



Crystal structure of UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir) phases

M. Daszkiewicz, P. Swatek, D. Kaczorowski*

Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocław, Poland

ARTICLE INFO

Article history:

Received 21 October 2011

Received in revised form

22 November 2011

Accepted 24 November 2011

Available online 2 December 2011

Keywords:

Crystal structure

Uranium alloys

Zinc-rich compounds

ABSTRACT

The crystal structures of the UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir) intermetallics have been refined from the single-crystal X-ray diffraction data. The compounds crystallize with a face-centered cubic structure of the $Mg_3Cr_2Al_{18}$ type.

© 2011 Elsevier B.V. All rights reserved.

1. Introduction

The uranium compounds UT_2Zn_{20} (T = d-electron transition metal) have recently been reported to exhibit a variety of intriguing physical phenomena, which arise due to strong electronic correlations [1–7]. The primary findings made for the phases with T = Co, Rh and Ir [1–3] have stimulated further comprehensive investigations on high-quality single crystals of these ternaries and also those with T = Fe and Ru [4–7]. Though all the hitherto identified UT_2Zn_{20} compounds were claimed to form with a cubic unit cell of the $Mg_3Cr_2Al_{18}$ type, up to date no precise information on their crystal structures has been available in the literature. The only exception is UIr_2Zn_{20} , which crystal structure was refined down to the residual $R_{wp} = 13.04\%$ from the neutron powder diffraction data taken at 0.6 K [1].

In the present paper we report on the structural studies carried out on single crystals of the UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir) compounds. The refined crystal structures are described with regard to the coordination polyhedra of the particular atoms. Moreover, some future prospects are outlined of preparing novel derivatives of the UT_2Zn_{20} phases.

2. Experimental

Single crystals of UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir) were synthesized in Zn flux [7]. Small specimens suitable for X-ray diffraction data collection were selected from each sample. Their isometric shape and size of about ~0.05 mm in length was a compromise between large absorption coefficient (the elemental constituents have large atomic scattering cross sections) and intensity of the measured diffraction

spots, together with reasonably large signal-to-noise ratios. Each crystal was glued on a thin glass fibre using epoxy resin.

The X-ray diffraction intensities were collected on a KUMA Diffraction KM-4 four-circle diffractometer equipped with a CCD detector, using graphite-monochromatized $MoK\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). The raw data were treated with the CrysAlis Data Reduction Program (version 1.172.32.6) taking into account an absorption correction. The measured intensities were corrected for Lorentz and polarization effects. The crystal structures were solved by direct methods and refined by a full-matrix least-squares method using SHELXL-97 program [8]. The experimental and structure refinement details are collected in Table 1.

3. Results and discussion

All the UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir) ternaries studied were found to crystallize in a face-centered cubic cell, space group $Fd\bar{3}m$, $Z = 8$, structure type $Mg_3Cr_2Al_{18}$. (Tables 1–4). The lattice parameters and the interatomic distances change in accord with the covalent radius of the T element. However, the interatomic distances are distinctly larger than the sums of the respective covalent radii [9].

In the unit cell, the uranium atom occupies a single position of high-symmetry, namely $\bar{4}3m$ (8a Wyckoff position), and is surrounded by as many as 16 zinc atoms (see Fig. 1a). This coordination sphere can be described as a Friauf-type icosaoctahedron [10,11]. In turn, the transition metal atom is located at a site with $\bar{3}m$ point site symmetry. Twelve zinc neighbours form a distorted icosahedral surrounding of Frank-Kasper type [12,13]. The zinc atoms in UT_2Zn_{20} have similar coordination spheres, which can be described as hexagonal (for Zn1) or pentagonal prisms (for Zn2 and Zn3) with two additional atoms located near the prism bases (cf. Fig. 1a). Since the Zn2 atom occupies the site of higher symmetry ($2mm$) than the Zn3 atom ($.m$), the bi-capped pentagonal prism of the latter atom is

* Corresponding author. Tel.: +48 71 34 350 21; fax: +48 71 34 410 19.
E-mail address: D.Kaczorowski@int.pan.wroc.pl (D. Kaczorowski).

