

Bis(μ -2-methylquinolin-1-ium-8-olato- κ^2 O:O')bis[(2-methylquinolin-1-ium-8-olato- κ O)tris(nitrato- κ^2 O,O')-lanthanum(III)]

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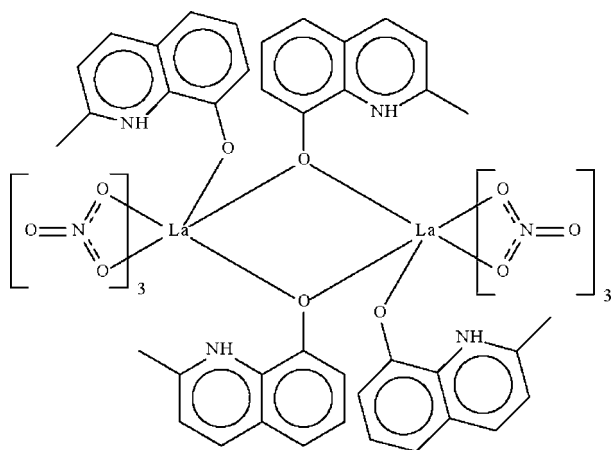
Received 19 May 2009; accepted 25 May 2009

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.022; wR factor = 0.057; data-to-parameter ratio = 15.3.

The two independent N -heterocycles in the centrosymmetric title compound, $[\text{La}_2(\text{C}_{10}\text{H}_9\text{NO})_4(\text{NO}_3)_6]$, exist in the zwitterionic form. One of these binds to one metal center, whereas the other bridges two metal centers. The La atom is chelated by three nitrate groups and is surrounded by nine O atoms in a coordination environment based on a distorted monocapped square-antiprism. The dinuclear structure is further stabilized by intramolecular $\text{N}-\text{H}\cdots\text{O}$ (nitrate) hydrogen bonds.

Related literature

The N -heterocycle exists in the deprotonated and neutral form in hexakis(μ -2-methylquinolin-8-oxido)bis(2-methylquinolin-8-oxido(2-methyl-8-quinolinol)(nitrato)trilanthanum methanol solvate; see: Katkova *et al.* (2005).



Experimental

Crystal data

$[\text{La}_2(\text{C}_{10}\text{H}_9\text{NO})_4(\text{NO}_3)_6]$
 $M_r = 1286.61$
 Monoclinic, $P2_1/n$
 $a = 10.7177$ (2) Å
 $b = 18.3308$ (3) Å
 $c = 12.4473$ (2) Å
 $\beta = 109.952$ (1)°

$V = 2298.67$ (7) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.93$ mm⁻¹
 $T = 100$ K
 $0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART APEX diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.699$, $T_{\max} = 0.830$

28922 measured reflections
 5258 independent reflections
 4897 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.057$
 $S = 1.05$
 5258 reflections
 344 parameters
 2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O4}^i$	0.88 (1)	2.39 (2)	3.115 (3)	140 (2)
$\text{N2}-\text{H2}\cdots\text{O3}$	0.87 (1)	2.08 (1)	2.950 (2)	173 (2)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2454).

References

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Acta Cryst. (2009). E65, m711 [doi:10.1107/S1600536809019746]

Bis(μ -2-methylquinolin-1-ium-8-olato- $\kappa^2O:O'$)bis[(2-methylquinolin-1-ium-8-olato- κO)tris(nitrato- κ^2O,O')]lanthanum(III)]

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Experimental

2-Methyl-8-hydroxyquinoline (0.32 g, 2 mmol) was added to lanthanum nitrate hexahydrate (0.43 g, 1 mmol) in methanol (10 ml). The mixture was stirred for an hour and then filtered. Slow evaporation of solution gave yellow crystals that are stable when heated up to 573 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 to 1.5 $U(C)$. The nitrogen-bound hydrogen atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H 0.88±01 Å; their temperature factors were freely refined.

Figures

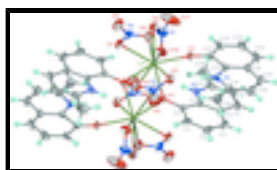


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $[La(NO_3)_3(C_{10}H_9NO)_2]_2$; ellipsoids are drawn at the 70% probability level and H atoms of arbitrary radius.

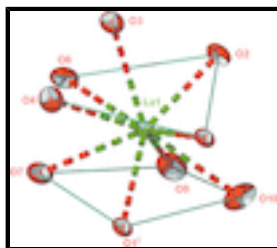


Fig. 2. Monocapped square-antiprismatic geometry of La.

