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Isothermal section of the Ce-Au-Sb system at 870 K

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Abstract

Phase equilibria in the Ce–Au–Sb system were derived from X-ray diffraction data and, optionally, from scanning electron microscope analysis of annealed at 870 K alloys. The structures of compounds were investigated using X-ray single crystal and powder diffraction methods. Five ternary compounds were found to exist within the investigated concentration region (0-50 at.% Ce). New $U_3Cu_2Sb_3$-type $Ce_3Au_2Sb_3$ compound (a = 4.5966(4) Å, c =24.005(2) Å, space group $P6_3/mmc$, no 194) was discovered and studied by X-ray single crystal diffraction. The existence and crystal structures of following compounds were confirmed at 870 K: the $ZrCuSi_2$-type $CeAu_{1-x}Sb_2$, UHg_2-type $Ce(Au_{1-x}Sb_x)_2$ and $Y_3Au_3Sb_4$-type $Ce_3Au_3Sb_4$. For the reported earlier UHg_2-type $Ce(Au_{1-x}Sb_x)_2$ and $ZrCuSi_2$-type $CeAu_{1-x}Sb_2$ compounds the homogeneity regions were established from annealed at 870 K alloys: $0.19 \leq x \leq 0.28$ and $0 \leq x \leq 0.21$ respectively. At 870 K, the structure of CeAuSb compound was found to be related to the $CaIn_2$-type from X-ray powder diffraction data. Moreover, the single crystal X-ray diffraction studies of the as-cast $CeAu_{1-x}Sb_2$ for x=0.118(2) and x=0.162(4) are given in present paper as well.

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1. Introduction

Investigation of ternary compounds with rare earths, transition metals and antimony is still of the great interest for researchers due to the interesting properties which these compounds can exhibit. Some specific compositions are already investigated, however these studies mainly were non-systematic and properties oriented. Although, the interactions between the components in the Ce–Au, Au–Sb and Ce–Sb binary systems have been studied in Refs.[1–6] and the ternary ZrCuSi$_2$-type CeAuSb$_2$ [7], Y$_3$Au$_3$Sb$_4$-type Ce$_3$Au$_3$Sb$_4$ [8], UHg2-type Ce(Au$_{1-x}$Sb$_x$)$_2$ [9] and CaIn$_2$-type CeAuSb compounds were reported earlier [10] (Table 1), no profound investigations of Ce-Au-Sb system were ever made. This work is devoted to the search and identification of new phases, precise structural characterization of compounds and construction of the isothermal section of Ce-Au-Sb system at 870 K within the concentration range 0-50 at.% Ce.

2. Experimental

The investigated alloys, in total number of 54, were prepared in an electric arc furnace under an argon atmosphere using a non-consumable tungsten electrode and a water-cooled copper tray. The ingots of cerium (Alfa Aesar Johnson Matthey Gmbh., 99.9%), gold drops (Ogüssa, Austria, 99.999%), and antimony pieces (Alfa Aesar Johnson Matthey Gmbh., 5N) were used as starting materials. Zirconium was used as a getter during the melting process. The alloys were re-melted three times in order to achieve complete fusion and homogeneous composition. The as-cast alloys were checked for crystals and subjected to anneal in evacuated quartz ampoules at 870 K for 1 week in a resistance furnace. The samples were quenched from annealing temperature in ice-cold water.

The phase equilibria in the Ce–Au–Sb system were determined from X-ray powder diffraction and optionally from scanning electron microscope analysis. X-ray powder investigations were made using Philips X'Pert diffractometer (Cu Kα radiation, 2θ range 10–120°, step width of 0.02°, a constant counting time of 10 s per step) on the annealed samples. Phase analyses, automatic indexing and lattice parameters refinements

were accomplished using the WinPlotr [11], PowderCell [12], FULLPROFF [13], TREOR [14] and DICVOL [15] programs.

Scanning electron microscopy and energy dispersive spectroscopy (SEM-EDS) were performed on pieces of samples embedded in resin and polished using SiC paper and diamond paste down to 1μm. A thin layer of carbon was deposited on their surfaces before metallographic analyses. The compositional contrast among the various phases was revealed by means of backscattered electron detector and chemical analyses were obtained with an Oxford link Isis spectrometer mounted on a 6400-JSM scanning electron microscope. At least three EDS point analysis were obtained for each phase The quantative analyses were performed by employing an accelerator voltage of 15 keV, a sample current of 20 nA and a counting time of 30 s.

