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Poly[aqua(μ_5-2-oxido-4-sulfonato-benzoato)lanthanum(III)]

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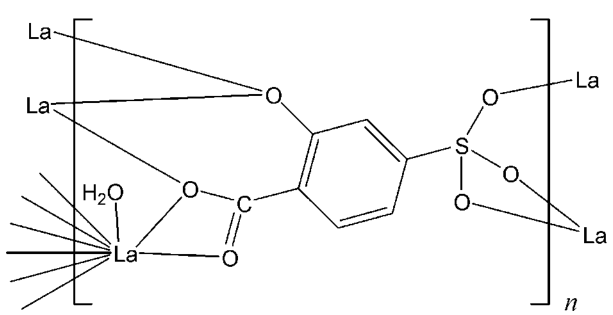
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 11.3.

The title compound, $[La(C_7H_3O_6S)(H_2O)]_n$, forms a three-dimensional framework in which the asymmetric unit contains one La^{III} atom, one 5-sulfosalicylate (2-oxido-4-sulfonato-benzoate) ligand and one coordinated water molecule. The La^{III} atom is coordinated by nine O atoms from three carboxylate, three sulfonate and two hydroxyl groups, and one water molecule, forming a distorted trigonal-prismatic square-face tricapped geometry.

Related literature

For the use of rigid carboxylate ligands in the design and synthesis of a variety of structures, see: Cao *et al.* (2002); Li *et al.* (2004, 2005). For the structure of the isotypic Nd compound, see: Wang *et al.* (2004).



Experimental

Crystal data

$[La(C_7H_3O_6S)(H_2O)]$
M_r = 372.08
Triclinic, $P\overline{1}$
a = 6.2297 (7) Å
b = 8.2390 (8) Å
c = 9.9157 (9) Å
α = 111.587 (2)°
β = 94.325 (2)°
γ = 93.785 (2)°
V = 469.47 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.79 mm^{-1}
T = 293 K
0.24 × 0.16 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.415, T_{max} = 0.563
2457 measured reflections
1633 independent reflections
1527 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.07
1633 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −1.66 e Å^{-3}

Table 1
Selected bond lengths (Å).

La1—O1^{i}	2.676 (5)	La1—O4	2.573 (5)
La1—O2^{ii}	2.449 (5)	La1—O5	2.970 (7)
La1—O2^{i}	2.561 (5)	La1—O6^{iv}	2.548 (5)
La1—O3^{iii}	2.478 (4)	La1—O7	2.501 (5)
La1—O3^{ii}	2.499 (4)		

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, y, z+1$; (iii) $-x+2, -y+1, -z$; (iv) $-x+2, -y+2, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2373).

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supporting information

Acta Cryst. (2009). E**65**, m383 [doi:10.1107/S1600536809007879]

Poly[aqua(μ_5-2-oxido-4-sulfonatobenzoato)lanthanum(III)]

Cheng-Feng Zhu, Xing Li and Enhong Sheng

S1. Comment

The carboxylate groups have a strong ability to bond various metal ions and afford abundant coordination modes, thus rigid carboxylate ligands have been widely used for the design and synthesis of a great variety of structures (Cao *et al.*, 2002; Li *et al.*, 2004). Introduction of a sulfonate group into rigid carboxylate ligands may result in the formation of unexpected frameworks as the sulfonic group has a different shape and properties in terms of its coordination ability compared to the carboxylate group (Li *et al.*, 2005).

Studies on the coordination chemistry of mixed carboxylate-sulfonic ligands are not very common. By employing 5-sulfoisophthalic acid as an organic ligand, we have successfully prepared one new metal-organic polymer $[La(C_7H_3O_6S)(H_2O)]_n$ with three dimensional framework by the bridging carboxylate and the sulfonate groups. Single X-ray diffraction analysis reveals that the title complex is isomorphous to the La-compound reported previously (Wang *et al.*, 2004). As Fig. 1 shown, the lanthanum(III) atom is surrounded by nine oxygen atoms, of which three come from carboxylate groups, three from sulfonates, two from hydroxyl groups and one from the coordinated water. The sulfosalicylate ligands serve as μ_5-bridge linking five La(III) ions (Fig. 2), resulting in a three dimensional framework.

S2. Experimental

A mixture of 5-sulfosalicylic acid (0.60 mmol, 0.15 g), La_2O_3 (0.2 mmol, 0.065 g) and H_2O (15 ml) was sealed in a 25 ml stainless steel reactor with Teflon linear and heated 433 K for 72 h. After cooling to room temperature, colorless crystals were isolated by filtering (yield 35%).