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$[La_2(C_{10}H_9NO)_4(NO_3)_6]$

$M_r = 1286.61$

Monoclinic, $P2_1/n$

$F_{000} = 1272$

$D_x = 1.859 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: -P 2yn
 $a = 10.7177$ (2) Å
 $b = 18.3308$ (3) Å
 $c = 12.4473$ (2) Å
 $\beta = 109.952$ (1)°
 $V = 2298.67$ (7) Å³
 $Z = 2$

Cell parameters from 9940 reflections
 $\theta = 2.3$ – 28.3 °
 $\mu = 1.93$ mm⁻¹
 $T = 100$ K
Block, yellow
 $0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART APEX
diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 100$ K
 ω scans
Absorption correction: Multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.699$, $T_{\max} = 0.830$
28922 measured reflections

5258 independent reflections
4897 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 27.5$ °
 $\theta_{\text{min}} = 2.1$ °
 $h = -13 \rightarrow 13$
 $k = -23 \rightarrow 23$
 $l = -16 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.057$
 $S = 1.05$
5258 reflections
344 parameters
2 restraints
Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring
sites
H atoms treated by a mixture of
independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 2.866P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³
Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
La1	0.627521 (11)	0.471863 (6)	0.661979 (10)	0.01366 (5)
O1	0.39482 (14)	0.47330 (8)	0.52498 (13)	0.0153 (3)
O2	0.55263 (15)	0.38409 (8)	0.76113 (14)	0.0197 (3)
O3	0.51647 (17)	0.53810 (9)	0.79000 (15)	0.0241 (3)
O4	0.57975 (17)	0.61199 (9)	0.68318 (15)	0.0259 (4)
O5	0.4652 (2)	0.65310 (11)	0.7854 (2)	0.0433 (5)
O6	0.81044 (17)	0.50974 (11)	0.84912 (14)	0.0281 (4)
O7	0.84706 (16)	0.54647 (10)	0.69668 (14)	0.0249 (3)

O8	0.97394 (18)	0.58366 (12)	0.86437 (17)	0.0380 (5)
O9	0.81082 (16)	0.37627 (10)	0.69806 (16)	0.0287 (4)
O10	0.63565 (19)	0.34935 (10)	0.55359 (15)	0.0311 (4)
O11	0.7770 (3)	0.26474 (13)	0.6382 (2)	0.0668 (8)
N1	0.31296 (18)	0.33149 (10)	0.50479 (16)	0.0185 (4)
H1	0.379 (2)	0.3456 (15)	0.483 (2)	0.026 (7)*
N2	0.37563 (17)	0.42049 (11)	0.86348 (15)	0.0178 (4)
H2	0.423 (2)	0.4525 (11)	0.842 (2)	0.017 (6)*
N3	0.51907 (19)	0.60337 (11)	0.75377 (18)	0.0234 (4)
N4	0.87999 (19)	0.54744 (12)	0.80494 (18)	0.0234 (4)
N5	0.7429 (2)	0.32815 (12)	0.62974 (19)	0.0313 (5)
C1	0.2499 (2)	0.38214 (12)	0.54963 (17)	0.0156 (4)
C2	0.2910 (2)	0.45585 (12)	0.55661 (17)	0.0151 (4)
C3	0.2200 (2)	0.50601 (13)	0.59584 (19)	0.0201 (4)
H3	0.2432	0.5562	0.5991	0.024*
C4	0.1140 (2)	0.48398 (15)	0.6309 (2)	0.0255 (5)
H4	0.0661	0.5197	0.6563	0.031*
C5	0.0788 (2)	0.41235 (15)	0.6292 (2)	0.0263 (5)
H5	0.0089	0.3982	0.6555	0.032*
C6	0.1471 (2)	0.35933 (13)	0.58808 (18)	0.0211 (4)
C7	0.1194 (2)	0.28332 (14)	0.5841 (2)	0.0281 (5)
H7	0.0524	0.2656	0.6114	0.034*
C8	0.1881 (3)	0.23603 (13)	0.5416 (2)	0.0290 (5)
H8	0.1694	0.1853	0.5408	0.035*
C9	0.2862 (2)	0.26032 (12)	0.49867 (19)	0.0235 (5)
C10	0.3615 (3)	0.21221 (14)	0.4471 (2)	0.0340 (6)
H10A	0.3016	0.1754	0.3991	0.051*
H10B	0.4328	0.1879	0.5078	0.051*
H10C	0.3997	0.2415	0.4001	0.051*
C11	0.3925 (2)	0.34856 (12)	0.84219 (18)	0.0176 (4)
C12	0.4870 (2)	0.33087 (12)	0.78824 (18)	0.0173 (4)
C13	0.5007 (2)	0.25687 (12)	0.76861 (19)	0.0213 (4)
H13	0.5619	0.2422	0.7327	0.026*
C14	0.4262 (3)	0.20362 (13)	0.8008 (2)	0.0265 (5)
H14	0.4391	0.1537	0.7868	0.032*
C15	0.3352 (3)	0.22155 (14)	0.8518 (2)	0.0280 (5)
H15	0.2859	0.1845	0.8727	0.034*
C16	0.3157 (2)	0.29544 (13)	0.87294 (19)	0.0222 (5)
C17	0.2211 (2)	0.32082 (15)	0.9205 (2)	0.0293 (5)
H17	0.1653	0.2866	0.9396	0.035*
C18	0.2081 (2)	0.39351 (15)	0.9397 (2)	0.0286 (5)
H18	0.1446	0.4093	0.9725	0.034*
C19	0.2892 (2)	0.44488 (14)	0.91067 (19)	0.0229 (5)
C20	0.2841 (3)	0.52479 (14)	0.9304 (2)	0.0278 (5)
H20A	0.3358	0.5506	0.8908	0.042*
H20B	0.3216	0.5349	1.0125	0.042*
H20C	0.1917	0.5414	0.9009	0.042*

