)Zn+0.6(1)Al)	16*n*	0	0.3484(3)	0.3234(1)	0.60(6)
T5(11.6(1)Zn+4.4(1)Al)	16*m*	0.1648(2)	x	0.4184(2)	0.86(6)

cube, formed by the T5 atoms, is the characteristic feature of the $HoZn_5Al_3$ structure (Fig. 1, i).

With the purpose of discovering isostructural compounds we have synthesized samples with the $RE_{11}Zn_{35-45}Al_{54-44}$ composition (RE = Y, Dy-Tm, Lu). X-ray diffraction analysis of these samples showed the formation of the ternary compounds. Their diffraction patterns were indexed with a tetragonal unit cell with lattice parameters shown in Table 4. The structures of all $RE(Zn,Al)_8$ compounds have been refined with the model of the $HoZn_5Al_3$ structure using X-ray powder diffraction analysis (Table 5). As

Atoms–	CN	Y	Dy	Ho*	Er	Tm	Yb	Lu
*RE*1–4T4	20	3.174(2)	3.178(2)	3.175(1)	3.161(3)	3.153(2)	3.195(2)	3.159(2)
–4T2		3.278(2)	3.265(2)	3.2605(9)	3.267(3)	3.257(3)	3.319(2)	3.253(3)
–4T3		3.299(3)	3.265(5)	3.258(2)	3.249(8)	3.252(5)	3.280(5)	3.263(4)
–8T5		3.476(2)	3.473(2)	3.475(1)	3.471(4)	3.463(2)	3.502(2)	3.464(2)
*RE*2–4T3	16	3.028(4)	3.047(5)	3.059(2)	3.034(8)	3.014(6)	3.111(5)	2.993(5)
–4T5		3.070(2)	3.087(3)	3.052(1)	3.039(5)	3.050(5)	3.030(2)	3.019(3)
–4T1		3.0877(4)	3.0725(3)	3.0753(3)	3.0722(5)	3.0654(8)	3.1305(3)	3.0647(3)
–4T4		3.107(2)	3.099(2)	3.0936(9)	3.085(4)	3.094(3)	3.110(2)	3.068(3)
T1–4T4	12	2.659(9)	2.626(1)	2.619(1)	2.609(2)	2.610(1)	2.6263(9)	2.593(1)
–4T3		2.815(2)	2.835(3)	2.827(1)	2.821(5)	2.801(3)	2.813(3)	2.786(3)
–2T5		2.953(2)	3.005(3)	2.992(1)	2.960(5)	2.957(3)	2.871(2)	2.933(3)
–2*RE*2		3.0877(4)	3.0725(3)	3.0753(3)	3.0722(5)	3.0654(8)	3.1305(3)	3.0647(3)
T2–2T5	10	2.579(2)	2.602(3)	2.599(1)	2.611(5)	2.589(3)	2.580(2)	2.592(3)
–2T2		2.601(3)	2.598(3)	2.610(1)	2.580(4)	2.592(4)	2.594(3)	2.595(4)
–4T3		2.745(3)	2.734(4)	2.733(2)	2.704(7)	2.728(5)	2.763(4)	2.725(4)
–2*RE*1		3.278(2)	3.265(2)	3.2605(9)	3.267(3)	3.257(1)	3.1305(3)	3.253(3)
T3–2T4	13	2.734(3)	2.715(5)	2.709(2)	2.724(7)	2.696(5)	2.721(4)	2.715(4)
–2T2		2.745(3)	2.734(4)	2.733(2)	2.704(7)	2.728(5)	2.763(4)	2.725(4)
–2T3		2.783(3)	2.805(5)	2.810(2)	2.790(8)	2.806(5)	2.882(4)	2.782(4)
–2T1		2.815(2)	2.835(3)	2.827(1)	2.821(5)	2.801(3)	2.813(3)	2.786(3)
–1*RE*2		3.028(4)	3.047(5)	3.059(2)	3.034(8)	3.014(6)	3.111(5)	2.993(5)
–1T4		3.206(4)	3.254(5)	3.229(2)	3.208(9)	3.184(5)	3.127(5)	3.140(5)
–2T5		3.148(2)	3.171(3)	3.172(1)	3.164(5)	3.156(3)	3.092(3)	3.161(3)
–1*RE*1		3.299(3)	3.265(2)	3.258(2)	3.249(8)	3.252(5)	3.280(5)	3.263(4)
T4–2T1	12	2.626(1)	2.626(1)	2.6194(6)	2.609(2)	2.610(1)	2.6263(9)	2.593(1)
–1T4		2.575(2)	2.590(3)	2.578(1)	2.590(5)	2.563(4)	2.604(3)	2.596(4)
–2T5		2.644(2)	2.643(3)	2.645(1)	2.631(5)	2.634(3)	2.645(2)	2.619(3)
–2T3		2.734(3)	2.715(5)	2.709(2)	2.724(7)	2.696(5)	2.721(4)	2.715(4)
–2T4		3.053(2)	3.095(3)	3.066(1)	3.046(4)	3.037(2)	2.998(2)	3.016(3)
–1*RE*2		3.107(2)	3.099(2)	3.0936(8)	3.085(4)	3.094(3)	3.110(2)	3.068(3)
–1T3		3.206(4)	3.254(5)	3.229(2)	3.208(9)	3.184(5)	3.127(5)	3.140(5)
–1*RE*1		3.174(2)	3.171(3)	3.1754(9)	3.161(3)	3.153(2)	3.195(2)	3.159(2)
T5–1T2	12(13**)	2.579(2)	2.602(3)	2.599(1)	2.611(5)	2.589(3)	2.580(2)	2.592(3)
–2T4		2.644(2)	2.643(3)	2.645(1)	2.631(5)	2.634(3)	2.645(2)	2.619(3)
–1T5		2.691(3)	2.659(4)	2.661(2)	2.657(7)	2.653(5)	2.772(2)	2.662(4)
–2T5		2.905(2)	2.828(3)	2.818(1)	2.823(5)	2.831(2)	3.033(3)	2.821(3)
–1T1		2.953(2)	3.005(3)	2.992(1)	2.960(5)	2.957(3)	2.871(2)	2.93393)
–1*RE*2		3.070(2)	3.087(3)	3.052(1)	3.039(5)	3.050(5)	3.030(2)	3.019(3)
–2T3		3.148(2)	3.171(3)	3.172(1)	3.164(5)	3.156(3)	3.092(3)	3.161(3)
–2*RE*1		3.476(2)	3.473(2)	3.475(1)	3.471(4)	3.463(2)	3.502(2)	3.464(2)
–1T6							2.553(2)	
T6–8T5	8**						2.553(2)	