S3. Refinement

Aromatic hydrogen atoms were assigned to calculated positions and allowed to ride on their respective parent C atoms with isotropic thermal displacement parameters. For the hydrogen atoms bonded to coordination water oxygen atom, The H7A was positioned geometrically and H7B was located in a difference map and constrained with O—H = 0.82 Å. The deepest residual electron density peak is located at 0.87 Å from atom La1.

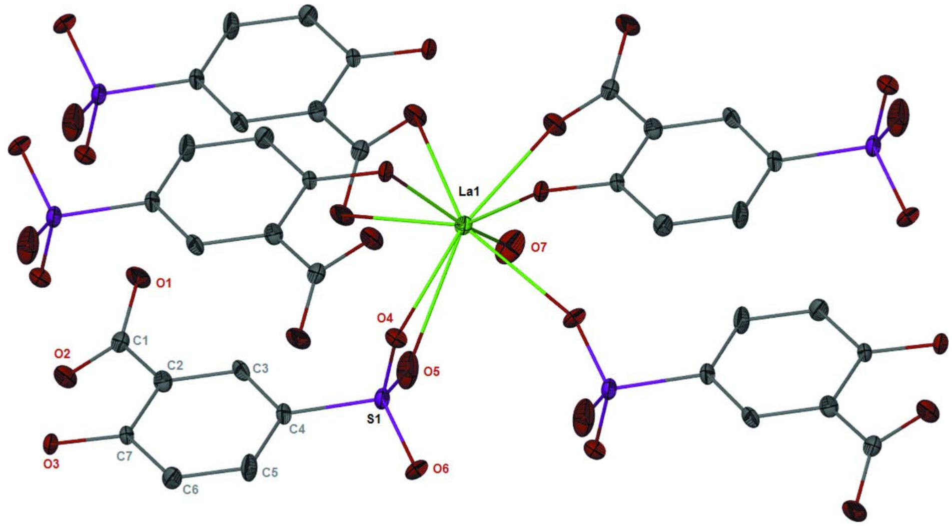

Figure 1

A view of the lanthanum ion coordination, Displacement ellipsoids are drawn at the 50% probability level.

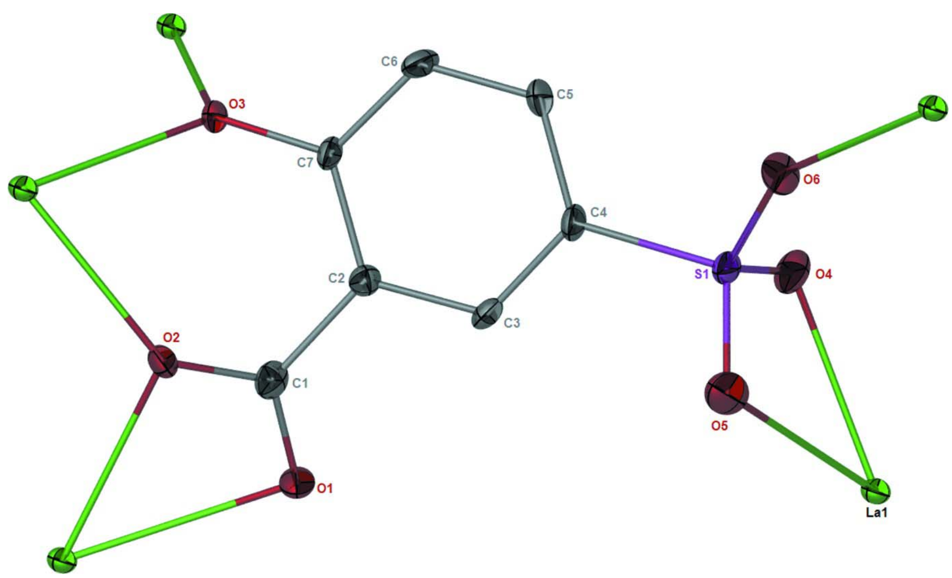

Figure 2

The sulfosalicylate ligands linking fashion.

Poly[aqua(μ_5-2-oxido-4-sulfonatobenzoato)lanthanum(III)]

Crystal data

[La($C_7H_3O_6S$)(H_2O)]
M_r = 372.08
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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c = 9.9157 (9) Å
α = 111.587 (2)°
β = 94.325 (2)°
γ = 93.785 (2)°
V = 469.47 (8) Å^3
Z = 2
F(000) = 352
D_x = 2.632 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2088 reflections
θ = 2.2–25.1°
μ = 4.79 mm^{-1}

