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Tetrasodium(I) pentaoxalatodilanthanate(III) dihydrate

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The La atom in the title compound, $Na_4[La_2(C_2O_4)_5]\cdot 2H_2O$, is chelated by five oxalate groups in a bicapped square-antiprismatic geometry; one oxalate ligand is located on a centre of inversion. All oxalate groups function in a μ_2-bridging mode, resulting in a three-dimensional network architecture. The Na^+ cations are octahedrally coordinated by oxalate O atoms and water molecules, the latter bridging pairs of cations.

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.025
wR factor = 0.080
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Crystal structures of monovalent polyoxalatolanthanates that have been reported include, for example, $M\mathrm{La}(H_2O)_2(C_2O_4)_2\cdot H_2O$ (M = K, NH_4; Bataille, Auffrédic & Louër, 2000), $K_3Ln(C_2O_4)_3\cdot 2H_2O$ (Ln = Eu, Gd, Nd, Sm, Tb), $K_8Ln_2(C_2O_4)_7.14H_2O$ (Ln = Dy, Er, Tb, Y, Yb) (Kahwa *et al.*, 1984), $NH_4Ln(C_2O_4)_2\cdot H_2O$ (Ln = Sm to Tm, Y; McDonald & Spink, 1967), $MLn(C_2O_4)_2\cdot nH_2O$ (M = Li, Ln = La to Gd, n = 2; M = Na, Ln = Ce to Nd, n = 3; Roméro *et al.*, 1995), $NH_4Gd(H_2O)(C_2O_4)_2$, $NH_4La(C_2O_4)_2$ (Trombe *et al.*, 2001), $NaY(H_2O)(C_2O_4)_2\cdot 3H_2O$ (Bataille & Louër, 1999) and $CsY(H_2O)(C_2O_4)_2$ (Bataille, Louër *et al.*, 2000). Recently, a series of oxalatolanthanates (La, Nd, Yb) with 1,2- or 1,3-diammoniumpropane as counter-ion has been reported in which the La atom is chelated by five oxalate groups (Mohanu

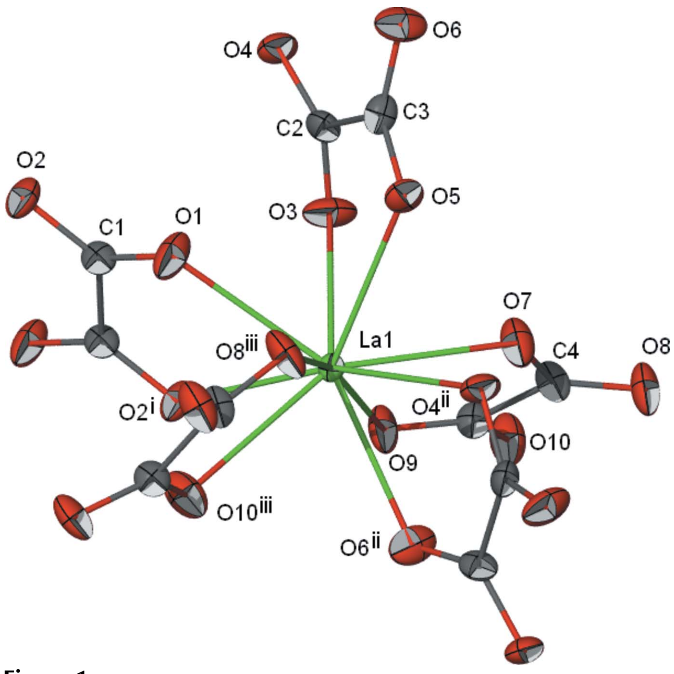

Figure 1
Fig. 1. The coordination of lanthanum with displacement ellipsoids drawn at the 50% probability level. Symmetry codes are given in Table 1.

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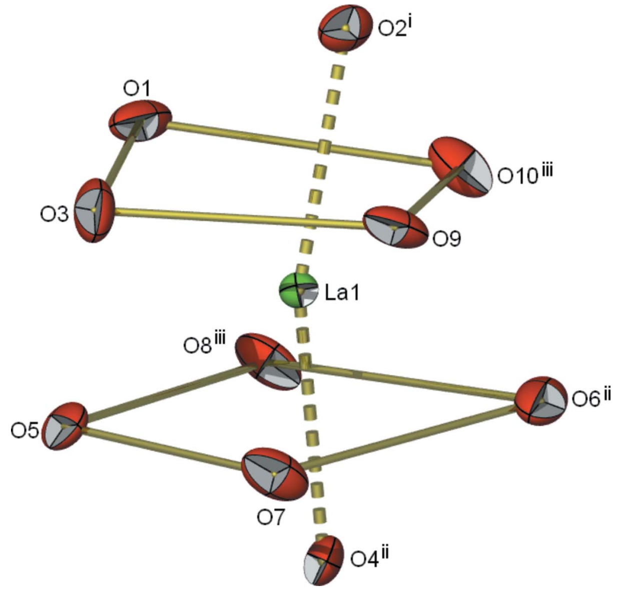

Figure 2

Fig. 2. Bicapped square-antiprismatic coordination geometry of La.

et al., 2006). Ten-coordinate lanthanum arising from chelation by five oxalate groups is also found in the title compound, $[(H_2O)_2Na_4][(C_2O_4)_5La_2]$ (Fig. 1). The O atoms that surround the central metal atom approximate a bicapped square-antiprismatic polyhedron. All oxalate groups function in a μ_2-bridging mode, resulting in a three-dimensional network architecture. One oxalate ligand is located on a centre of inversion. The Na^+ cations are octahedrally coordinated by oxalate O atoms and water molecules, the latter bridging pairs of cations. The network is further consolidated by hydrogen bonds (Table 2).