For the X-ray single crystal data collections, the single crystals were isolated from the annealed alloys in case of $Ce_3Au_2Sb_3$ and from the samples in as-cast conditions for $CeAu_{1-x}Sb_2$, glued on the top of the glass fibers and mounted on the goniometer head. X-ray diffraction intensities data were collected at room temperature with a Nonius Kappa CCD four-circle diffractometer (MoKα radiation, ω-scan). The complete strategy to fill more than a hemisphere was automatically calculated with the use of the program COLLECT [16].

3. Phase relations in the Ce-Au-Sb system at 870 K

The results obtained during the systematic investigation of the Ce-Au-Sb ternary phase diagram by powder diffraction method and optionally by SEM were used in the construction of the isothermal section of the Ce–Au–Sb system at 870 K. Phase compositions and lattice parameters for identified phases in chosen samples from the derived equilibrium fields are presented in Table 2. The partial isothermal section obtained at 870 K is reported in Fig. 1, and the crystal structure data relevant to the ternary phases are listed in Table 1.

The existence of the binary phases reported in the literature was confirmed with the exception of $CeAu_2$ [5] for which the investigation was severely hampered by high rates of sample oxidation in the vicinity of composition 32 at.% Ce- 68 at.% Au up to ~ 7 at

% of Sb. All the binaries were found to have negligible extensions into the ternary system.

Phase relations in the investigated concentration region at 870 K are characterized by formation of five ternary compounds. The formation of $CeAu_{1-x}Sb_2$ (1), $Ce_3Au_3Sb_4$ (2) and $Ce(Au_{1-x}Sb_x)_2$ (3) was confirmed. The boundaries of the homogeneity regions for the $Ce(Au_{1-x}Sb_x)_2$ [9] ($0.19 \leq x \leq 0.28$) and $CeAu_{1-x}Sb_2$ ($0 \leq x \leq 0.21$) were determined from Rietveld refinements of X-ray powder diffraction data and SEM-EDS measurements (Table 2) while constructing the phase equilibria. The $CeAu_{1-x}Sb_2$ was found to be in equilibrium with Sb; SEM-EDS analyses carried out on the samples located in the region around this compound, yielded the values $\sim Ce_{25}Au_{25}Sb_{50}$ and $\sim Ce_{26}Au_{21}Sb_{53}$ as the limit compositions for its homogeneity field (Fig. 2).

The existence of equiatomic CeAuSb (4) [10] compound was confirmed from X-ray powder diffraction data of alloys in corresponding concentration fields as well as from SEM-EDS analyses (Table 2). However the X-ray powder diffraction pattern, calculated on the basis of $CaIn_2$ structure, differed from the one obtained in our experiments, and the additions of small amounts of secondary phases such as $Ce_{14}Au_{51}$ (*P6/m* space group) and $Ce_3Au_3Sb_4$ (*I-43d* space group) were observed in all samples within corresponding equilibrium fields. For new compound $Ce_3Au_2Sb_3$ (5) no homogeneity region was observed. In the vicinity of Au-Sb binary system, a region of liquidus was found to exist in ternary system and is probably induced by the low temperature eutectic (638 K) in the binary Au-Sb system.

3. Crystal structures of ternary compounds derived from the X-ray single crystal diffraction

Several specimens selected from the alloy with a nominal composition 3Ce:2Au:3Sb were tested and showed hexagonal unit cells with lattice parameters $a \cong 4.62$, $c \cong 24.01$. One single crystal of good quality was chosen and measured. The experimental details on single crystal data collection are given in Table 3. For space group determination, crystal structure solution and refinement, the program package WinGX 1.70 [17] was used. The space group extinctions lead to the possible *P6₃/mmc*

(no. 194) space group, which was found to be correct during the refinement. The structure was solved with the aid of SHELXS-97 [18] using direct methods, which resulted in the positions of all atoms. The structural refinement was performed with a full-matrix least-square program package. The distribution of atoms on atomic sites was found to correspond to that which is typical for $U_3Cu_2Sb_3$ [19] structure type. Obtained atomic model was refined with SHELXL-97 [20] and converged to the satisfactory agreement indexes (see Table 3) giving the final stoichiometric composition. Final values of the atomic positional (standardized with STIDY [21]) and displacement parameters are given in Table 4; interatomic distances are presented in Table 5.

