Crystal structure of decacerium pentagallium tetrabromide, $Ce_{10}Ga_5Br_4$

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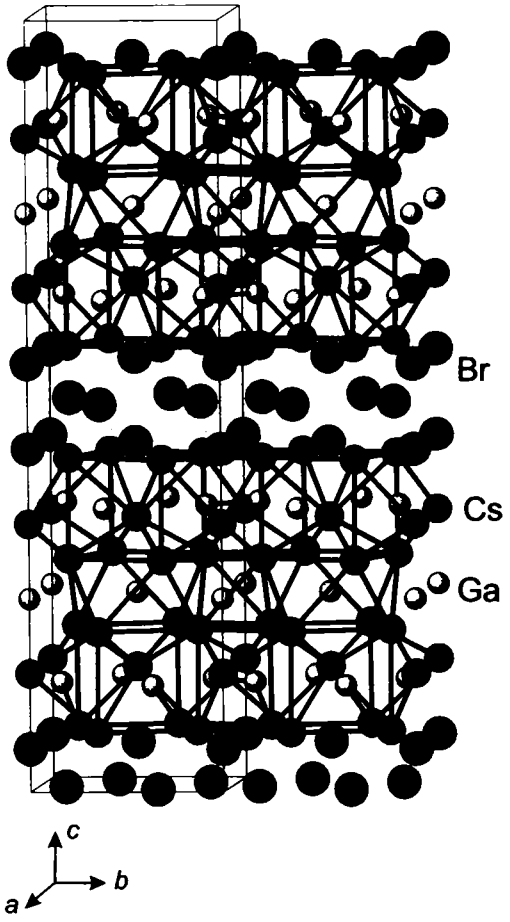

Abstract

$Br_4Ce_{10}Ga_5$, tetragonal, *I*4/*mcm* (no. 140), $a = 8.0937(3)$ Å, $c = 32.129(3)$ Å, $V = 2104.7$ Å^3, $Z = 4$, $R_{gt}(F) = 0.047$, $wR_{ref}(F^2) = 0.114$, $T = 293$ K.

Source of material

$Ce_{10}Ga_5Br_4$ was prepared by heating of a mixture of $CeBr_3$, Ce and Ga (molar ratio 4:26:15) under Ar atmosphere in a silica jacked sealed Ta capsule at 890 °C for 36 days, yielding a pure phase. $Ce_{10}Ga_5Br_4$ forms silver colored plates stable in air and moisture.

Discussion

$Ce_{10}Br_4Ga_5$ is isostructural to $La_{10}Cl_4Ga_5$, $La_{10}Br_4Ga_5$ [1], $Ce_{10}Cl_4Ga_5$ [2] and $La_{10}Br_4Al_5$ [3]. It crystallizes in a layered structure consisting of Ce-Ga slabs separated by Br sheets. There are two types of layer topological arrangements which have frequent occurrence in intermetallic phases. The first is type 4^4 in the Schläfli notation, and the second one 3^2434. The center of the slab contains the Ga2 atom in a square antiprismatic coordination to Ce2. This part of the structure is similar to a planar section of the $CuAl_2$-type structure [4]. Ce2 and Ce1 form cube-shaped as well as trigonal prismatic cavities. The cubic cavity is occupied by Ce3 at the center, and the trigonal prismatic one by Ga1. This substructure corresponds to a two-dimensional section of the intermetallic structure type U_3Si_2 [5]. The Ga1 atoms are interlinked to form dimers with a distance d(Ga1—Ga1′) = 2.783 Å. The compound exhibits metallic conductivity.

Table 1. Data collection and handling.

Crystal:	silver plate, size 0.03 × 0.10 × 0.14 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	349.69 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω/φ
$2\theta_{max}$:	49.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6397, 508
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 507
$N(param)_{refined}$:	32
Programs:	SIR97 [6], SHELXTL [7]

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}
Ce(1)	16*l*	0.6712(1)	x+½	0.42636(4)	0.0137(5)	U_{11}	0.0206(8)	0.0010(5)	−0.0018(4)	−0.0018(4)
Ce(2)	16*l*	0.6670(1)	x+½	0.29569(4)	0.0167(6)	U_{11}	0.0214(8)	0.0006(5)	0.0002(4)	0.0002(4)
Ce(3)	8*f*	½	½	0.34674(6)	0.0199(7)	U_{11}	0.0189(9)	0	0	0
Ga(1)	16*l*	0.3784(2)	−x+½	0.36411(8)	0.0136(8)	U_{11}	0.019(1)	0.001(1)	−0.0008(7)	0.0008(7)
Ga(2)	4*a*	½	½	¼	0.013(2)	U_{11}	0.023(3)	0	0	0
Br(1)	8*f*	0	0	0.9437(1)	0.016(1)	U_{11}	0.020(2)	0	0	0
Br(2)	8*h*	0.8565(3)	x+½	½	0.022(1)	U_{11}	0.024(2)	−0.003(2)	0	0

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