Crystal structure of dekalanthanum tetrabromide pentaaluminide, $\text{La}_{10}\text{Br}_4\text{Al}_5$

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Abstract

$\text{Al}_5\text{Br}_4\text{La}_{10}$, tetragonal, $I4/mcm$ (No. 140), $a = 8.2713(8)$ Å, $c = 32.835(5)$ Å, $V = 2246.4$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.027$, $wR_{\text{ref}}(F^2) = 0.058$, $T = 293$ K.

Source of material

$\text{La}_{10}\text{Br}_4\text{Al}_5$ 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

$\text{La}_{10}\text{Br}_4\text{Al}_5$ is isotypic with $\text{La}_{10}\text{X}_4\text{Ga}_5$ ($\text{X} = \text{Cl}, \text{Br}$) and $\text{Ce}_{10}\text{Cl}_4\text{Ga}_5$ [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 $0.06 \times 0.20 \times 0.20$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	258.45 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, ω/θ
$2\theta_{\text{max}}$:	57.98°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	6957, 822
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 794
$N(\text{param})_{\text{refined}}$:	32
Programs:	SHELXL-97 [3], ATOMS [4]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
La(1)	16l	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)	16l	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)	8f	1/2	1/2	0.34817(2)	0.0183(2)	U_{11}	0.0150(3)	0	0	0
Br(1)	8f	0	0	0.94471(3)	0.0128(3)	U_{11}	0.0177(4)	0	0	0
Br(2)	8h	0.85785(9)	$x+1/2$	1/2	0.0188(3)	U_{11}	0.0211(5)	−0.0028(4)	0	0
Al(1)	16l	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)	4a	1/2	1/2	1/4	0.015(1)	U_{11}	0.015(2)	0	0	0

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