Crystal structure of trieuropium octacopper tetrastannide, $Eu_3Cu_8Sn_4$

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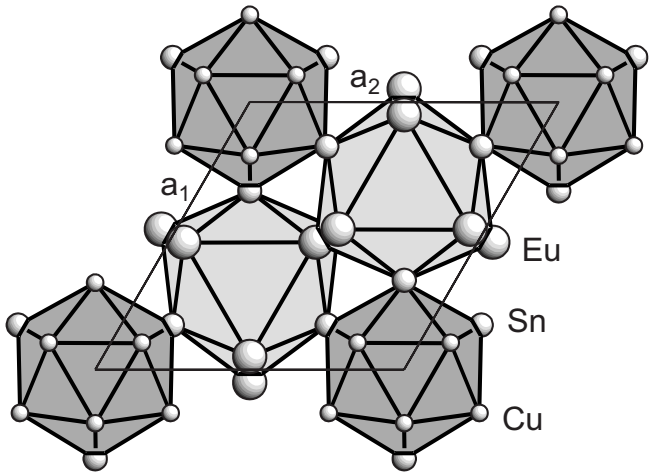

Abstract

$Cu_8Eu_3Sn_4$, hexagonal, $P6_3mc$ (No. 186), a = 9.251(2) Å, c = 7.801(1) Å, V = 578.2 Å^3, Z = 2, $R_{gt}(F)$ = 0.026, $wR_{all}(F^2)$ = 0.062, T = 293 K.

Source of material

The title compound has been obtained from a sample of composition $Eu_3Cu_4Sn_4$ starting from elemental commercial products (Eu 99.8 wt.%, Cu 99.99 wt.% and Sn 99.999 wt.%). The metals were melted in a Mo crucible sealed by arc welding under argon and the resulting alloy was examined by differential thermal analysis. A subsequent annealing at 1073 K was applied for 15 days.

Experimental details

The Flack parameter, used for establishing the absolute structure, indicated a possible twinning by inversion. An inversion matrix was applied and the refined batch scale factor (BASF) resulted to be 0.21(4). After the structure solution a Guinier powder pattern was indexed using the program LAZY PULVERIX [1] and lattice parameters were determined, in good agreement with the single crystal data.

Discussion

The new $Eu_3Cu_8Sn_4$ stannide (Pearson code *hP*30) crystallizes with the ordered structure already found for the $R_3Co_8Sn_4$ phases and refined by single crystal methods for R = Nd, Gd, Yb, Lu and Y [2]. The structure can be considered a ternary derivative of the $BaLi_4$ type [3], with a change of the space group from $P6_3/mmc$ to $P6_3mc$, to allow a splitting of some atomic positions and an ordered distribution of all atoms. In the figure a projection along [001] is given and the icosahedron around Cu4 (dark stippling) and the CN10 polyhedron around Cu3 (light stippling) are outlined. These polyhedra, which share Sn1 atoms, are chosen because not interpenetrating and involving all atoms. The Cu4 icosahedra (9Cu+3Sn) form columns along [001] by sharing faces, while the Cu3 polyhedra (4Sn+6Eu) are connected through Eu vertices. The shortest interatomic distances are d(Cu2—Cu4) = 2.523(3) Å, d(Cu3—Sn1) = 2.688(2) Å, d(Eu—Cu1) = 3.203(2) Å, d(Eu—Sn1) = 3.301(1) Å and d(Eu—Eu) = 3.950(1) Å.

Table 1. Data collection and handling.

Crystal:	metallic grey prism, size 0.05 × 0.09 × 0.10 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	387.70 cm^{-1}
Diffractometer, scan mode:	Bruker-Nonius MACH3, ω/θ
$2\theta_{max}$:	59.84°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2508, 658
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 629
$N(param)_{refined}$:	35
Programs:	LAZY PULVERIX [1], SHELXL-97 [4]

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	6*c*	0.47567(4)	–x	0	0.0075(2)	U_{11}	0.0075(3)	0.0029(2)	–0.0004(2)	–U_{13}
Cu(1)	6*c*	0.8375(2)	–x	0.8293(3)	0.0111(7)	U_{11}	0.0137(8)	0.0050(8)	0.0012(4)	–U_{13}
Cu(2)	6*c*	0.8996(1)	–x	0.5235(2)	0.0123(5)	U_{11}	0.0106(9)	0.0063(6)	–0.0007(4)	–U_{13}
Cu(3)	2*b*	1/3	2/3	0.6685(5)	0.008(1)	U_{11}	0.017(2)	U_{11}/2	0	0
Cu(4)	2*a*	0	0	0.2743(4)	0.0132(8)	U_{11}	0.013(2)	U_{11}/2	0	0
Sn(1)	6*c*	0.8335(1)	–x	0.2055(2)	0.0073(3)	U_{11}	0.0075(4)	0.0046(4)	–0.0001(2)	–U_{13}
Sn(2)	2*b*	1/3	2/3	0.3151(2)	0.0086(6)	U_{11}	0.0089(8)	U_{11}/2	0	0

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