Experimental

A mixture of lanthanum(III) nitrate *x*-hydrate (0.217 g, 0.5 mmol), oxalic acid dihydrate ((0.252 g, 2 mmol), nicotinic acid (0.123 g, 1 mmol), sodium hydroxide (0.200 g, 5 mmol) and water (10 ml) was placed in a 15-ml Teflon-lined stainless-steel Parr bomb. The bomb was heated at 433 K for 72 h. Colourless crystals were isolated from the cool solution in about 50% yield.

Crystal data

$Na_4[La_2(C_2O_4)_5]\cdot 2H_2O$
$M_r = 845.91$
Monoclinic, $P2_1/n$
$a = 7.8410\ (4)$ Å
$b = 11.6990\ (7)$ Å
$c = 12.0084\ (7)$ Å
$\beta = 100.943\ (1)^\circ$
$V = 1081.5\ (1)$ Å^3

$Z = 2$
$D_x = 2.598$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.09$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.23 × 0.16 × 0.13 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.453$, $T_{\max} = 0.619$ (expected range = 0.430–0.588)

5919 measured reflections
2400 independent reflections
2277 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.080$
$S = 1.23$
2400 reflections
180 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 5.3936P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.76$ e Å^{-3}
$\Delta\rho_{\min} = -0.77$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

La1—O1	2.553 (4)	La1—O6^{ii}	2.551 (4)
La1—O2^{i}	2.568 (3)	La1—O7	2.553 (4)
La1—O3	2.541 (4)	La1—O8^{iii}	2.565 (4)
La1—O4^{ii}	2.701 (4)	La1—O9	2.670 (4)
La1—O5	2.605 (3)	La1—O10^{iii}	2.693 (4)
O1—La1—O2^{i}	63.6 (1)	O3—La1—O10^{iii}	134.7 (1)
O1—La1—O3	68.7 (1)	O4^{ii}—La1—O5	64.4 (1)
O1—La1—O4^{ii}	122.1 (1)	O4^{ii}—La1—O6^{ii}	62.2 (1)
O1—La1—O5	75.8 (1)	O4^{ii}—La1—O7	62.5 (1)
O1—La1—O6^{ii}	146.0 (1)	O4^{ii}—La1—O8^{iii}	59.9 (1)
O1—La1—O7	137.7 (1)	O4^{ii}—La1—O9	115.2 (1)
O1—La1—O8^{iii}	68.3 (1)	O4^{ii}—La1—O10^{iii}	100.8 (1)
O1—La1—O9	120.8 (1)	O5—La1—O6^{ii}	125.2 (1)
O1—La1—O10^{iii}	73.9 (1)	O5—La1—O7	69.9 (1)
O2^{i}—La1—O3	76.2 (1)	O5—La1—O8^{iii}	70.4 (1)
O2^{i}—La1—O4^{ii}	163.3 (1)	O5—La1—O9	120.5 (1)
O2^{i}—La1—O5	130.7 (1)	O5—La1—O10^{iii}	129.8 (1)
O2^{i}—La1—O6^{ii}	103.9 (1)	O6^{ii}—La1—O7	76.0 (1)
O2^{i}—La1—O7	125.7 (1)	O6^{ii}—La1—O8^{iii}	92.3 (1)
O2^{i}—La1—O8^{iii}	114.7 (1)	O6^{ii}—La1—O9	74.6 (1)
O2^{i}—La1—O9	65.9 (1)	O6^{ii}—La1—O10^{iii}	72.2 (1)
O2^{i}—La1—O10^{iii}	64.6 (1)	O7—La1—O8^{iii}	119.6 (1)
O3—La1—O4^{ii}	120.4 (1)	O7—La1—O9	61.9 (1)
O3—La1—O5	63.4 (1)	O7—La1—O10^{iii}	148.2 (1)
O3—La1—O6^{ii}	142.3 (1)	O8^{iii}—La1—O9	166.2 (1)
O3—La1—O7	74.2 (1)	O8^{iii}—La1—O10^{iii}	61.6 (1)
O3—La1—O8^{iii}	122.5 (1)	O9—La1—O10^{iii}	109.4 (1)
O3—La1—O9	71.3 (1)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1···O3^{iv}	0.85 (1)	2.06 (3)	2.865 (6)	159 (7)
O1w—H2···O6^{v}	0.85 (1)	1.97 (2)	2.811 (5)	168 (6)

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

The water H atoms were located in a difference Fourier map and were refined with distance restraints of O–H 0.85 (1) and H···H 1.39 (1) Å. The displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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