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demchenko@franko.lviv.ua**Key indicators**

Single-crystal X-ray study

T = 295 K

Mean  $\sigma(\text{Ni}-\text{Al}) = 0.003 \text{ \AA}$ 

R factor = 0.028

wR factor = 0.073

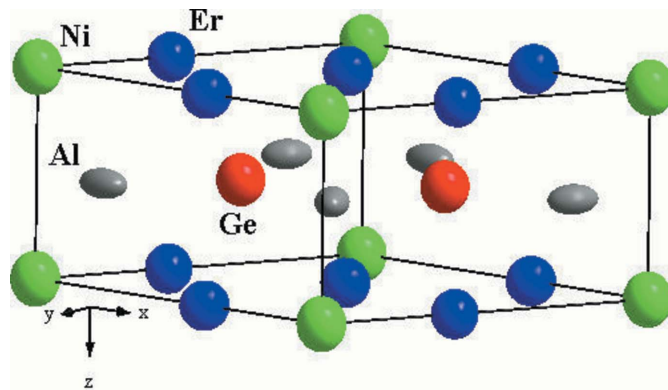
Data-to-parameter ratio = 17.4

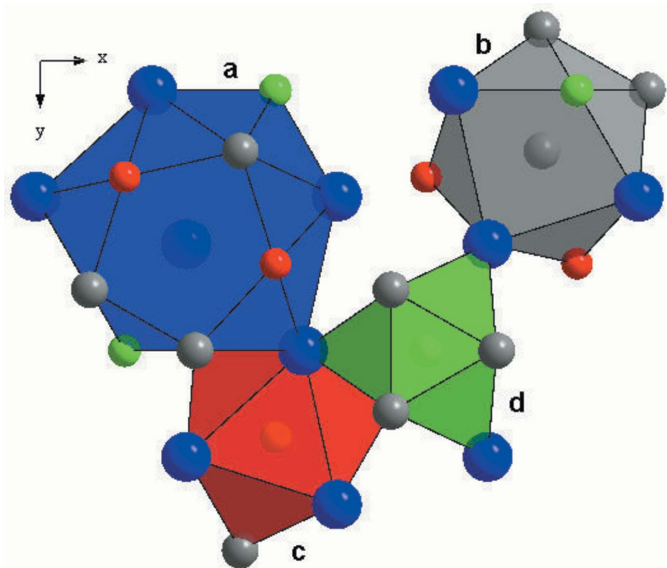
For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Trierbium nickel trialuminium digermanide,  
Er<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub>**Single crystals of Er<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> were synthesized from the corresponding elements by arc-melting. The new quaternary intermetallic compound crystallizes in the primitive hexagonal space group  $P\bar{6}2m$  and adopts the Y<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> structure type [Zhao & Parthé (1990). *Acta Cryst. C* **46**, 2273–2276], with all atoms in special positions: Er and Al with site symmetry  $m2m$ , Ni with site symmetry  $\bar{6}2m$ , and Ge with  $\bar{6}$ .. site symmetry.

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In memory of Professor Dr  
Oksana Bodak.**Comment**The Fe<sub>2</sub>P structure type (Hendricks & Kosting, 1930; Rundqvist & Jellinek, 1959) is a widespread type among intermetallic phases. About 450 compounds crystallize with this type of structure (Villars & Calvert, 1997). Moreover, its ternary substitution variant, ZrNiAl (Kripyakevich *et al.*, 1967), and its quaternary substitution variant, Y<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> (Zhao & Parthé, 1990), are also known.Rare earth intermetallics of different composition have received attention due to their interesting magnetic and electric properties. The accurate determination of the crystal structure is a basic requirement for the better understanding of their physical properties. The new compound Er<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> was obtained during the systematic investigation of the quaternary Er–Ni–Al–Ge system. We present here the results of a single-crystal structure study.Er<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> adopts the Y<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> structure type which is a quaternary substitution variant of the Fe<sub>2</sub>P type (Zhao & Parthé, 1990). A clinographic projection of the unit-cell contents is shown in Fig. 1. The coordination sphere around Er (site symmetry  $m2m$ ) consists of 16 atoms if bonding interactions are considered for distances  $<4.1 \text{ \AA}$ , resulting in a polyhedron with 16 apices [ErNi<sub>2</sub>Ge<sub>4</sub>Al<sub>6</sub>Er<sub>4</sub>] (Fig. 2a). The**Figure 1**A clinographic projection of the Er<sub>3</sub>NiAl<sub>3</sub>Ge<sub>2</sub> unit-cell contents, with displacement ellipsoids drawn at the 95% probability level.