The projection of the unit cell of $Ce_3Au_2Sb_3$ on YZ plane and coordination polyhedra of atoms are given in Fig. 3. The nearest neighborhood of Ce1 atom consists of 14 atoms: 6 Sb, 6 Au and 2 atoms of Ce2. The coordination sphere of Ce2 is formed by six antimony atoms which are located at the distances 3.214(1) Å and 3.257(1) Å from the central atom, three atoms of gold (3.746(7) Å) and one Ce1 (4.186(3) Å). For the atom of gold the coordination polyhedron has a shape of trigonal prism formed by 6 Ce atoms capped with four additional atoms: three Sb1 and one Au. Sb1 is surrounded by a trigonal prism formed by cerium atoms with the additional Au atom against each rectangular face. Sb2 is surrounded by six Ce2 atoms, which form a tetragonal bi-pyramid.

The crystal structures of the $CeAu_{1-x}Sb_2$ compound for x=0.118(2) and x=0.162(4) were investigated in the way described above. Two single crystals of good quality were chosen from the as cast multiphase samples and measured. Structure solution in *P4/nmm* space group revealed the 4 atoms arrangement typical for the $ZrCuSi_2$ structure for both crystals. Numerical data on the refinement of crystals, crystallographic characteristics, standardized atomic positions and occupancies for atoms are presented in Table 6. The results showed the existence of homogeneity field for this compound also in the as cast conditions.

4. Summary

The partial isothermal section of the ternary Ce-Au-Sb system at 870 K (0-50 at.% Ce) has been experimentally investigated and the tie-triangles have been drawn. Besides the region in the proximity of $CeAu_2$ not yet studied, five ternary phases were found. The already known phases $CeAu_{1-x}Sb_2$ (1), $Ce_3Au_3Sb_4$ (2) and $Ce(Au_{1-x}Sb_x)_2$ (3) were confirmed. Two ternary compounds, $CeAu_{1-x}Sb_2$ (1) and $Ce(Au_{1-x}Sb_x)_2$ (3) exhibit the certain ranges of homogeneity. The new ternary compound $Ce_3Au_2Sb_3$ (5) was found and studied by X-ray single crystal diffraction. The crystal structure of CeAuSb (4) reported in the literature [10] as $CaIn_2$-type compound was not confirmed from powder X-ray diffraction of alloys at 870 K. Given presentation is complemented by the single crystal X-ray diffraction studies of the as-cast $CeAu_{1-x}Sb_2$ compound.

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Figure Captions.

Fig. 1. The isothermal section of Ce-Au-Sb system at 870 K. The two-phase regions are shaded. Large figures correspond to the codes of compounds, small figures show the codes of samples.

Fig. 2. (a) Micrograph of the $Ce_{23}Au_{18}Sb_{69}$ sample (27) showing $CeAu_{1-x}Sb_2$ (26.38 at.% at Ce : 20.84 at.% Au : 52.77 at.% Sb; light grey phase) and Sb (0.62 at.% Ce : 0.65% at. Au : 98.73 at.% Sb; dark grey phase); (b) micrograph of the $CeAuSb_3$ sample (13) showing $CeAuSb_2$ (25.07 at.% Ce : 24.89 at.% Au : 50.11 at.% Sb; light grey phase) and Sb (0.32 at.% Ce : 0.85 at.% Au : 98.83 at.% Sb; dark grey phase).

Fig. 3. 2D cell projection of $Ce_3Au_2Sb_3$ (a) and coordination polyhedra for Ce1 (b), Ce2 (c), Au (d), Sb1 (e), Sb2 (f). Large dark gray spheres correspond to Ce atoms, small dark gray spheres correspond to Au atoms and light gray spheres correspond to Sb atoms.

Table 1 Crystallographic data on the unary, binary and ternary compounds in the Ce–Au–
Sb (Ce<50 at.%) system at 870 K

