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Key indicators

Single-crystal X-ray study

$T = 295$ K

Mean $\sigma(\text{Si}-\text{Si}) = 0.004$ Å

R factor = 0.022

wR factor = 0.050

Data-to-parameter ratio = 12.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Erbium dicobalt disilicide, ErCo_2Si_2

Single crystals of erbium dicobalt disilicide were synthesized from the corresponding elements by arc melting. The ternary intermetallic compound crystallizes in the body-centred tetragonal space group $I4/mmm$ and adopts the CeGa_2Al_2 structure type, with all atoms in special positions.

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Comment

Ternary intermetallics of rare earth metals with the general formula $\text{RE}T_2X_2$ (where RE is a rare earth metal, T is a transition metal or, in a few cases, a p -block element, and X is a p -block element) crystallize mostly in ten structure types: tetragonal CeGa_2Al_2 (also called ThCr_2Si_2), CaBe_2Ge_2 and YB_2C_2 , trigonal $\text{La}_2\text{O}_2\text{S}$, orthorhombic CaRh_2B_2 , LaRe_2Si_2 , HfFe_2Si_2 and ScB_2C_2 , and monoclinic LaPt_2Ge_2 and HoNi_2B_2 . In the majority of cases, $\text{RE}T_2X_2$ phases belong to the CeGa_2Al_2 structure type (body-centred tetragonal) or to the very similar CaBe_2Ge_2 structure type (primitive tetragonal), which are both ordered derivatives of the BaAl_4 structure (Parthé *et al.*, 1983).

The $\text{RE}T_2X_2$ phases have received special attention due to their interesting physical properties. The compound CeCu_2Si_2 (CeGa_2Al_2 type) was the first representative of a heavy-fermion system. The accurate determination of the crystal structure for phases of this composition is necessary for a better understanding of their physical properties. The existence of the ErCo_2Si_2 phase was first reported by Rossi *et al.* (1978), and the crystal structure was determined by means of X-ray powder diffraction measurements. Subsequently,

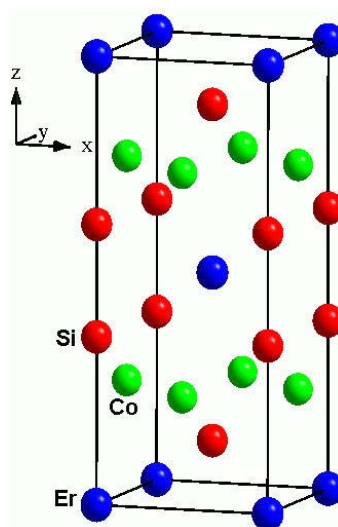


Figure 1

A clinographic projection of the ErCo_2Si_2 unit cell, with displacement ellipsoids drawn at the 95% probability level.

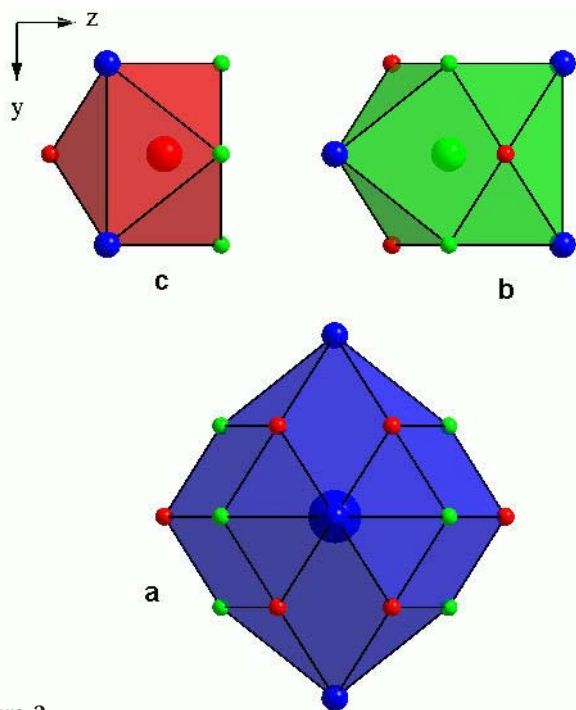


Figure 2
Coordination polyhedra around (a) the Er atom, (b) the Co atom and (c) the Si atom. Er atoms are blue, Co atoms are red and Si atoms are green.

neutron powder diffraction measurements and structure refinements have been performed by Yakinthos *et al.* (1983) and Leciejewicz *et al.* (1983). In view of the close relation of the structure types CeGa_2Al_2 (space group $I4/mmm$) and CaBe_2Ge_2 (space group $P4/nmm$), it was necessary to determine precisely the structure type for ErCo_2Si_2 on the basis of single-crystal diffraction data, and we present these results here.

ErCo_2Si_2 adopts the CeGa_2Al_2 structure type. A clino-graphic projection of the unit cell is shown in Fig. 1. The coordination sphere around Er (site symmetry $4/mmm$) consists of 22 atoms, resulting in a polyhedron with 22 vertices $[\text{ErSi}_8\text{Co}_8\text{Si}_2\text{Er}_4]$ (Fig. 2a), and 12 quadrangular and 24 triangular faces. The coordination polyhedron of the Co atom (site symmetry $\bar{4}m2$) is a distorted cuboctahedron $[\text{CoSi}_4\text{Co}_4\text{Er}_4]$ (Fig. 2b). The coordination polyhedron for Si (site symmetry $4mm$) is a monocapped tetragonal antiprism $[\text{SiCo}_4\text{Si}_1\text{Er}_4]$ with one additional Si as the capping atom (Fig. 2c). The interatomic distances are in good agreement with the sums of the atomic radii (Pauling, 1967). The shortest distance (Table 1) is observed between Co and Si atoms (94% of the sum of the atomic radii of the corresponding atoms).