Table 6. Interatomic distances (δ, Å) and coordination numbers (CN) of atoms in the *RE*(Zn,Al)$_8$ and $Yb_4Zn_{20.3}Al_{12.7}$ structures.

* Single crystal data; ** only for $Yb_4Zn_{20.3}Al_{12.7}$.

one can see from Table 4, the Zn content in the compounds grows up in the Dy(Zn,Al)$_8$ - Lu(Zn,Al)$_8$ line. This could indicate some homogeneity ranges for these compounds, but to determine their exact extent additional investigations are required.

The diffraction pattern of Yb(Zn,Al)$_8$ was also well indexed with a tetragonal unit cell with slightly bigger lattice parameters (Table 4), but the intensity refinement did not yield satisfactory results ($R_I \approx 0.15$). On the difference Fourier synthesis an additional electron density maximum, which coincides with the center of the vacant hexahedron, typical for the $HoZn_5Al_3$ structure, was observed. This allowed us to suppose that the deformed hexahedron in the Yb(Zn,Al)$_8$ structure may be centered by additional atoms. Occupancy of the 2*b* position with a statistical mixture of Zn and Al reduces the value of R_I to 0.087, which confirms that the $Yb_4Zn_{20.3}Al_{12.7}$ structure belongs to the $Yb_8Cu_{17}Al_{49}$ type [15], closely related with the $HoZn_5Al_3$ structure. It is noteworthy that in the $Yb_4Zn_{20.3}Al_{12.7}$ structure the deformation of the hexahedron is stronger than in the Ho(Zn,Al)$_8$ structure. The atomic coordinates in the structure of $Yb_4Zn_{20.3}Al_{12.7}$ are shown in Table 5. Interatomic distances of all investigated structures are shown in Table 6. They are in good agreement with the sum of the atomic radii of the elements.

Discussion

The new $HoZn_5Al_3$ structure type is closely related with the $Yb_8Cu_{17}Al_{49}$ structure type. The main difference is the existence of distorted vacant hexahedra in the $HoZn_5Al_3$ structure and of deformed Cu centered hexahedra in the $Yb_8Cu_{17}Al_{49}$ structure. Thus, the $Yb_8Cu_{17}Al_{49}$ structure is a filled-up version of the $HoZn_5Al_3$ type. This difference has a considerable influence on the way the coordination polyhedra (CP) of the *RE*2 atoms are connected. In the $Yb_8Cu_{17}Al_{49}$ structure [***RE***16T] polyhedra are connected by the [***T***8T] hexahedron only in the 0*z* direction, and in the 0*x* direction they are connected by the T6 atom, placed in the 2*b* position (Fig. 2a). In the $HoZn_5Al_3$ structure the connection of the *RE* atoms in both directions is by means of the empty deformed hexahedron (Fig. 2b).