Compound	Structure type	Space group	Lattice parameters, Å			T [K][a]	Ref.
			a	b	c		
Au	Cu	Fm-3m	4.0773			**1337**	[1]
Sb	As	R-3m	4.3000		11.251	**904**	[2]
$CeAu_6$	$PrAu_6$	C2/c	7.800	7.780 $\beta=100.6°$	9.08	*1173*	[3]
$Ce_{14}Au_{51}$	$Gd_{14}Ag_{51}$	P6/m	12.808		9.327	**1423**	[4]
$CeAu_2$	KHg_2	Imma	4.528	7.203	8.068	**1403**	[5]
CeAu	TlI	Cmcm	3.90	11.14	4.75	**1645**	[4]
$CeSb_2$	$LaSb_2$	Cmca	6.280	6.130	18.240	*1773*	[6]
CeSb	NaCl	Fm-3m	6.426			**2073**	[6]
$CeAu_{1-x}Sb_2$ (1) $0≤x≤0.21$	$ZrCuSi_2$	P4/nmm	4.4081 4.4079(2)- 4.3560(1)		10.339 10.3588(1)- 10.2405(1)		[7] *, PD
$Ce_3Au_3Sb_4$ (2)	$Y_3Au_3Sb_4$	I-43d	10.058 10.0567(3)				[8] *, PD
$Ce(Au_{1-x}Sb_x)_2$ (3) $0.19≤x≤0.28$	UHg_2	P6/mmm	4.743(1) – 4.712(2)		3.567(1) – 3.768(1)		[9]
CeAuSb (4)	$CaIn_2$ $CaIn_2$-related	$P6_3/mmc$ hexagonal	4.616		8.322		[10] *, PD
$Ce_3Au_2Sb_3$ (5)	$U_3Cu_2Sb_3$	$P6_3/mmc$	4.5966(4) 4.609		24.005(2) 24.04		*, SC *, PD

[a] Temperature of melting (**bold font**) or peritectic reaction (*italic font*)

* corresponds to the data obtained in this work; SC – single crystal diffraction data; PD –
powder diffraction data

Table 2. Crystallographic data of selected Ce-Au-Sb alloys annealed at 870 K

N	Nominal composition Ce-Au-Sb, at.%	Ce:Au:Sb, at.% (EDS analysis)	X-ray phase analysis	Space group	Structure type	Lattice parameters in Å, a	b	c
12	20-40-40	25:25:50 0:100:0	$CeAu_{1-x}Sb_2$ Sb (traces) Au	P4/nmm R-3m Fm-3m	$ZrCuSi_2$ As Cu	4.410(2) 4.297(3) 4.0709(2)		10.359(3) 11.263(5)
13	20-20-60	25:25:50 0:0:100	$CeAu_{1-x}Sb_2$ Sb	P4/nmm R-3m	$ZrCuSi_2$ As	4.408(2) 4.297(2)		10.356(4) 11.263(4)
15	20-55-25		$Ce_3Au_3Sb_4$ Au $CeAu_6$ (traces)	I-43d Fm-3m C2/c	$Y_3Au_3Sb_4$ Cu $PrAu_6$	10.049(1) 4.050(1)		
20	25-50-25	30:30:40 22:78:0	$Ce_3Au_3Sb_4$ $Ce_{14}Au_{51}$ $CeAu_6$	I-43d P6/m C2/c	$Y_3Au_3Sb_4$ $Gd_{14}Ag_{51}$ $PrAu_6$	10.0567(3) 12.801(4) 7.822(5)	 7.779(4) $\beta=100.8(1)°$	 9.323(3) 9.079(5)
22	30-50-20		$Ce_3Au_2Sb_3$ (5) $Ce_{14}Au_{51}$ CeAuSb	$P6_3/mmc$ P6/m	$U_3Cu_2Sb_3$ $Gd_{14}Ag_{51}$ $CaIn_2$-related	4.613(4) 12.802(5)		24.039(7) 9.315(5)
25	30-40-30	30:30:40 22:78:0 33:33:33	$Ce_3Au_3Sb_4$ $Ce_{14}Au_{51}$ CeAuSb	I-43d P6/m	$Y_3Au_3Sb_4$ $Gd_{14}Ag_{51}$ $CaIn_2$-related	10.0555(5) 12.810(6)		 9.332(5)
27	25-18-57	0:0:100 26:21:53	$CeAu_{1-x}Sb_2$ Sb $CeSb_2$ (traces)	P4/nmm R-3m	$ZrCuSi_2$ As	4.362(2) 4.293(4)		10.269(4) 11.260(6)
38	35-45-20	33:49:117 50:50:0	$Ce_3Au_2Sb_3$ (5) (traces) $Ce(Au_{1-x}Sb_x)_2$ (4) CeSb	$P6_3/mmc$ P6/mmc Fm-3m	$U_3Cu_2Sb_3$ UHg_2 NaCl	 4.711(3) 6.437(5)		 3.769(2)
39	33-34-33		$Ce_3Au_3Sb_4$ CeAuSb $Ce_3Au_2Sb_3$ (5)	I-43d $P6_3/mmc$	$Y_3Au_3Sb_4$ $CaIn_2$-related $U_3Cu_2Sb_3$	10.0562(2) 4.6096(3)		 24.045(5)

