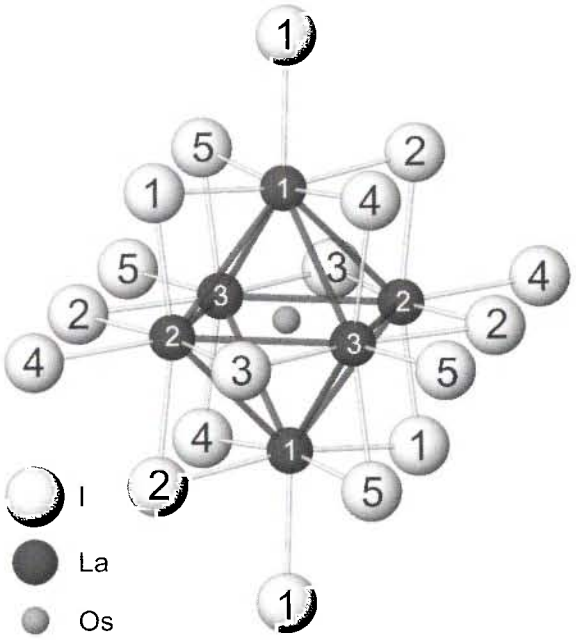
Crystal structure of hexalanthanum osmium decaiodide, La_6OsI_{10}

Hj. Mattausch* and A. Simon

Max-Planck-Institut fur Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Received February 15, 2005, accepted and available on-line March 23, 2005; CSD no. 409817



Abstract

$I_{10}La_6Os$, triclinic, $P\bar{1}$ (no. 2), $a = 8.033(1)$ Å, $b = 9.861(1)$ Å, $c = 10.048(1)$ Å, $\alpha = 108.62(2)°$, $\beta = 97.62(2)°$, $\gamma = 106.02(2)°$, $V = 703.4$ Å^3, $Z = 1$, $R_{gt}(F) = 0.022$, $wR_{ref}(F^2) = 0.055$, $T = 293$ K.

Source of material

Single crystals of $La_6I_{10}Os$ are obtained by reacting a stoichiometric mixture of LaI_3, La and Os (10:8:3 molar ratio) under Ar atmosphere in sealed Ta capsules at 1170 K for 12 days, yielding a pure phase. $La_6I_{10}Os$ forms black colored platelets sensitive to moisture.

Discussion

The crystal structure of $La_6I_{10}Os$ consists of La octahedra centered by Os atoms. The iodine atoms coordinate the La_6Os octahedra above the edges I(i) and the corners I(a) in the fashion of the $M_6I(i)_{12}I(a)_6$ cluster and do connect the clusters as $(La_6Os)I(i)_2I(i\text{-}i)_{4/2}I(i\text{-}a)_{6/2}I(a\text{-}i)_{6/2}$. The La—La distances range from 3.93 Å to 4.21 Å, the La—I distances are between 3.11 Å and 3.45 Å. The distances of La to Os vary between 2.71 Å and 2.97 Å. The title structure is isotypic to Y_6OsI_{10} [1], Y_6RuI_{10} [2] and Y_6IrI_{10} [2].

Table 1. Data collection and handling.

Crystal:	black platelet, size 0.03 × 0.16 × 0.2 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	129.29 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	18746, 4733
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4042
$N(param)_{refined}$:	80
Programs:	SHELXL-97 [3], ATOMS [4]

References

1. Hughbanks, T.; Corbett, J. D.: Encapsulation of Heavy Transition Metals in Iodide Clusters. Synthesis, Structure, and Bonding of Unusual Cluster Phase $Y_6I_{10}Ru$. Inorg. Chem. **28** (1989) 631-635.
2. Payne, M. W.; Corbett, J. D.: Encapsulation of the Platinum and Neighboring Metals within Cluster Iodides of Rare Earth Elements. Inorg. Chem. **29** (1990) 2246-2251.
3. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
4. Dowty, E.: ATOMS. A Complete Program for Displaying Atomic Structures. V. 5.0. Shape Software, Kingsport, Tennessee, USA 1999.

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}
Os(1)	1*f*	½	0	½	0.0092(1)	0.01091(9)	0.01013(8)	0.00391(7)	0.00308(6)	0.00459(6)
La(1)	2*i*	0.61890(3)	0.04092(3)	0.24896(2)	0.0143(1)	0.0167(1)	0.01645(9)	0.00642(8)	0.00404(7)	0.00718(8)
La(2)	2*i*	0.12869(3)	0.85702(3)	0.31902(2)	0.0110(1)	0.0177(1)	0.01513(9)	0.00530(8)	0.00358(7)	0.00659(8)
La(3)	2*i*	0.52624(3)	0.71825(3)	0.41575(2)	0.0137(1)	0.0176(1)	0.0180(1)	0.00636(8)	0.00487(8)	0.00831(8)
I(1)	2*i*	0.22558(5)	0.91087(5)	0.03556(3)	0.0199(2)	0.0538(2)	0.0182(1)	0.0008(2)	0.0022(1)	0.0184(1)
I(2)	2*i*	−0.05061(4)	0.81496(3)	−0.40980(3)	0.0126(1)	0.0208(1)	0.0214(1)	0.0059(1)	0.00395(9)	0.0096(1)
I(3)	2*i*	0.13134(5)	0.52533(4)	0.22100(4)	0.0256(2)	0.0167(1)	0.0453(2)	0.0037(1)	−0.0074(1)	0.0007(1)
I(4)	2*i*	−0.30739(4)	0.72410(3)	−0.86281(3)	0.0199(2)	0.0198(1)	0.0175(1)	0.0081(1)	0.00547(9)	0.00359(9)
I(5)	2*i*	0.58841(6)	0.37089(4)	0.31692(4)	0.0574(3)	0.0215(2)	0.0327(2)	0.0215(2)	0.0246(2)	0.0169(1)

* Correspondence author (e-mail: hj.mattausch@fkf.mpg.de)