Table 1
Crystal data and structure refinement details for UT_2Zn_{20} (R = Fe, Co, Ru, Rh, and Ir).

Chemical formula	UFe ₂ Zn ₂₀	UCo ₂ Zn ₂₀	URu ₂ Zn ₂₀	URh ₂ Zn ₂₀	UIr ₂ Zn ₂₀
M_r	1657.13	1663.29	1747.57	1751.25	1929.83
a (Å)	14.110 (1)	14.056 (2)	14.227 (1)	14.204 (1)	14.208 (1)
V (Å ³)	2809.3(3)	2777.2 (6)	2879.8 (4)	2865.6 (3)	2868.1 (4)
μ (mm ⁻¹)	46.84	47.68	45.78	46.20	62.40
Crystal size (mm)	0.05 × 0.05 × 0.04	0.05 × 0.04 × 0.03	0.05 × 0.05 × 0.04	0.06 × 0.05 × 0.04	0.05 × 0.04 × 0.04
T_{min}, T_{max}	0.254, 0.416	0.120, 0.375	0.210, 0.439	0.176, 0.410	0.254, 0.416
Z , calculated density (g cm ⁻³)	8, 7.836	7.956	8.061	8.118	8.938
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9102, 180, 179	8113, 170, 167	7603, 183, 179	6025, 190, 188	9097, 176, 176
R_{int}	0.116	0.170	0.134	0.079	0.142
θ range (°)	2.5–27.0	2.5–26.7	4.1–27.1	4.1–27.4	4.1–26.7
Range of h, k, l	$h = -18 \rightarrow 18$ $k = -18 \rightarrow 18$ $l = -18 \rightarrow 18$	$h = -17 \rightarrow 17$ $k = -17 \rightarrow 17$ $l = -17 \rightarrow 17$	$h = -17 \rightarrow 18$ $k = -18 \rightarrow 18$ $l = -18 \rightarrow 18$	$h = -17 \rightarrow 18$ $k = -18 \rightarrow 18$ $l = -17 \rightarrow 18$	$h = -17 \rightarrow 17$ $k = -17 \rightarrow 17$ $l = -17 \rightarrow 17$
$R[F^2 > 2s(F^2)], wR(F^2), S$	0.047, 0.115, 1.54	0.049, 0.112, 1.50	0.038, 0.086, 1.31	0.038, 0.070, 1.36	0.038, 0.092, 1.33
Data/restraints/parameters	180/0/17	170/0/17	183/0/17	190/0/16	176/0/17
Extinction coefficient	0.00019 (5)	0.00076 (11)	0.00011 (3)	None	0.00019 (3)
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	1.64, -0.93	1.62, -1.06	1.53, -1.13	1.20, -1.40	1.86, -1.38

more distorted than that of the former one. The point site symmetry of the Zn1 atom is $\bar{3}m$, i.e. same as that of the T atom.

The coordination spheres of the uranium and T atoms can be considered as assemblies of smaller polyhedra. As demonstrated in Fig. 1b, four nearest Zn1 neighbours of the U atom form a tetrahedron, whereas twelve Zn3 atoms form a truncated tetrahedron. Together, these two polygons result in an icosahedral arrangement with the coordination number CN = 16. In the case of T atom, its coordination sphere with CN = 12 is constructed by the Zn2 and Zn3 atoms transformed by a $\bar{3}$ rotoinversion axis (see Fig. 1b). For each UT_2Zn_{20} compound, the T–Zn2 interatomic distance is significantly shorter than the T–Zn3 distance. As a result, elongated (Zn2)₆ and compressed (Zn3)₆ trigonal antiprisms are formed along the $\bar{3}$

rotoinversion axis, which jointly outline the icosahedron around the T atom.