42	40-35-25	50:0:50 33:54:12	CeAu (traces) $Ce(Au_{1-x}Sb_x)_2$ (4) CeSb	Cmcm P6/mmc Fm-3m	TlI UHg_2 NaCl	3.912(4) 4.741(3) 6.431(3)	11.145(3)	4.749(4) 3.568(2)
45	35-20-45	30:30:40 50:0:50 26:21:53	$Ce_3Au_3Sb_4$ CeSb $CeAu_{1-x}Sb_2$	I-43d Fm-3m P4/nmm	$Y_3Au_3Sb_4$ NaCl $ZrCuSi_2$	10.0559(4) 6.430(4) 4.408(1)		10.359(2)
51	40-15-45		$Ce_3Au_3Sb_4$ CeSb $Ce_3Au_2Sb_3$ (5)	I-43d Fm-3m $P6_3$/mmc	$Y_3Au_3Sb_4$ NaCl $U_3Cu_2Sb_3$	10.0567(2) 6.433(1) 4.6089(5)		24.040(7)

Table 3 Parameters for the single crystal X-ray data collection and refinement for the $Ce_3Au_2Sb_3$ compound

Crystal	$Ce_3Au_2Sb_3$
Lattice parameters (Å)	a=4.5966(4), c = 24.005(2)
Cell volume ($Å^3$)	439.24(7)
Space group, Z	$P6_3/mmc$ (no. 194), 2
Calculated density (Mg/m^3)	8.918
Absorption coefficient (mm^{-1})	57.444
Theta range for data collection (deg)	5.10 – 27.50
Data set	$-5 \leq h \leq 5$, $-5 \leq k \leq 5$, $-31 \leq l \leq 26$
Number of measured reflections / unique reflections	4441 / 230 [Rint=0.1132]
Number of reflections with $I>2\sigma(I_0)$	197
Refinement method	Full-matrix least-squares on F^2
Number of refined parameters	19
Goodness of fit on F^2	1.189
R_1, wR_2 (all data)	R1=0.0712, wR2=0.1551
R_1, wR_2 ($I>2\sigma(I_0)$)	R1=0.0575, wR2=0.1462
Largest diffraction peak and hole (e/$Å^{3)}$)	3.643/-2.835

Table 4. Atomic coordinates and displacement parameters for $Ce_3Au_2Sb_3$ obtained from single crystal X-ray diffraction

Atom	Wyckoff position	x	Y	z	Occupancy, (%)	$U_{eq}x10^2$ (Å^2)
Ce1	2(c)	1/3	2/3	¼	100	1.03(13)
Ce2	4(f)	1/3	2/3	0.0756(1)	100	0.84(9)
Au	4(e)	0	0	0.1858(1)	100	1.05(7)
Sb1	4(f)	1/3	2/3	0.6542(1)	100	0.79(9)
Sb2	2(a)	0	0	0	100	0.68(8)

Table 5. Selected interatomic distances for atoms in $Ce_3Au_2Sb_3$

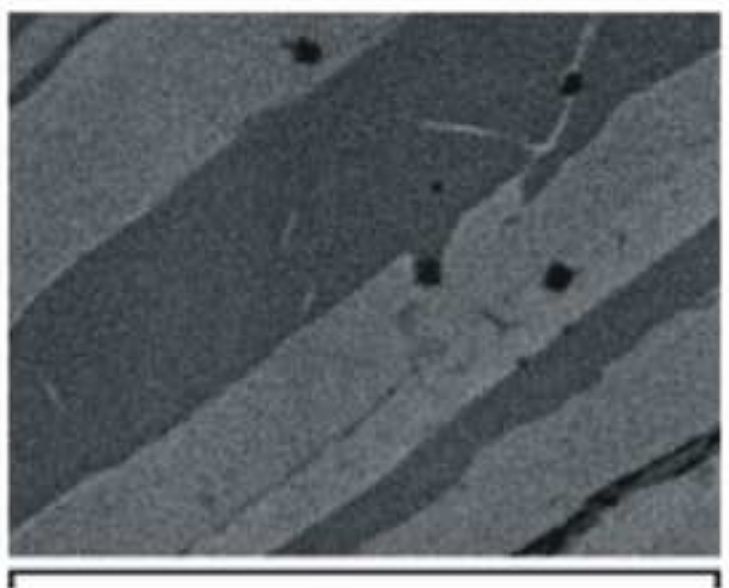| ATOM	Distance, Å	CN	ATOM	Distance, Å	CN
Ce1 – 6Sb1	3.509(7)	14	Sb1 – 3Au	2.759(4)	9
- 6Au	3.068(3)		- 3Ce1	3.257(1)	
- 2Ce2	4.186(3)		- 3Ce2	3.509(7)	
Ce2 – 3Sb2	3.214(1)	10	Sb2 – 6Ce2	3.214(1)	6
– 3Sb1	3.257(1)				
- 3Au	3.746(7)				
- 1Ce1	4.186(3)				
Au – 3Sb1	2.759(1)	10			
- 1Au	3.068(7)				
- 3Ce2	3.081(7)				
- 3Ce1	3.746(7)				