**Figure 2**  
Coordination polyhedra around (a) the Er atom, (b) the Al atom, (c) the Ge atom and (d) the Ni atom. Er atoms are blue, Ni atoms are green, Al atoms are grey and Ge atoms are red.

coordination polyhedron around Al (site-symmetry  $m2m$ ) is a distorted cuboctahedron  $[\text{AlNi}_2\text{Ge}_2\text{Al}_2\text{Er}_6]$  (Fig. 2b). The coordination polyhedron around Ge (site-symmetry  $\bar{6}$ ) is a tricapped trigonal prism  $[\text{GeAl}_3\text{Er}_6]$ , with three additional Al as the capping atoms (Fig. 2c), and a tricapped trigonal prism  $[\text{NiAl}_6\text{Er}_3]$  is also observed around the Ni atom (site symmetry  $\bar{6}2m$ ), with three additional Er atoms as the capping atoms (Fig. 2d). The interatomic distances (Table 1) are in good agreement with the sums of the atomic radii (Emsley, 1991). The shortest distance with the highest deviation (93% of the sum of the atomic radii) is observed between Er and Ni atoms, with  $\text{Er}-\text{Ni} = 2.7931$  (9) Å.

## Experimental

The single crystal used in this work was extracted from an alloy with nominal composition  $\text{Er}_{35}\text{Ni}_{10}\text{Al}_{35}\text{Ge}_{20}$ , which was prepared by arc melting of the initial components (purity better than 99.9%) in an electric arc furnace with a water-cooled copper bottom (Ti-getter) under an argon atmosphere and annealed at 870 K. A preliminary crystal investigation was performed using Laue and rotation methods (RKV-86 and RGNS-2 chambers, Mo  $K\alpha$  radiation).

### Crystal data

$\text{Er}_3\text{NiAl}_3\text{Ge}_2$   
 $M_r = 786.61$   
Hexagonal,  $P\bar{6}2m$   
 $a = 6.8360$  (10) Å  
 $c = 4.1480$  (9) Å  
 $V = 167.87$  (5) Å<sup>3</sup>  
 $Z = 1$   
 $D_x = 7.781$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 1298 reflections  
 $\theta = 4.9$ – $32.3^\circ$   
 $\mu = 48.92$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
Needle, metallic light grey  
 $0.22 \times 0.04 \times 0.03$  mm

### Data collection

Oxford Diffraction XCALIBUR3  
CCD diffractometer  
 $\omega$  scans  
Absorption correction: analytical  
(*CrysAlis RED*; Oxford Diffraction, 2005)  
 $T_{\min} = 0.105$ ,  $T_{\max} = 0.237$   
1371 measured reflections

244 independent reflections  
244 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$   
 $\theta_{\text{max}} = 32.3^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -9 \rightarrow 9$   
 $l = -6 \rightarrow 3$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.073$   
 $S = 1.21$   
244 reflections  
14 parameters  
 $w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 2.9965P]$   
where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 2.98$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.85$  e Å<sup>-3</sup>  
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.012 (2)  
Absolute structure: Flack (1983), 93  
Friedel pairs  
Flack parameter: 0.09 (8)

**Table 1**

Selected interatomic distances (Å).

Er–Ni	2.7931 (9)	Er–Er <sup>iii</sup>	3.5853 (7)
Er–Ge <sup>i</sup>	2.9302 (4)	Ge–Al	2.686 (4)
Er–Al <sup>i</sup>	3.1925 (7)	Ni–Al <sup>iv</sup>	2.617 (4)
Er–Al <sup>ii</sup>	3.208 (4)	Al–Al <sup>v</sup>	2.763 (10)

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $-y, x-y, z+1$ ; (iii)  $-x+y-1, -x, z$ ; (iv)  $-x+y+1, -x+1, z+1$ ; (v)  $-x+y+2, -x+1, z$ .

Atomic coordinates were standardized using the *STRUCTURE-TIDY* program (Gelato & Parthé, 1987). The highest maximum residual electron density is 2.06 Å<sup>-3</sup> from the Ge atom and the deepest hole is 1.92 Å<sup>-3</sup> from the Al atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

## References

- Brandenburg, K. (1999). *DIAMOND*. Version 2.1e. Crystal Impact, Bonn, Germany.
- Emsley, J. (1991). *The Elements*, 2nd ed., p. 251. Oxford: Clarendon Press.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
- Hendricks, S. B. & Kosting, P. R. (1930). *Z. Kristallogr.* **74**, 511–533.
- Kripyakevich, P. I., Markiv, V. Ya. & Mel'nyk, E. V. (1967). *Dopov. Akad. Nauk Ukr. RSR Ser. A*, **8**, 750–753. (In Russian.)
- Oxford Diffraction (2004). *CrysAlis CCD*. Version 1.170. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
- Oxford Diffraction (2005). *CrysAlis RED*. Version 1.171. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
- Rundqvist, S. & Jellinek, F. (1959). *Acta Chem. Scand.* **13**, 425–432.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Villars, P. & Calvert, L. D. (1997). *Pearsons Handbook of Crystallographic Data for Intermetallic Phases*, Desk Edition. Materials Park, Ohio, USA: American Society for Metals.
- Zhao, J. T. & Parthé, E. (1990). *Acta Cryst.* **C46**, 2273–2276.