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## Structure Reports

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Zr<sub>3</sub>NiSb<sub>7</sub>: a new antimony-enriched ZrSb<sub>2</sub> derivativeV. Romaka,<sup>a\*</sup> A. Tkachuk<sup>b</sup> and L. Romaka<sup>a</sup><sup>a</sup>Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya Street 6, 79005 Lviv, Ukraine, and <sup>b</sup>Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{Sb-Ni}) = 0.001$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.054; data-to-parameter ratio = 25.3.

Single crystals of trizirconium nickel heptaantimonide were synthesized from the constituent elements by arc-melting. The compound crystallizes in a unique structure type and belongs to the family of two-layer structures. All crystallographically unique atoms ( $3 \times \text{Zr}$ ,  $1 \times \text{Ni}$  and  $7 \times \text{Sb}$ ) are located at sites with  $m$  symmetry. The structure contains 'Zr<sub>2</sub>Ni<sub>2</sub>Sb<sub>5</sub>' and 'Zr<sub>4</sub>Sb<sub>9</sub>' fragments and might be described as a new ZrSb<sub>2</sub> derivative with a high Sb content.

## Related literature

The structure of ZrSb<sub>2</sub> was described by Garcia & Corbett (1988). For related antimonides, see: Romaka *et al.* (2007); Tkachuk *et al.* (2007). For related literature, see: Emsley (1991).

## Experimental

## Crystal data

Zr<sub>3</sub>NiSb<sub>7</sub>  $V = 990.22$  (18) Å<sup>3</sup>  
 $M_r = 1184.62$   $Z = 4$   
 Orthorhombic,  $Pnma$   $\text{Mo } K\alpha$  radiation  
 $a = 17.5165$  (19) Å  $\mu = 23.56$  mm<sup>-1</sup>  
 $b = 3.9266$  (4) Å  $T = 295$  (2) K  
 $c = 14.3968$  (15) Å  $0.37 \times 0.06 \times 0.04$  mm

## Data collection

Bruker SMART 1000  $\text{Absorption correction: numerical}$   
 diffractometer  $(\text{SHELXTL}; \text{Sheldrick, 2008})$   
 $T_{\min} = 0.057$ ,  $T_{\max} = 0.426$

11118 measured reflections  
 1722 independent reflections

1500 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.053$   
 $S = 1.18$   
 1722 reflections

68 parameters  
 $\Delta\rho_{\text{max}} = 2.12$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -2.89$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Zr1—Sb4 <sup>i</sup>	2.9620 (6)	Zr3—Sb6 <sup>v</sup>	2.9975 (8)
Zr1—Sb6	2.9876 (8)	Zr3—Sb3 <sup>vi</sup>	3.1616 (9)
Zr1—Sb1 <sup>ii</sup>	3.0669 (8)	Ni1—Sb7	2.5728 (10)
Zr1—Sb3 <sup>iii</sup>	3.0720 (7)	Ni1—Sb2 <sup>iv</sup>	2.5875 (7)
Zr1—Sb7 <sup>iii</sup>	3.0960 (6)	Ni1—Sb1 <sup>iv</sup>	2.6140 (7)
Zr1—Sb5	3.1324 (8)	Ni1—Sb4 <sup>vi</sup>	2.7141 (10)
Zr2—Sb6 <sup>iv</sup>	2.9478 (6)	Sb1—Sb2	3.1998 (8)
Zr2—Sb4 <sup>iii</sup>	2.9499 (6)	Sb1—Sb3 <sup>vii</sup>	3.2645 (6)
Zr2—Sb2 <sup>iv</sup>	2.9604 (6)	Sb1—Sb4 <sup>viii</sup>	3.2981 (6)
Zr2—Sb2 <sup>ii</sup>	3.0029 (8)	Sb2—Sb2 <sup>ix</sup>	3.2250 (7)
Zr2—Sb5	3.0044 (8)	Sb2—Sb4 <sup>viii</sup>	3.3111 (6)
Zr3—Sb1 <sup>iv</sup>	2.9569 (6)	Sb5—Sb7 <sup>iii</sup>	3.1380 (6)
Zr3—Sb3 <sup>iv</sup>	2.9944 (7)	Sb5—Sb6 <sup>iv</sup>	3.1387 (6)
Zr3—Sb5 <sup>iv</sup>	2.9958 (6)	Sb6—Sb7 <sup>i</sup>	3.1393 (6)

Symmetry codes: (i)  $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, y, -z + \frac{1}{2}$ ; (iii)  $-x + \frac{1}{2}, -y, z - \frac{1}{2}$ ; (iv)  $-x + \frac{1}{2}, -y, z + \frac{1}{2}$ ; (v)  $x, y, z + 1$ ; (vi)  $x + \frac{1}{2}, y, -z + \frac{1}{2}$ ; (vii)  $-x, -y + 1, -z + 1$ ; (viii)  $-x, -y, -z + 1$ ; (ix)  $-x, -y, -z$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2000); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1999); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2182).

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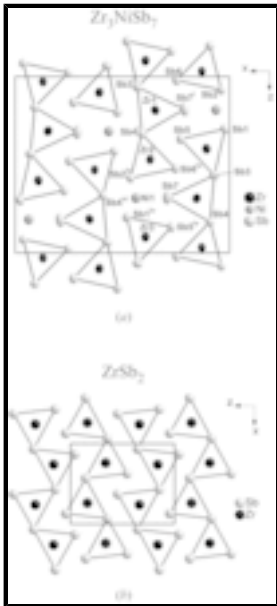
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