T = 293 K	0.24 × 0.16 × 0.12 mm
Block, colorless	

Data collection

Siemens SMART CCD area-detector diffractometer	2457 measured reflections
Radiation source: fine-focus sealed tube	1633 independent reflections
Graphite monochromator	1527 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.029
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.1°, θ_{min} = 2.2°
T_{min} = 0.415, T_{max} = 0.563	$h = -4 \rightarrow 7$
	$k = -9 \rightarrow 9$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.090	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 4.598P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
1633 reflections	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −1.66 e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
La1	0.76441 (5)	0.64763 (5)	0.46004 (4)	0.01280 (16)
S1	0.9837 (3)	0.8865 (2)	0.28204 (17)	0.0167 (4)
O1	0.4823 (8)	0.4571 (7)	−0.2043 (5)	0.0258 (12)
O2	0.5737 (8)	0.5722 (7)	−0.3605 (5)	0.0215 (11)
O3	1.0224 (7)	0.6040 (6)	−0.3536 (5)	0.0139 (9)
O4	1.0612 (9)	0.7528 (6)	0.3353 (5)	0.0229 (11)
O5	0.7603 (9)	0.9023 (8)	0.3122 (6)	0.0360 (14)
O6	1.1278 (9)	1.0487 (6)	0.3439 (5)	0.0237 (11)
O7	0.4427 (9)	0.8190 (7)	0.5052 (7)	0.0332 (13)
H7A	0.3472	0.7722	0.4375	0.040*
H7B	0.4185	0.9029	0.5766	0.040*
C1	0.6163 (12)	0.5488 (9)	−0.2412 (7)	0.0181 (14)
C2	0.8185 (11)	0.6385 (9)	−0.1475 (7)	0.0150 (13)
C3	0.8153 (11)	0.7035 (9)	0.0033 (7)	0.0153 (13)

H3A	0.6938	0.6777	0.0437	0.018*
C4	0.9937 (11)	0.8069 (9)	0.0930 (7)	0.0168 (14)
C5	1.1779 (12)	0.8448 (10)	0.0340 (7)	0.0210 (15)
H5A	1.2964	0.9148	0.0953	0.025*
C6	1.1846 (11)	0.7790 (9)	−0.1142 (8)	0.0192 (14)
H6A	1.3085	0.8041	−0.1526	0.023*
C7	1.0069 (11)	0.6740 (8)	−0.2089 (7)	0.0141 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0098 (2)	0.0143 (2)	0.0121 (2)	−0.00092 (15)	0.00131 (14)	0.00277 (16)
S1	0.0185 (8)	0.0174 (8)	0.0098 (8)	−0.0033 (7)	0.0027 (6)	0.0005 (6)
O1	0.023 (3)	0.034 (3)	0.019 (3)	−0.016 (2)	−0.001 (2)	0.012 (2)
O2	0.017 (2)	0.031 (3)	0.016 (3)	−0.009 (2)	−0.005 (2)	0.012 (2)
O3	0.015 (2)	0.015 (2)	0.009 (2)	0.0004 (18)	0.0007 (18)	0.0012 (18)
O4	0.034 (3)	0.019 (2)	0.017 (3)	−0.002 (2)	0.005 (2)	0.009 (2)
O5	0.025 (3)	0.047 (4)	0.022 (3)	0.001 (3)	0.008 (2)	−0.004 (3)
O6	0.031 (3)	0.014 (2)	0.020 (3)	−0.010 (2)	−0.001 (2)	0.001 (2)
O7	0.023 (3)	0.030 (3)	0.037 (3)	0.010 (2)	0.003 (2)	0.000 (3)
C1	0.024 (4)	0.014 (3)	0.014 (3)	0.000 (3)	0.004 (3)	0.002 (3)
C2	0.014 (3)	0.018 (3)	0.014 (3)	0.004 (3)	0.003 (3)	0.005 (3)
C3	0.017 (3)	0.019 (3)	0.012 (3)	0.003 (3)	0.007 (3)	0.007 (3)
C4	0.022 (3)	0.018 (3)	0.008 (3)	−0.002 (3)	0.001 (3)	0.003 (3)
C5	0.019 (3)	0.028 (4)	0.010 (3)	−0.003 (3)	−0.001 (3)	0.001 (3)
C6	0.017 (3)	0.020 (3)	0.017 (3)	−0.003 (3)	0.008 (3)	0.002 (3)
C7	0.019 (3)	0.014 (3)	0.008 (3)	−0.001 (3)	0.002 (3)	0.003 (3)

Geometric parameters (Å, º)

