Crystal structure of dekalanthanum tetrabromide pentaaluminide, $La_{10}Br_4Al_5$

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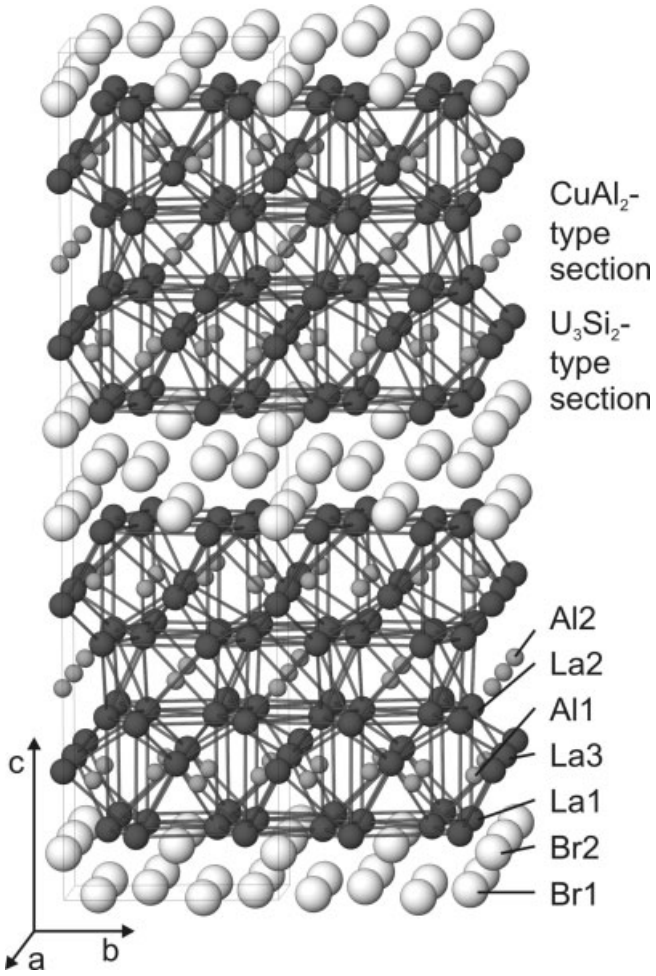
Received May 19, 2003, accepted and available on-line July 23, 2003; CSD-No. 409704



Abstract

$Al_5Br_4La_{10}$, tetragonal, *I*4/*mcm* (No. 140), a = 8.2713(8) Å, c = 32.835(5) Å, V = 2246.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.027, $wR_{ref}(F^2)$ = 0.058, T = 293 K.

Source of material

$La_{10}Br_4Al_5$ is prepared by heating stoichiometric amounts of $LaBr_3$, La and Al under Ar atmosphere in sealed Ta-capsules at 1125 K for 7 days.

Discussion

$La_{10}Br_4Al_5$ is isotypic with $La_{10}X_4Ga_5$ (X= Cl, Br) and $Ce_{10}Cl_4Ga_5$ [1,2]. The crystal structure consists of La–Al slabs separated by layers of Br ions. The two types of the metal layer topology correspond to a planar section of the $CuAl_2$-type structure condensed with a 2-dimensional section of the U_3Si_2- structure type. The distances La—La range from 4.022(1) Å to 4.104(1) Å, La—Br from 3.110(1) Å to 3.170(1) Å, and La—Al from 3.210(2) Å to 3.350(2) Å.

Table 1. Data collection and handling.

Crystal:	silver platelet, size 0.06 × 0.20 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	258.45 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, ω/θ
$2\theta_{max}$:	57.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6957, 822
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 794
$N(param)_{refined}$:	32
Programs:	SHELXL-97 [3], ATOMS [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}
La(1)	16*l*	0.67194(3)	x+1/2	0.42846(1)	0.0127(2)	U_{11}	0.0166(2)	0.0010(1)	–0.00181(9)	U_{13}
La(2)	16*l*	0.66757(4)	x+1/2	0.29608(1)	0.0157(2)	U_{11}	0.0189(2)	0.0007(1)	0.0008(1)	U_{13}
La(3)	8*f*	1/2	1/2	0.34817(2)	0.0183(2)	U_{11}	0.0150(3)	0	0	0
Br(1)	8*f*	0	0	0.94471(3)	0.0128(3)	U_{11}	0.0177(4)	0	0	0
Br(2)	8*h*	0.85785(9)	x+1/2	1/2	0.0188(3)	U_{11}	0.0211(5)	–0.0028(4)	0	0
Al(1)	16*l*	0.3814(2)	–x+1/2	0.36506(6)	0.0133(6)	U_{11}	0.015(1)	0.0003(8)	0.0001(5)	–U_{13}
Al(2)	4*a*	1/2	1/2	1/4	0.015(1)	U_{11}	0.015(2)	0	0	0

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