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Crystal structure of lanthanum triiodate iodic acid, $La(IO_3)_3(HIO_3)$

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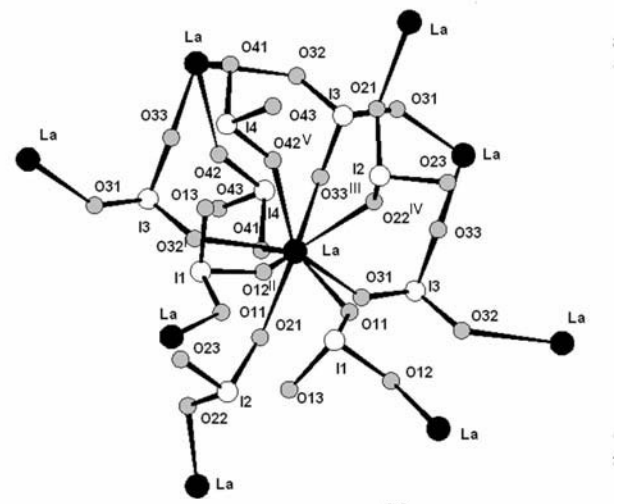

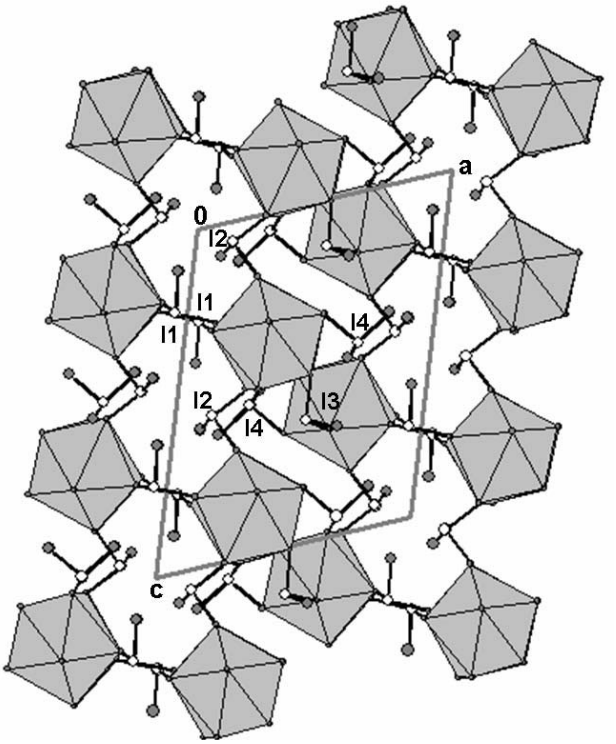

Abstract

HI_4LaO_{12}, monoclinic, $P12_1/c1$ (no. 14), a = 10.685(1) Å, b = 7.626(1) Å, c = 14.314(1) Å, β = 110.23(1)°, V = 1094.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.019, $wR_{ref}(F^2)$ = 0.040, T = 293 K.

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Source of material

0.5 mmol of anhydrous lanthanum chloride and 2.5 mmol of lithium iodate were dissolved in 40 ml of 7 M nitric acid . The solution was evaporated slowly at 323 K. After six days, transparent and colourless prismatic crystals suitable for X-ray crystal structure analysis were obtained. They were filtered, washed with deionised water and dried at room temperature (yield 0.33 g, 78 %).

Experimental details

Hydrogen atom from iodic acid molecule could not be located by difference Fourier analysis.

Discussion

Until now, $La(IO_3)_3(HIO_3)$ was only characterized by powder XRD (JCPDS file no 51-0075). The asymmetric unit of the title compound is made up of one lanthanum(III) cation, three iodate anions and one iodic acid ligand. The coordination number of the lanthanum cation is nine according to the bond valence sum concept with a valence value of 3.054 (for the expected value of 3) [1,2]. The La—O bond lengths are in the range of 2.428(3) to 2.674(3) Å and the O–La–O angles vary from 65.00(1)° to 143.98(1)°. The nine oxygen atoms come from seven iodate anions (two $I1O_3$, two $I2O_3$, three $I3O_3$ groups) and two iodic acid molecules ($HI4O_3$) (figure, top). The polyhedron can be described as a monocapped square antiprism with the O42^v (symmetry code v: $2-x,2-y,2-z$) capping atom corresponding to the longest La—O bond length. The mean deviations from calculated mean planes of the two square faces (O11–O21–O31–O41) and (O12^{ii}–O22^{iv}–O32^i–O33^{iii}) are equal to 0.480(3) Å and 0.122(3) Å, respectively (symmetry code i: $x,y+1,z$; ii: $-x,y+1/2,1/2-z$; iii: $1-x,-y,1-z$; iv: $x,1/2-y,z+1/2$). The dihedral angle between these faces is equal to 3.1(4)°. The environment of iodine is formed by three I—O strong bonds (mean bond length is 1.810(3) Å, except for the I4—O43 longest bond length of the iodic acid for which O43 is protonated with d(I4—O43) = 1.896(3) Å corresponding to an AX_3E configuration of the iodate anion and three additional weak bonds (bond lengths in the range 2.468(3) Å to 3.215(3) Å). This coordination is described as an octahedral with the iodine atom displaced off centre along the ternary axis [3]. Iodate groups shows two different coordination scheme towards lanthanum atom: $I1O_3$, $I2O_3$ and $I4O_3$ groups bridge two cations in a bis-monodentate way *via* O11, O12 , O21 , O22, O41 and O42 respectively, and $I3O_3$ group bridge three cations in a tris-monodentate way *via* its three oxygens. The crystal structure reveals a three-dimensional packing in which each lanthanum atom is connected to eight other lanthanum atoms through iodate bridges (figure, bottom). One lanthanum neighbour is linked *via* two $I3O_3$ and two $I4O_3$ groups, through an inversion centre, leading to eight-membered rings and to the shortest La···La distance equal to