Interestingly, in the crystal structure of the UT_2Zn_{20} phases, the [U(Zn1)₄] tetrahedrons are mutually connected by their vertices, which gives rise to the appearance of three-dimensional polymeric network [UZn1]_∞ (marked by red lines in Fig. 2a) (for interpretation of the references to color in this sentence, the reader is referred to the web version of the article). At the same time, each of the four (Zn3)₆ hexagonal faces of the [U(Zn3)₁₂] truncated tetrahedron is a base of the coordination sphere of the Zn1 atom. In consequence, the [UZn1]_∞ lattice appears submerged in the (Zn3)_∞ cages. Besides, the latter cages are connected to the [T(Zn2)₆(Zn3)₆] icosahedra by their vertices.

Table 2
Atomic coordinates and equivalent isotropic displacement parameters for UT_2Zn_{20} (T = Fe, Co, Ru, Rh, and Ir). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms		x	y	z	U _{eq}
UFe ₂ Zn ₂₀					
U	8a	1/8	1/8	1/8	0.0056(7)
Fe	16d	1/2	1/2	1/2	0.0059(12)
Zn1	16c	0	0	0	0.0205(12)
Zn2	48f	0.48952(19)	1/8	1/8	0.0105(7)
Zn3	96g	0.05894(9)	0.05894(9)	0.32593(13)	0.0133(7)
UCo ₂ Zn ₂₀					
U	8a	1/8	1/8	1/8	0.0061(8)
Co	16d	1/2	1/2	1/2	0.0080(13)
Zn1	16c	0	0	0	0.0250(14)
Zn2	48f	0.4891(2)	1/8	1/8	0.0116(8)
Zn3	96g	0.05908(9)	0.05908(9)	0.32557(14)	0.0135(8)
URu ₂ Zn ₂₀					
U	8a	1/8	1/8	1/8	0.0060(5)
Ru	16d	1/2	1/2	1/2	0.0051(6)
Zn1	16c	0	0	0	0.0185(9)
Zn2	48f	0.48863(15)	1/8	1/8	0.0128(6)
Zn3	96g	0.05932(7)	0.05932(7)	0.32485(10)	0.0134(5)
URh ₂ Zn ₂₀					
U	8a	1/8	1/8	1/8	0.0056(4)
Rh	16d	1/2	1/2	1/2	0.0049(5)
Zn1	16c	0	0	0	0.0188(8)
Zn2	48f	0.48776(13)	1/8	1/8	0.0109(4)
Zn3	96g	0.05978(6)	0.05978(6)	0.32406(8)	0.0129(4)
UIr ₂ Zn ₂₀					
U	8a	1/8	1/8	1/8	0.0070(6)
Ir	16d	1/2	1/2	1/2	0.0066(5)
Zn1	16c	0	0	0	0.0184(12)
Zn2	48f	0.48704(19)	1/8	1/8	0.0119(7)
Zn3	96g	0.05991(9)	0.05991(9)	0.32339(13)	0.0134(6)

Table 3
Anisotropic displacement parameters [\AA^2] for $\text{UT}_2\text{Zn}_{20}$ (T = Fe, Co, Ru, Rh, and Ir).