Table 6. Parameters for the single crystal X-ray data collection and refinement for the as-cast $CeAu_{1-x}Sb_2$ compound

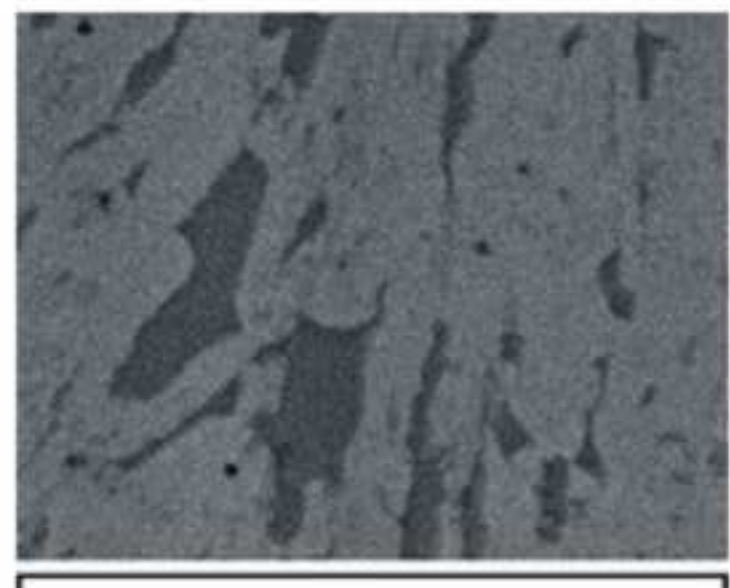| Crystal	I	II
Lattice parameters (Å)	a = 4.440(1) c = 10.183(3)	a = 4.41870(1) c = 10.2167(6)
Cell volume (Å^3)	200.74(5)	199.48(1)
Space group, Z	P4/nmm (no. 129), 2	P4/nmm (no. 129), 2
Calculated density (Mg/m^3)	9.605	9.666
Theta range (deg)	4.00 – 41.95	3.99 – 34.95
Data set	$-7{\leq}h{\leq}8$, $-6{\leq}k{\leq}8$, $-19{\leq}l{\leq}13$	$-7{\leq}h{\leq}4$, $-7{\leq}k{\leq}7$, $-16{\leq}l{\leq}15$
Number of measured reflections / unique reflections	4476 / 468	3158 / 303
Number of reflections with $I>2\sigma(I_0)$	439	276
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Number of refined parameters	15	15
Goodness of fit on F^2	1.122	1.109
R_1, wR_2 (all data)	R1=0.0483, wR2=0.1091	R1=0.0262, wR2=0.0450
R_1, wR_2 ($I>2\sigma(I_0)$)	R1=0.0452, wR2=0.1070	R1=0.0214, wR2=0.0430
Ce; occupancy	2c; z=0.25021(6); 1.00 Ce	2c; z=0.25159(5); 1.00 Ce
Au; occupancy	2b; 0.838(4)Au	2b; 0.882(2) Au
Sb1; occupancy	2c; z=0.8305(1); 1.00 Sb	2c; z=0.82885(8); 1.00 Sb
Sb2; occupancy	2a; 1.00 Sb	2a; 1.00 Sb
Largest diffr. peak and hole (e/Å^3)	4.16/-3.98	1.630/-1.474

Figure 1

Ce - Au - Sb
Isotherm 870 K

Figure 2

30 μm

a

30 μm

b

Figure 3 colour

a

b

c   d   e   f

Figure 3 black and white

a

b

c

d

e

f