Crystal structure of dilanthanum pentaiodide, La_2I_5

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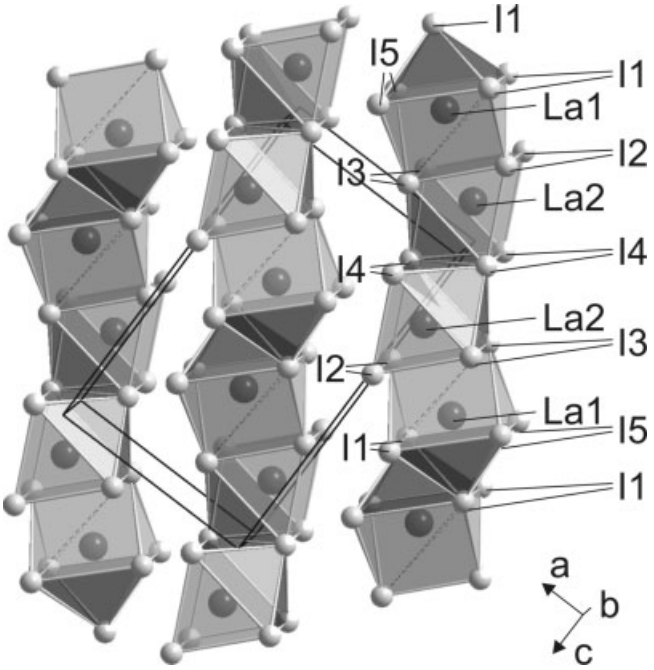
Received May 19, 2003, accepted and available on-line July 23, 2003; CSD-No. 409702



Abstract

I_5La_2, monoclinic, $P12_1/m1$ (No. 11), $a = 8.618(2)$ Å, $b = 4.4038(9)$ Å, $c = 14.580(3)$ Å, $\beta = 90.20(3)°$, $V = 553.3$ Å^3, $Z = 2$, $R_{gt}(F) = 0.026$, $wR_{ref}(F^2) = 0.059$, $T = 293$ K.

Source of material

Reaction of La metal and LaI_3 in Ta capsules in Ar atmosphere for 12d at 1225 K leads to single crystals of La_2I_5.

Discussion

La_2I_5 is isotypic with Pr_2I_5 [1], La_2Br_5 [2], and Pr_2X_5 (X = Br, I) [3]. The La atoms are coordinated by seven iodine atoms for La(1) and eight for La(2) trigonal prismatically including positions above the rectangular prism faces.

Table 1. Data collection and handling.

Crystal:	bronze, needle, size 0.024 × 0.024 × 0.190 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	214.88 cm^{-1}
Diffractometer, scan mode:	Stoe IPDSII, φ
$2\theta_{max}$:	58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10418, 1642
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1475
$N(param)_{refined}$:	44
Programs:	SHELXL-97 [4], DIAMOND [5]

References

1. Warkentin, E.: Zur Strukturchemie des Systems Pr–PrI_3, Dissertation, Universität Karlsruhe 1977.
2. Krämer, K.; Schleid, T.; Schulze, M.; Urland, W.; Meyer, G.: Three Bromides of Lanthanum: $LaBr_2$, La_2Br_6, and $LaBr_3$. Z. Anorg. Allg. Chem. **575** (1989) 61-70.
3. Krämer, K.; Meyer, G.; Fischer, P.; Hewat, A. W.; Güdel, H. U.: Neutron Diffraction Investigation of Magnetic Phase Transitions to Longe-Range Antiferromagnetic Ordering in the 'Free-Electron' Praseodymium Halides Pr_2X_5 (X = Br, I). J. Solid State Chem. **95** (1991) 1-13.
4. Sheldrick, G. M.: SHELXL-97. Program for Refining Crystal Structures. University of Göttingen, Germany 1997.
5. Brandenburg, K.: DIAMOND - Visual Crystal Structure Information System. Crystal Impact, Germany 2000.

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)	2*e*	0.42084(5)	1/4	0.65836(3)	0.0233(2)	0.0225(2)	0.0202(2)	0	0.0038(2)	0
La(2)	2*e*	0.91707(6)	1/4	0.15865(3)	0.0403(3)	0.0178(2)	0.0239(2)	0	0.0085(2)	0
I(1)	2*e*	0.69529(6)	1/4	0.49188(3)	0.0266(2)	0.0228(3)	0.0209(2)	0	0.0041(2)	0
I(2)	2*e*	0.04689(6)	1/4	0.67838(3)	0.0238(2)	0.0261(3)	0.0233(2)	0	0.0030(2)	0
I(3)	2*e*	0.35660(6)	1/4	0.87902(3)	0.0299(3)	0.0278(3)	0.0234(2)	0	0.0051(2)	0
I(4)	2*e*	0.84783(6)	1/4	0.92992(3)	0.0298(3)	0.0238(3)	0.0210(2)	0	0.0041(2)	0
I(5)	2*e*	0.33452(6)	1/4	0.27313(4)	0.0294(2)	0.0213(3)	0.0308(3)	0	0.0006(2)	0

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