The CP of the *RE* atoms are similar to those of the larger atoms in the structures of other intermetallic compounds. Specifically, the Ho1 coordination polyhedron is similar to that of Th in the $ThMn_{12}$ type structure and to the CP of the Ba atom in the $BaHg_{11}$ type structure. The common feature of the $HoZn_5Al_3$ and $BaHg_{11}$ structure types is also the existence of vacant hexahedra in both structures. A centered hexahedron is the CP of the Ru2 atom in the $Y_3Ru_4Al_{12}$ [16] structure. The coordination polyhedra of the *T*1 and *T*4 atoms are distorted icosahedra (Figs 1d and g). Thus, the $HoZn_5Al_3$ type structure is similar to a large group of structures of intermetallic compounds

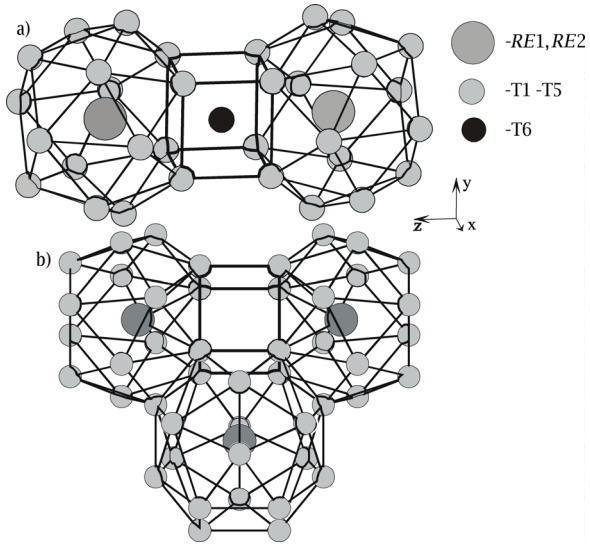

Fig. 2. The connection of the coordination polyhedra of *RE*2 atoms in the $Yb_8(Zn,Al)_{66}$ (a) and $HoZn_5Al_3$ (b) structures.

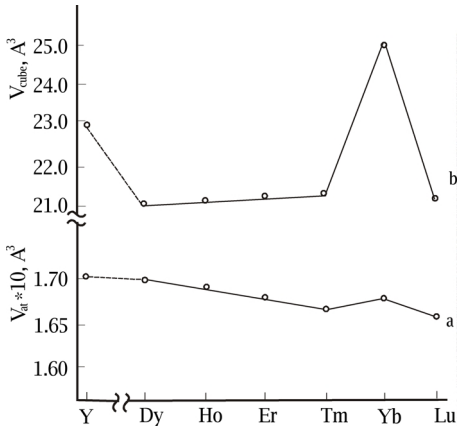

Fig. 3. The relation between atomic volume (a), distorted cubes [8T] volume (b) and the atomic number of *RE* atoms in a number of $RE(Zn,Al)_8$ or $Yb_8(Zn,Al)_{66}$ compounds.

with icosahedra as the main CP of the smaller atoms: the $CaCu_5$ and the Th_2Ni_{17}-structure types, the Laves phases, *etc.* [17].

With the purpose of determining the reasons for the filling of the deformed hexahedra in the $Yb_4Zn_{20.3}Al_{12.7}$ structure we calculated the volumes of vacant and filled hexahedra in all investigated structures taking into consideration the values of the lattice parameters and the refined atomic coordinates. As one can see from Fig. 3b, the hexahedron volume in the $Yb_4Zn_{20.3}Al_{12.7}$ structure is much larger than the volume of the same hexahedra in other structures. If one admits that this hexahedron is filled by the Zn and Al atoms in the ratio of 1 : 1 and takes the averaged values of the atomic radii of Zn and Al ($r_{Zn} = 1.332$ Å, $r_{Al} = 1.431$ Å [18]), then a *T* atom with the averaged radius 1.382 Å could sufficiently easily fill up the hexahedron in the $Yb_4Zn_{20.3}Al_{12.7}$ structure. But for the vacant hexahedra in the $RE(Zn,Al)_8$ structures it would be too big. Thus one can believe that the reason why the inclusion structure to the $HoZn_5Al_3$ structure type exists is the sterie factor.

The analysis of interatomic distances shows that in all investigated structures no significant reduction of the *RE*-*T* and *T*-*T* distances in relation to the radii of the respective atoms is observed. These reductions are not larger then 5 – 7%, which is usual in the structures of intermetallic compounds.

In order to receive information about the valence state of the *RE* atoms in the new compounds the average atomic volume $V_{av} = \frac{a^2c}{N}$, (N – number of atoms per unit cell) was calculated. As one can

see from Fig. 3a, a slight maximum, which could indicate an intermediate valence of the Yb atoms (Yb^{+2}-Yb^{+3}) in the structure of $Yb_4Zn_{20.3}Al_{12.7}$, is observed.

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