5.739 Å. An other lanthanum neighbour is linked *via* two $I3O_3$ groups leading also to eight-membered ring and to a La···La distance equal to 6.045 Å. The six other lanthanum neighbours are connected by simple iodate bridges. The distances La···La are equivalent to two by two and they vary from 7.161 to 7.626 Å.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.10 × 0.11 × 0.12 mm
Wavelength:	Ag K_α radiation (0.56087 Å)
μ:	80.66 cm^{-1}
Diffractometer, scan mode:	Nonius Kappa CCD, φ/ω
$2\theta_{max}$:	42.82°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	20421, 2509
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2348
$N(param)_{refined}$:	154
Programs:	SIR92 [5], SHELXL-97 [6]

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	4*e*	0.31892(2)	0.26551(3)	0.36111(2)	0.0057(1)	0.0069(1)	0.0060(1)	0.00031(8)	0.00166(9)	–0.00025(9)
I(1)	4*e*	–0.04958(3)	0.13711(4)	0.22986(2)	0.0080(1)	0.0091(1)	0.0103(1)	–0.0013(1)	0.0026(1)	0.0005(1)
I(2)	4*e*	0.14970(3)	0.33711(4)	0.06055(2)	0.0098(1)	0.0082(1)	0.0073(1)	0.0004(1)	0.0033(1)	0.0002(1)
I(3)	4*e*	0.46513(2)	–0.23389(4)	0.36078(2)	0.0062(1)	0.0074(1)	0.0081(1)	0.00030(9)	0.0029(1)	0.0002(1)
I(4)	4*e*	0.70401(3)	0.31737(4)	0.44496(2)	0.0088(1)	0.0075(1)	0.0086(1)	0.00114(9)	0.0018(1)	–0.0001(1)
O(11)	4*e*	0.1215(3)	0.0701(4)	0.2887(3)	0.006(1)	0.012(2)	0.027(2)	–0.002(1)	–0.003(1)	0.003(1)
O(12)	4*e*	–0.1045(3)	–0.0864(4)	0.1922(3)	0.009(1)	0.011(2)	0.022(2)	–0.002(1)	0.003(1)	–0.001(1)
O(13)	4*e*	–0.0558(3)	0.2143(5)	0.1089(2)	0.018(2)	0.023(2)	0.013(2)	–0.002(1)	0.004(1)	0.007(1)
O(21)	4*e*	0.2673(3)	0.2699(5)	0.1800(2)	0.018(2)	0.025(2)	0.008(2)	0.008(1)	0.005(1)	0.005(1)
O(22)	4*e*	0.2738(3)	0.3996(4)	0.0056(2)	0.019(2)	0.014(2)	0.015(2)	0.001(1)	0.011(1)	0.002(1)
O(23)	4*e*	0.1071(3)	0.5509(4)	0.0924(2)	0.023(2)	0.009(2)	0.018(2)	0.005(1)	0.007(1)	–0.000(1)
O(31)	4*e*	0.3724(3)	–0.0356(4)	0.3175(2)	0.023(2)	0.011(2)	0.017(2)	0.009(1)	0.003(1)	0.001(1)
O(32)	4*e*	0.3362(3)	–0.3978(4)	0.3197(2)	0.015(2)	0.014(2)	0.016(2)	–0.007(1)	0.003(1)	–0.001(1)
O(33)	4*e*	0.4703(3)	–0.2195(4)	0.4900(2)	0.010(1)	0.020(2)	0.008(2)	–0.000(1)	0.003(1)	–0.001(1)
O(41)	4*e*	0.5539(3)	0.2930(5)	0.3362(2)	0.009(1)	0.032(2)	0.009(2)	–0.001(1)	–0.001(1)	0.002(1)
O(42)	4*e*	0.6721(3)	0.5311(4)	0.4845(3)	0.026(2)	0.007(2)	0.018(2)	0.003(1)	0.011(1)	–0.002(1)
O(43)	4*e*	0.8180(3)	0.4000(5)	0.3783(3)	0.016(2)	0.020(2)	0.022(2)	–0.002(1)	0.012(1)	0.005(1)

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