Atoms	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
UFe₂Zn₂₀						
U	0.0056(7)	0.0056(7)	0.0056(7)	0.00000	0.00000	0.00000
Fe	0.0059(12)	0.0059(12)	0.0059(12)	0.0007(12)	0.0007(12)	0.0007(12)
Zn1	0.0205(12)	0.0205(12)	0.0205(12)	−0.0042(12)	−0.0042(12)	−0.0042(12)
Zn2	0.0108(14)	0.0104(9)	0.0104(9)	0.00000	0.00000	−0.0020(11)
Zn3	0.0152(8)	0.0152(8)	0.0096(11)	−0.0036(8)	−0.0006(5)	−0.0006(5)
UCo₂Zn₂₀						
U	0.0061(8)	0.0061(8)	0.0061(8)	0.00000	0.00000	0.00000
Co	0.0080(13)	0.0080(13)	0.0080(13)	0.0001(12)	0.0001(12)	0.0001(12)
Zn1	0.0250(14)	0.0250(14)	0.0250(14)	−0.0042(14)	−0.0042(14)	−0.0042(14)
Zn2	0.0119(15)	0.0115(10)	0.0115(10)	0.00000	0.00000	−0.0024(12)
Zn3	0.0156(9)	0.0156(9)	0.0093(12)	−0.0030(9)	−0.0010(6)	−0.0010(6)
URu₂Zn₂₀						
U	0.0060(5)	0.0060(5)	0.0060(5)	0.00000	0.00000	0.00000
Ru	0.0051(6)	0.0051(6)	0.0051(6)	0.0003(5)	0.0003(5)	0.0003(5)
Zn1	0.0185(9)	0.0185(9)	0.0185(9)	−0.0049(9)	−0.0049(9)	−0.0049(9)
Zn2	0.0132(11)	0.0126(7)	0.0126(7)	0.00000	0.00000	−0.0024(8)
Zn3	0.0154(6)	0.0154(6)	0.0094(8)	−0.0043(6)	−0.0013(4)	−0.0013(4)
URh₂Zn₂₀						
U	0.0056(4)	0.0056(4)	0.0056(4)	0.00000	0.00000	0.00000
Rh	0.0049(5)	0.0049(5)	0.0049(5)	−0.0005(4)	−0.0005(4)	−0.0005(4)
Zn1	0.0188(8)	0.0188(8)	0.0188(8)	−0.0055(8)	−0.0055(8)	−0.0055(8)
Zn2	0.0105(9)	0.0110(6)	0.0110(6)	0.00000	0.00000	−0.0043(7)
Zn3	0.0153(5)	0.0153(5)	0.0082(7)	−0.0050(5)	−0.0008(3)	−0.0008(3)
UIr₂Zn₂₀						
U	0.0070(6)	0.0070(6)	0.0070(6)	0.00000	0.00000	0.00000
Ir	0.0066(5)	0.0066(5)	0.0066(5)	−0.0004(3)	−0.0004(3)	−0.0004(3)
Zn1	0.0184(12)	0.0184(12)	0.0184(12)	−0.0037(12)	−0.0037(12)	−0.0037(12)
Zn2	0.0123(14)	0.0117(9)	0.0117(9)	0.00000	0.00000	−0.0041(12)
Zn3	0.0155(8)	0.0155(8)	0.0093(11)	−0.0050(8)	−0.0003(6)	−0.0003(6)

4. Future prospects

The available literature data on the $\text{UT}_2\text{Zn}_{20}$ compounds report on interesting physical properties, which are closely related to their crystal structures [1–7]. One may expect that intentional changes in the composition of these alloys would yield some significant modifications in their physical behaviour. For example one may attempt to partially fill the voids, which exist in the crystal lattice

of the parent material. As discussed above, the crystal structure of the $\text{UT}_2\text{Zn}_{20}$ ternaries can be depicted as a vertex-sharing network of the $[\text{U}(\text{Zn}_1)_4(\text{Zn}_3)_{12}]$ and $[\text{T}(\text{Zn}_2)_6(\text{Zn}_3)_6]$ polyhedra (Fig. 2; see also Ref. [14]). Such a description of the crystal lattice implies the appearance of some voids, which eventually could be filled by small enough guest atoms [15–17]. As a result, new quaternary compounds of the same $Fd\bar{3}m$ symmetry like the parent structure can be obtained. Obviously, general chemical formula of such a quaternary

Table 4
Interatomic distances in $\text{UT}_2\text{Zn}_{20}$ (T = Fe, Co, Ru, Rh, and Ir).

