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Letter

New ternary CeScSi-type RZrSb compounds (R=Y, Gd–Tm, Lu)

A.V. Morozkin*, I.A. Sviridov

Department of Chemistry, Moscow Lomonosov State University, Leninskie Gory V-234, GSP-3, Moscow 119899, Russia

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Abstract

Investigations made by powder X-ray diffraction on eight new ternary RZrSb compounds (R=Y, Gd–Tm, Lu) are reported. The YZrSb (a=0.4245(1) nm, c=1.6306(3) nm), GdZrSb (a=0.4261(1) nm, c=1.6455(2) nm), TbZrSb (a=0.4251(1) nm, c=1.6380(2) nm), DyZrSb (a=0.4240(1) nm, c=1.6349(2) nm), HoZrSb (a=0.4201(1) nm, c=1.6143(2) nm), ErZrSb (a=0.4204(1) nm, c=1.6159(2) nm), TmZrSb (a=0.4174(1) nm, c=1.5997(2) nm) and LuZrSb (a=0.4178(1) nm, c=1.5952(3) nm) crystallize in the tetragonal CeScSi-type structure (space group *I4/mmm*).

Keywords: Rare earth compounds; Crystal structure; X-ray diffraction

In the present investigation the RZrSb compounds were made in an electric arc furnace under an argon atmosphere using a non-consumable tungsten electrode and water-cooled copper tray. Antimony (purity: 99.99%), yttrium

Table 1
Lattice parameters a, c (nm), c/a, unit cell volume V (nm^3) and atomic position parameters of RZrSb compounds (R=Y, Gd–Tm, Lu) (the reliability factors R_F are given in %)

Compound	a	c	c/a	V	Z_R	Z_{Sb}	R_F
YZrSb	0.4245(1)	1.6306(3)	3.8415	0.2938	0.335(2)	0.143(3)	5.3
GdZrSb	0.4261(1)	1.6455(2)	3.8618	0.2988	0.324(2)	0.134(2)	6.0
TbZrSb	0.4251(1)	1.6380(2)	3.8534	0.2960	0.325(2)	0.136(2)	4.4
DyZrSb	0.4240(1)	1.6349(2)	3.8556	0.2940	0.325(2)	0.139(2)	5.7
HoZrSb	0.4201(1)	1.6143(2)	3.8430	0.2848	0.322(2)	0.137(3)	6.8
ErZrSb	0.4204(1)	1.6159(2)	3.8435	0.2856	0.326(2)	0.141(2)	3.5
TmZrSb	0.4174(1)	1.5997(2)	3.8330	0.2787	0.322(2)	0.140(2)	3.1
LuZrSb	0.4178(1)	1.5952(3)	3.8177	0.2785	0.324(2)	0.140(2)	5.2

Table 2
Interatomic distances in RZrSb compounds $D\pm10^{-4}$–10^{-3} nm

R		Y	Gd	Tb	Dy	Ho	Er	Tm	Lu
R	–4Sb	0.302	0.309	0.307	0.306	0.304	0.302	0.301	0.301
	–1Sb	0.313	0.313	0.310	0.304	0.299	0.299	0.291	0.294
	–4Zr	0.343	0.360	0.357	0.356	0.356	0.351	0.353	0.350
	–4R	0.409	0.387	0.388	0.387	0.377	0.386	0.374	0.378
Zr	–4Zr	0.300	0.301	0.301	0.300	0.297	0.297	0.295	0.296
	–4Sb	0.315	0.307	0.308	0.311	0.305	0.310	0.306	0.306
	–4R	0.343	0.360	0.357	0.356	0.356	0.351	0.353	0.350
Sb	–4Zr	0.315	0.307	0.308	0.304	0.305	0.310	0.350	0.306
	–4R	0.302	0.309	0.307	0.306	0.304	0.302	0.301	0.301
	–1R	0.313	0.313	0.310	0.311	0.299	0.299	0.293	0.294

*Corresponding author.
E-mail address: morozkin@general.chem.msu.ru (A.V. Morozkin).