La1—O1^{i}	2.676 (5)	O2—C1	1.279 (9)
La1—O2^{ii}	2.449 (5)	O3—C7	1.349 (8)
La1—O2^{i}	2.561 (5)	O7—H7A	0.8200
La1—O3^{iii}	2.478 (4)	O7—H7B	0.8200
La1—O3^{ii}	2.499 (4)	C1—C2	1.480 (10)
La1—O4	2.573 (5)	C2—C3	1.393 (9)
La1—O5	2.970 (7)	C2—C7	1.424 (9)
La1—O6^{iv}	2.548 (5)	C3—C4	1.385 (10)
La1—O7	2.501 (5)	C3—H3A	0.9300
S1—O4	1.478 (5)	C4—C5	1.395 (10)
S1—O5	1.450 (6)	C5—C6	1.372 (10)
S1—O6	1.457 (5)	C5—H5A	0.9300
S1—C4	1.751 (7)	C6—C7	1.405 (10)
O1—C1	1.251 (9)	C6—H6A	0.9300
O2^{ii}—La1—O3^{iii}	103.65 (16)	O6—S1—O4	110.7 (3)
O2^{ii}—La1—O3^{ii}	68.47 (15)	O5—S1—C4	109.1 (3)
O3^{iii}—La1—O3^{ii}	67.24 (16)	O6—S1—C4	107.0 (3)

O2^{ii}—La1—O7	72.75 (19)	O4—S1—C4	107.5 (3)
O3^{iii}—La1—O7	158.70 (17)	C1—O1—La1^{i}	93.1 (4)
O3^{ii}—La1—O7	127.17 (17)	C1—O2—La1^{v}	139.2 (4)
O2^{ii}—La1—O6^{iv}	87.98 (17)	C1—O2—La1^{i}	97.8 (4)
O3^{iii}—La1—O6^{iv}	131.23 (16)	La1^{v}—O2—La1^{i}	116.49 (18)
O3^{ii}—La1—O6^{iv}	74.06 (16)	C7—O3—La1^{iii}	121.3 (4)
O7—La1—O6^{iv}	70.05 (18)	C7—O3—La1^{v}	123.5 (4)
O2^{ii}—La1—O2^{i}	63.51 (18)	La1^{iii}—O3—La1^{v}	112.76 (16)
O3^{iii}—La1—O2^{i}	86.88 (16)	S1—O4—La1	110.1 (3)
O3^{ii}—La1—O2^{i}	116.96 (15)	S1—O5—La1	93.3 (3)
O7—La1—O2^{i}	72.64 (18)	S1—O6—La1^{iv}	151.0 (3)
O6^{iv}—La1—O2^{i}	138.33 (17)	La1—O7—H7A	109.5
O2^{ii}—La1—O4	162.22 (17)	La1—O7—H7B	130.5
O3^{iii}—La1—O4	73.55 (15)	H7A—O7—H7B	119.7
O3^{ii}—La1—O4	94.76 (16)	O1—C1—O2	119.2 (6)
O7—La1—O4	116.21 (18)	O1—C1—C2	122.1 (6)
O6^{iv}—La1—O4	81.48 (16)	O2—C1—C2	118.6 (6)
O2^{i}—La1—O4	132.71 (16)	C3—C2—C7	120.0 (6)
O2^{ii}—La1—O1^{i}	110.68 (15)	C3—C2—C1	118.6 (6)
O3^{iii}—La1—O1^{i}	88.69 (16)	C7—C2—C1	121.1 (6)
O3^{ii}—La1—O1^{i}	154.12 (16)	C4—C3—C2	119.7 (6)
O7—La1—O1^{i}	73.65 (18)	C4—C3—H3A	120.1
O6^{iv}—La1—O1^{i}	131.55 (17)	C2—C3—H3A	120.1
O2^{i}—La1—O1^{i}	49.19 (15)	C3—C4—C5	120.7 (6)
O4—La1—O1^{i}	86.95 (15)	C3—C4—S1	118.5 (5)
O2^{ii}—La1—O5	139.80 (16)	C5—C4—S1	120.8 (5)
O3^{iii}—La1—O5	115.64 (15)	C6—C5—C4	120.1 (6)
O3^{ii}—La1—O5	134.13 (15)	C6—C5—H5A	120.0
O7—La1—O5	67.57 (18)	C4—C5—H5A	120.0
O6^{iv}—La1—O5	72.93 (16)	C5—C6—C7	120.9 (6)
O2^{i}—La1—O5	108.88 (15)	C5—C6—H6A	119.5
O4—La1—O5	49.58 (16)	C7—C6—H6A	119.5
O1^{i}—La1—O5	64.08 (16)	O3—C7—C6	119.5 (6)
O5—S1—O6	115.5 (3)	O3—C7—C2	122.0 (6)
O5—S1—O4	106.9 (3)	C6—C7—C2	118.4 (6)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, y, z+1$; (iii) $-x+2, -y+1, -z$; (iv) $-x+2, -y+2, -z+1$; (v) $x, y, z-1$.