	C.N.	UFe ₂ Zn ₂₀	UCo ₂ Zn ₂₀	URu ₂ Zn ₂₀	URh ₂ Zn ₂₀	UIr ₂ Zn ₂₀
U						
4Zn1	16	3.0549(2)	3.0433(4)	3.0803(2)	3.0752(2)	3.0761(3)
12Zn3		3.1266(19)	3.109(2)	3.1355(15)	3.1162(12)	3.1074(19)
T						
6Zn2	12	2.4987(2)	2.4896(3)	2.5203(2)	2.5169(2)	2.5184(3)
6Zn3		2.7233(19)	2.719(2)	2.7630(15)	2.7726(12)	2.7830(19)
Zn1						
2U	14	3.0549(2)	3.0433(4)	3.0803(2)	3.0752(2)	3.0761(3)
12Zn3		3.0179(10)	3.0033(12)	3.0342(8)	3.0212(7)	3.0177(10)
Zn2						
2T	12	2.4987(2)	2.4896(3)	2.5203(2)	2.5169(2)	2.5184(3)
4Zn2		2.703(4)	2.702(4)	2.744(3)	2.757(3)	2.772(4)
2Zn3		2.658(3)	2.646(3)	2.679(2)	2.669(2)	2.668(3)
4Zn3		2.7718(17)	2.7634(18)	2.8019(14)	2.8050(12)	2.8079(17)
Zn3						
1U	12	3.1266(19)	3.109(2)	3.1355(15)	3.1162(12)	3.1074(19)
1T		2.7233(19)	2.719(2)	2.7630(15)	2.7726(12)	2.7830(19)
2Zn1		3.0178(10)	3.0033(12)	3.0342(8)	3.0212(7)	3.0177(10)
1Zn2		2.658(3)	2.646(3)	2.679(2)	2.669(2)	2.668(3)
2Zn2		2.7718(17)	2.7634(18)	2.8019(14)	2.8050(12)	2.8079(17)
1Zn3		2.637(3)	2.621(4)	2.643(3)	2.620(2)	2.616(4)
2Zn3		2.691(3)	2.677(3)	2.699(2)	2.688(2)	2.678(3)
2Zn3		2.836(2)	2.831(2)	2.8776(16)	2.8859(14)	2.898(2)

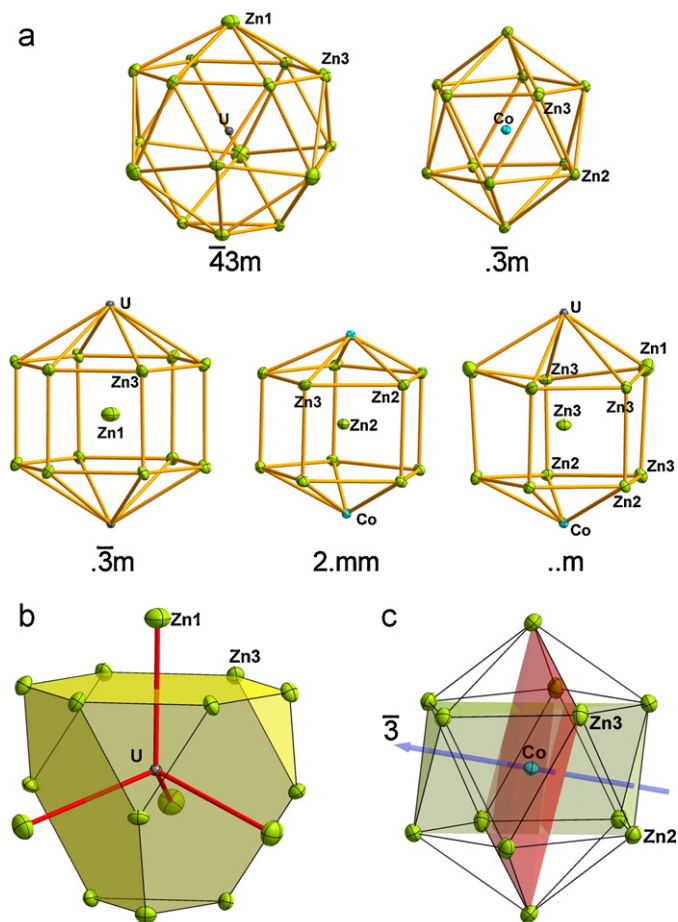


Fig. 1. (a) Coordination spheres of all the atoms in UCo_2Zn_{20} . (b) Icosaohedral coordination sphere of the uranium atom shown as an assembly of $[U(Zn1)_4]$ tetrahedron and $[U(Zn3)_{12}]$ truncated tetrahedron. (c) Icosaohedral coordination of the cobalt atom presented as a combination of two trigonal antiprisms created by the Zn2 and Zn3 atoms.