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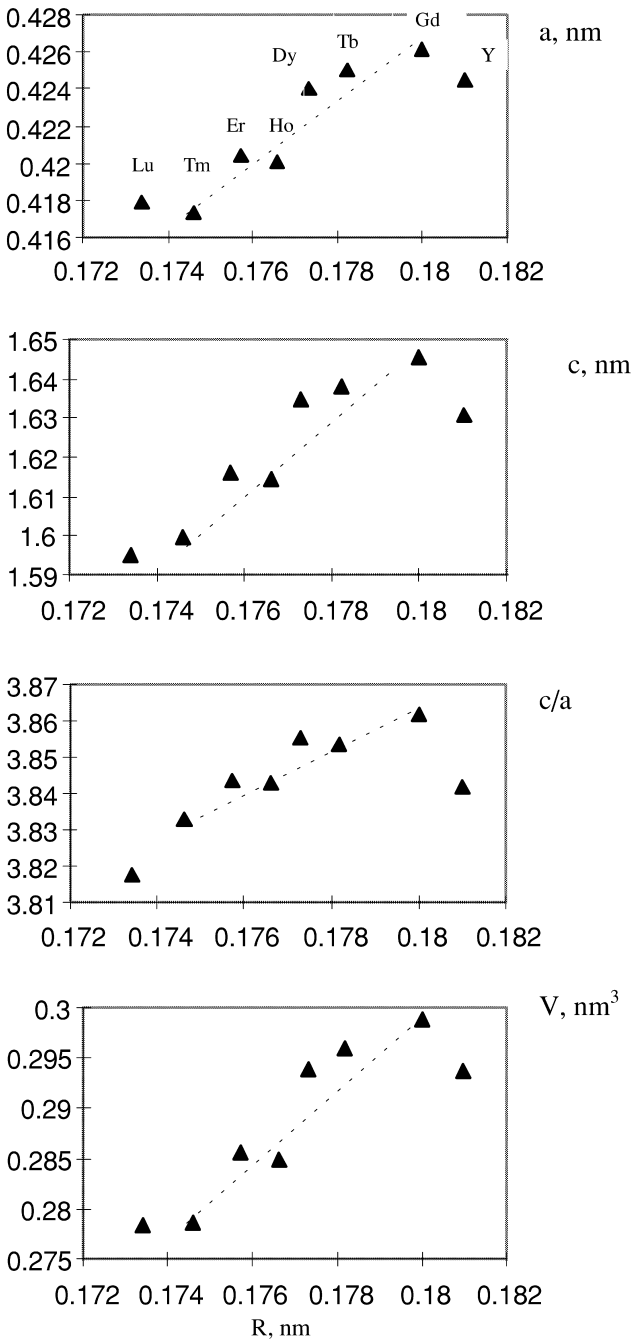

Fig. 1. The lattice parameters of RZrSb compounds vs. the atomic radii of the rare earths.

(purity: 99.98%), gadolinium (purity: 99.98%), terbium (purity: 99.99%), dysprosium (purity: 99.99%), holmium (purity: 99.98%), erbium (purity: 99.99%), thulium (purity: 99.99%), lutetium (purity: 99.99%) and zirconium (purity: 99.99%) were used as the starting components. Titanium was used as a getter during melting.

X-ray powder diffraction analyses were obtained on an DRON-3.0 (Cu Kα radiation, 2θ=20–70°, step: 0.05°, 1002 points). The obtained diffractograms were identified and intensity calculations were made in the isotropic approximation using the Rietan programs [1].

Analysis of the powder X-ray diffractograms shows that the new ternary RZrSb compounds (R=Y, Gd–Tm, Lu) crystallize in the tetragonal CeScSi-type structure (*I4*/*mmm*). In the CeScSi-type structure the rare-earth and antimony atoms occupy the 4(*e*) site (0, 0, *z*) and the Zr atoms occupy the special position 4(*c*) (0, 1/2, 0) [2]. The lattice parameters of the compounds, refined at room temperature, the atomic position parameters of the compounds and the reliability factors R_F resulting from the refinements are given in Table 1. Interatomic distances in RZrSb compounds are given in Table 2.

The cell parameters of RZrSb compounds are proportional to the rare earths atomic radii [3], as a rule, excepting the YZrSb compound (Fig. 1).

Acknowledgements

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