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Refinement of the crystal structure of lanthanum digallide, $LaGa_2$

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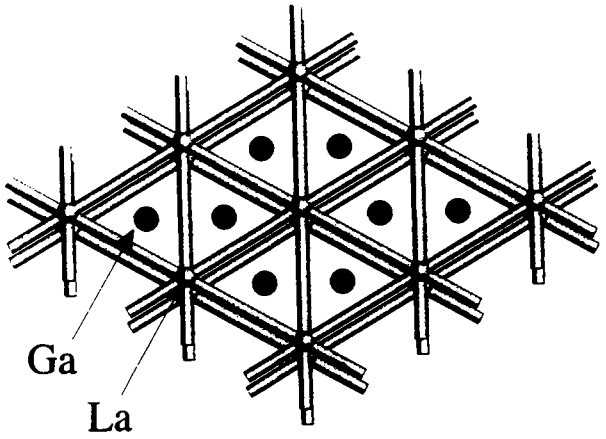

Abstract

Ga_2La, hexagonal, *P6/mmm* (No. 191), $a = 4.3092(6)$ Å, $c = 4.4251(9)$ Å, $V = 71.2$ Å^3, $Z = 1$, $R_{gt}(F) = 0.019$, $wR_{ref}(F^2) = 0.044$, $T = 293$ K.

Source of material

Single crystals of the title compound was grown from a mixture of elemental La and Ga in $LaBr_3$ flux under Ar atmosphere in sealed Ta ampoule at 1173 K for 12 days.

Experimental details

Absorption correction was applied using the ψ-scan method [1].

Discussion

La and Ga form a number of binary compounds: La_3Ga, La_5Ga_3, LaGa, $LaGa_2$ and $LaGa_6$ [2]. Of these, $LaGa_2$ is interesting because its electronic structure is known [3] and has been reported to possess a homogeneity range of 66.7 at. % – 80.0 at. % of Ga [4]. Although its structure has been determined from powder data [2], the single crystal structure has not been reported. We present here the single crystal structure of $LaGa_2$.

Our structure refinement did not show excess Ga. The La—Ga distance in the title compound is 3.3294(4) Å, much larger than the sum of the covalent radii of La (1.69 Å) and Ga (1.25 Å). This indicates that the La–Ga interaction is significantly ionic. The Ga—Ga distance is 2.4879(3) Å, close to the sum of covalent radii of Ga. It is also comparable to the Ga—Ga distance of 2.465 Å in α-Ga, which is the thermodynamically stable allotrope at room temperature [5]. However, it is smaller than the Ga—Ga distance in many Ga-containing intermetallic compounds that are characterized by multi-center, delocalized bonding. For example, the Ga—Ga distance in the superconducting V_2Ga_5 solid is 2.683(2) Å [6]. This fact implies that the Ga—Ga bond is close to the localized two-center, two-electron type. It should be also noted that the thermal ellipsoid of Ga is elongated along the *c*-axis, indicating the larger degree of freedom for motion along this direction which is not blocked by the La atoms.

Table 1. Data collection and handling.

Crystal:	metallic dark grey plate, size 0.04 × 0.12 × 0.12 mm
Wavelength:	Ag K_α radiation (0.56085 Å)
μ:	174.39 cm^{-1}
Diffractometer, scan mode:	CAD4, ω
$2\theta_{max}$:	53.9°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	368, 86
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 78
$N(param)_{refined}$:	6
Programs:	SIR97 [7], SHELXTL [8]

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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*a*	0	0	0	0.0056(2)	U_{11}	0.0069(3)	$U_{11}/2$	0	0
Ga	2*d*	2/3	1/3	1/2	0.0051(3)	U_{11}	0.0184(5)	$U_{11}/2$	0	0

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