phase depends on the void to be occupied. The voids available in the UT_2Zn_{20} unit cell are those at the $\bar{4}3m$ site (x, y, z : $3/8, 3/8, 3/8$; 8b Wyckoff position; see Fig. 2), the $\bar{3}m$ site (x, y, z : $0.28275, 0.28275, 0.28275$; 32e Wyckoff position) and the $..m$ site (x, y, z : $0.31525, 0.31525, 0.12868$; 96g Wyckoff position). As the distance between the geometry centers of these voids and the adjacent zinc atoms is approximately 1.9 \AA , hypothetically they might be occupied for example by carbon or boron atoms, hence leading to the formation of the novel compounds, e.g., $UT_2Zn_{20}C$, $UT_2Zn_{20}C_4$, $UT_2Zn_{20}C_{12}$, $UT_2Zn_{20}C_5$, $UT_2Zn_{20}C_{13}$ and/or $UT_2Zn_{20}C_{17}$.

Another route of synthesizing novel phases is to substitute some of the atoms in the parent material [15–17]. For example, in the UT_2Zn_{20} compounds, one may attempt to replace part of the Zn atoms by indium atoms. Because the Zn constituents occupy three independent Wyckoff positions, i.e. 16c, 48f and 96g, one can speculate on the existence of $UT_2Zn_{18}In_2$, $UT_2Zn_{14}In_6$ and $UT_2Zn_8In_{12}$, when one of these sites is entirely substituted by the In atoms, respectively. In case of full replacement on two Wyckoff positions, $UT_2Zn_{12}In_8$ (16c+48f), $UT_2Zn_6In_{14}$ (16c+96g) and $UT_2Zn_2In_{18}$ (48f+96g) might be formed.

Despite simplicity of the above considerations, similar approach has already been proven to be a powerful method for designing “new compounds with predictable structure and with new (or predictable) properties” [17]. In the present context, it should be recalled that recently a series of non-stoichiometric alloys $YMn_{2+\delta}Zn_{20-x-\delta}In_x$ ($x=2.96\text{--}3.99$, $\delta=0.44\text{--}1.24$) was synthesized

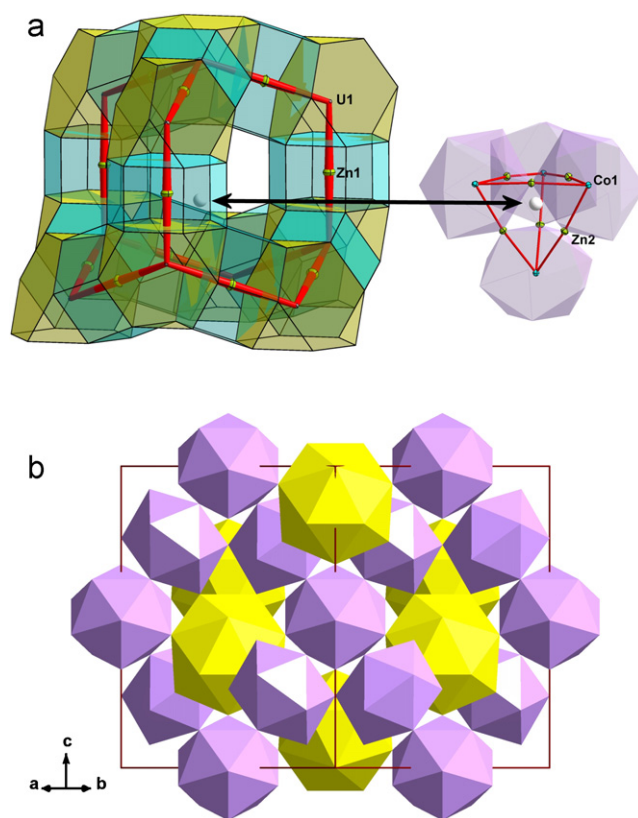


Fig. 2. (a) Three-dimensional polymeric network of $[UZn1]_{\infty}$ polyhedra submerged in $(Zn3)_{\infty}$ cages (left) and fragment of vertex-sharing lattice constructed by $[Co(Zn2)_6(Zn3)_6]$ icosahedra (right). Exemplary void of $\bar{4}3m$ point symmetry is indicated as a white sphere. (b) Unit cell viewed down the $[110]$ crystallographic axis.