Experimental

The single crystal used in this work was extracted from an alloy with nominal composition $\text{Er}_{20}\text{Co}_{40}\text{Si}_{40}$, 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

Co_2ErSi_2
 $M_r = 341.30$
Tetragonal, $I4/mmm$
 $a = 3.874(2) \text{ \AA}$
 $c = 9.704(4) \text{ \AA}$
 $V = 145.64(12) \text{ \AA}^3$
 $Z = 2$
 $D_x = 7.783 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
Cell parameters from 561 reflections
 $\theta = 2.4\text{--}29.3^\circ$
 $\mu = 40.29 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
Plate, metallic light grey
 $0.14 \times 0.13 \times 0.04 \text{ mm}$

Data collection

Oxford Xcalibur3 CCD area-detector diffractometer
 ω scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
 $T_{\min} = 0.008$, $T_{\max} = 0.261$
694 measured reflections

109 independent reflections
106 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\text{max}} = 33.8^\circ$
 $h = -4 \rightarrow 6$
 $k = -5 \rightarrow 6$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.050$
 $S = 1.17$
109 reflections
9 parameters
 $w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 2.3748P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 2.09 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -2.41 \text{ e \AA}^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.018 (3)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Er—Si ⁱ	2.9977 (17)	Co—Co ⁱⁱⁱ	2.7393 (14)
Er—Co ⁱ	3.1044 (10)	Si—Si ^{iv}	2.435 (6)
Co—Si ⁱⁱ	2.2831 (17)		
Si ⁱ —Er—Si ^v	180.0	Si ^x —Co—Co ⁱⁱⁱ	53.14 (3)
Si ⁱ —Er—Si ^{vi}	132.07 (10)	Co ⁱⁱⁱ —Co—Co ⁱⁱ	180.0
Si ^v —Er—Si ^{vi}	47.93 (10)	Co ⁱⁱⁱ —Co—Co ^{xii}	90.0
Si ⁱ —Er—Si ^{vii}	80.51 (4)	Si ⁱⁱⁱ —Co—Er	65.57 (5)
Si ^v —Er—Si ^{vii}	99.49 (4)	Si ^x —Co—Er	160.56 (6)
Si ⁱ —Er—Co ⁱ	43.90 (4)	Si—Co—Er	83.35 (7)
Si ^v —Er—Co ⁱ	136.10 (4)	Co ⁱⁱ —Si—Co ^{xii}	73.73 (6)
Si ^{vi} —Er—Co ⁱ	94.92 (5)	Co ⁱⁱ —Si—Co ^v	116.08 (13)
Si ^{viii} —Er—Co ⁱ	85.08 (5)	Co ⁱⁱ —Si—Si ^{iv}	121.96 (6)
Co ⁱ —Er—Co ^{ix}	52.36 (2)	Co ⁱⁱ —Si—Er ^{xiii}	139.747 (19)
Si ⁱⁱ —Co—Si ^x	106.27 (6)	Co ^v —Si—Er ^{xiii}	70.54 (2)
Si ⁱⁱ —Co—Si ^v	116.08 (13)	Si ^{iv} —Si—Er ^{xiii}	66.04 (5)
Si ⁱⁱⁱ —Co—Co ⁱⁱⁱ	126.86 (3)	Er ^{xiii} —Si—Er ^{xiv}	132.07 (10)

Symmetry codes: (i) $x - \frac{1}{2}, y - \frac{1}{2}, z - \frac{1}{2}$; (ii) $-\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$; (iii) $\frac{1}{2} - x, \frac{3}{2} - y, \frac{1}{2} - z$; (iv) $-x, -y, 1 - z$; (v) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$; (vi) $\frac{1}{2} + x, \frac{1}{2} + y, z - \frac{1}{2}$; (vii) $x - \frac{1}{2}, \frac{1}{2} + y, z - \frac{1}{2}$; (viii) $-\frac{1}{2} - x, -\frac{1}{2} - y, \frac{1}{2} - z$; (ix) $-x, -y, -z$; (x) $x, 1 + y, z$; (xi) $-\frac{1}{2} - x, \frac{3}{2} - y, \frac{1}{2} - z$; (xii) $x, y - 1, z$; (xiii) $\frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} + z$; (xiv) $x - \frac{1}{2}, y - \frac{1}{2}, \frac{1}{2} + z$.

The structure refinement of ErCo_2Si_2 clearly indicated that this phase crystallizes in the tetragonal crystal system in space group $I4/mmm$, adopting the CeGa_2Al_2 structure type. Refinement in space group $P4/nmm$ (CaBe_2Ge_2 structure type) was less satisfactory and resulted in higher values of the R factors and atomic displacement factors. The highest maximum residual electron density is located at a distance of 0.73 \AA from the Er atom, and the deepest hole is 1.80 \AA from the same atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); 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*.

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