Crystal structure of europium cobalt aluminide (1/2/9), $EuCo_2Al_9$

V. M. T. Thiede and W. Jeitschko*

Universität Münster, Anorganisch-Chemisches Institut, Wilhelm-Klemm-Straße 8, D-48149 Münster, Germany

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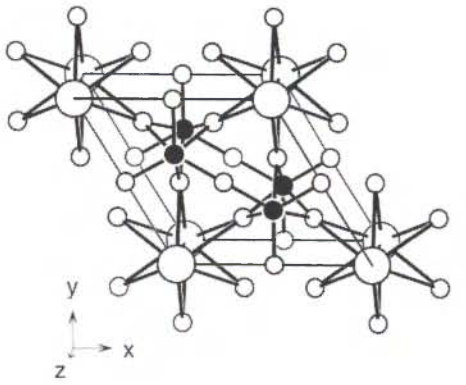
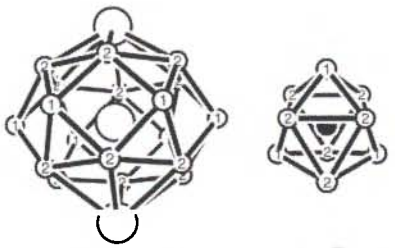
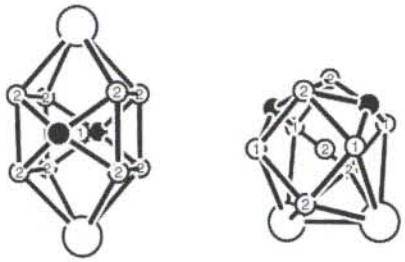




Eu (6/mmm) Co ($\bar{6}$m2)



Al(1) (mmm) Al(2) (mm2)

Abstract

Al_9Co_2Eu, hexagonal, *P6/mmm* (No. 191), $a = 7.865(2)$ Å, $c = 3.898(1)$ Å, $V = 208.8$ Å^3, $Z = 1$, $R(F) = 0.014$, $R_w(F^2) = 0.035$, $T = 293$ K.

Source of material

The elemental components in the ratio Eu:Co:Al = 1:1:8 were enclosed in an alumina crucible and sealed in a silica tube under argon. The sample was annealed at 1123 K for 60 h and slowly (20 K/h) cooled to room temperature. The matrix was dissolved by hydrochloric acid.

Discussion

$EuCo_2Al_9$ is a new compound, which is isotypic with $BaFe_2Al_9$ [1]. The europium atoms are coordinated by 12 Al(2) atoms at 349.2 pm, two Eu atoms at 389.8 pm, and six Al(1) atoms at 393.2 pm. The cobalt atoms have 9 aluminum neighbors at distances of 227.0 pm (3x) and 254.9 pm (6x) in the form of a tricapped trigonal prism. Both aluminum atoms have two Eu and two Co neighbors. In addition, the Al(1) atoms have eight Al(2) neighbors at 281.5 pm, and the Al(2) atoms have 4Al(1) (281.5 pm), 2 Al(2) (284.5 pm), and 2 Al(2) (289.8 pm) neighbors. Other isotypic compounds are $CaCo_2Al_9$ [2] and $SrNi_2Al_9$, $SrCo_2Al_9$, $BaNi_2Al_9$, $BaCo_2Al_9$ [1].

Table 1. Data collection and handling.

Crystal:	silvery, needle-shaped, size 0.022 x 0.022 x 0.033 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	122.02 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω/2θ
$2\theta_{max}$:	69.88°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2052, 220
Criterion for I_{obs}:	$I_{obs} > 2\,\sigma(I_{obs})$, 178
$N(param)_{refined}$:	13
Programs:	SHELXS-86 [3], SHELXL-93 [4], DIAMOND [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu(1)	1*a*	0	0	0	0.0220(2)	U_{11}	0.0093(2)	$U_{11}/2$	0	0
Co(1)	2*c*	1/3	2/3	0	0.0049(2)	U_{11}	0.0061(3)	$U_{11}/2$	0	0
Al(1)	3*f*	1/2	0	0	0.0121(5)	0.0061(6)	0.0088(5)	$U_{22}/2$	0	0
Al(2)	6*m*	0.21273(7)	2*x*	1/2	0.0073(3)	0.0072(4)	0.0082(4)	$U_{22}/2$	0	0

* Correspondence author

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