[18], which derives from the hypothetical YMn_2Zn_{20} compound. The chemical formula of these materials can be written as $YMn_2(In_{2.96}Mn_{0.44}Zn_{16.60})\text{--}YMn_2(In_{3.99}Mn_{1.24}Zn_{14.77})$ to emphasize the fact that they arise by replacement of the Zn1 atoms at the 16c position and the Zn3 atoms at the 96g position by the In atoms and a mixture of Mn/In atoms, respectively. Worth mentioning are also two series of rare-earth-based compounds $REMn_2Zn_{20-x}In_x$ and $REMn_2Zn_{20-x}Al_x$ (RE = Ce, Pr, Nd, Sm, Gd, Dy, Er, Yb), in which Zn atoms are partially substituted by In or Al atoms [19]. Interestingly, in the former alloys preferential occupation of the Zn sites was observed, whereas statistical distribution of the substituent was established for the latter one.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jallcom.2011.11.124.

References

- [1] E.D. Bauer, A.D. Christianson, J.S. Gardner, V.A. Sidorom, J.D. Thompson, J.L. Sarrao, M.F. Hundley, Phys. Rev. B 74 (2006) 155118.
- [2] E.D. Bauer, J.D. Thompson, J.L. Sarrao, M.F. Hundley, J. Magn. Magn. Mater. 310 (2007) 449.
- [3] E.D. Bauer, C. Wang, V.R. Fanelli, J.M. Lawrence, E.A. Goremychkin, N.R. de Souza, F. Ronning, J.D. Thompson, A.V. Silhanek, V. Vildosola, A.M. Lobos, A.A. Aligia, S. Bobev, J.L. Sarrao, Phys. Rev. B 78 (2008) 115120.
- [4] C.H. Wang, A.D. Christianson, J.M. Lawrence, E.D. Bauer, E.A. Goremychkin, A.I. Kolesnikov, F. Trouw, F. Ronning, J.D. Thompson, M.D. Lumsden, N. Ni, E.D. Mun, S. Jia, P.C. Canfield, Y. Qiu, J.R.D. Copley, Phys. Rev. B 82 (2010) 184407.
- [5] P. Swatek, D. Kaczorowski, J. Phys. Soc. Jpn. 80 (2011) SA106.
- [6] P. Swatek, D. Kaczorowski, J. Phys.: Condensed Matter 23 (2011) 466001.
- [7] P.C. Canfield, Z. Fisk, Philos. Mag. B 65 (1992) 1117.
- [8] G.M. Sheldrick, Acta Crystallogr. A 64 (2008) 112.
- [9] P. Pykkö, M. Atsumi, Chem. Eur. J. 15 (2009) 186.

- [10] I.B. Friauf, J. Am. Chem. Soc. 49 (1927) 3107.
[11] J.B. Friauf, Phys. Rev. 29 (1927) 35.
[12] S. Samson, Acta Crystallogr. 11 (1958) 851.
[13] M.A. Ebner, K.-J. Range, J. Alloys Compd. 236 (1996) 50.
[14] T. Nasch, W. Jeitschko, U. Ch Rodewald, Z. Naturforsch. 52b (1997) 1023.
[15] L.D. Gulay, M. Daszkiewicz, V. Ya Shemet, Z. Anorg. Allg. Chem. 634 (2008) 1887.
[16] L.D. Gulay, M. Daszkiewicz, M.R. Huch, J. Solid State Chem. 181 (2008) 2626.
[17] L.D. Gulay, M. Daszkiewicz, in: K.A. Gschneidner Jr., J.-C.G. Bünzli, V.K. Pecharsky (Eds.), Handbook on the Physics and Chemistry of Rare Earths, vol. 41, 2011, Ch. 250.
[18] Y. Okamoto, T. Shimizu, J. Yamaura, Y. Kiuchi, Z. Hiroi, J. Phys. Soc. Jpn. 79 (2010) 093712.
[19] E.M. Benbow, S.E. Lattner, J. Solid State Chem. 179 (2006) 3989.