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Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.01291 (7)	0.01585 (7)	0.01372 (7)	-0.00115 (4)	0.00648 (5)	0.00089 (4)
O1	0.0135 (7)	0.0175 (7)	0.0165 (7)	-0.0023 (5)	0.0073 (6)	0.0011 (6)
O2	0.0205 (7)	0.0183 (7)	0.0243 (8)	0.0005 (6)	0.0129 (6)	0.0048 (6)
O3	0.0275 (9)	0.0219 (8)	0.0293 (9)	-0.0028 (6)	0.0182 (7)	-0.0025 (7)
O4	0.0336 (9)	0.0189 (8)	0.0277 (9)	-0.0011 (7)	0.0135 (7)	0.0016 (7)
O5	0.0421 (11)	0.0277 (10)	0.0687 (15)	0.0063 (8)	0.0302 (11)	-0.0141 (10)
O6	0.0249 (9)	0.0433 (10)	0.0175 (8)	-0.0090 (8)	0.0092 (7)	-0.0023 (7)
O7	0.0203 (8)	0.0363 (9)	0.0202 (8)	-0.0081 (7)	0.0094 (6)	-0.0026 (7)
O8	0.0248 (9)	0.0518 (12)	0.0333 (10)	-0.0167 (8)	0.0045 (8)	-0.0121 (9)
O9	0.0206 (8)	0.0328 (9)	0.0354 (10)	0.0050 (7)	0.0129 (7)	0.0039 (8)
O10	0.0399 (10)	0.0305 (9)	0.0211 (9)	0.0092 (8)	0.0079 (8)	-0.0024 (7)
O11	0.105 (2)	0.0392 (13)	0.0404 (13)	0.0431 (14)	0.0049 (13)	-0.0060 (10)
N1	0.0187 (9)	0.0173 (9)	0.0174 (9)	-0.0025 (7)	0.0035 (7)	0.0021 (7)
N2	0.0171 (8)	0.0223 (9)	0.0157 (9)	-0.0016 (7)	0.0078 (7)	0.0035 (7)
N3	0.0192 (9)	0.0204 (9)	0.0304 (11)	0.0000 (7)	0.0083 (8)	-0.0055 (8)
N4	0.0171 (9)	0.0310 (10)	0.0226 (10)	-0.0028 (8)	0.0073 (8)	-0.0048 (8)
N5	0.0433 (13)	0.0308 (11)	0.0245 (11)	0.0161 (10)	0.0175 (10)	0.0032 (9)
C1	0.0131 (9)	0.0205 (10)	0.0115 (9)	-0.0013 (7)	0.0020 (7)	0.0037 (8)
C2	0.0127 (9)	0.0200 (10)	0.0125 (9)	-0.0018 (7)	0.0043 (7)	0.0022 (8)
C3	0.0174 (10)	0.0232 (11)	0.0190 (11)	0.0020 (8)	0.0056 (8)	-0.0012 (9)
C4	0.0157 (10)	0.0415 (14)	0.0202 (11)	0.0039 (9)	0.0073 (8)	-0.0029 (10)
C5	0.0150 (10)	0.0476 (15)	0.0190 (11)	-0.0069 (10)	0.0094 (8)	0.0013 (10)
C6	0.0151 (10)	0.0315 (12)	0.0145 (10)	-0.0068 (9)	0.0024 (8)	0.0056 (9)
C7	0.0245 (11)	0.0354 (14)	0.0196 (11)	-0.0144 (10)	0.0012 (9)	0.0093 (10)
C8	0.0333 (13)	0.0218 (11)	0.0222 (12)	-0.0125 (10)	-0.0029 (10)	0.0082 (9)
C9	0.0296 (12)	0.0175 (10)	0.0157 (10)	-0.0024 (9)	-0.0021 (9)	0.0013 (8)
C10	0.0449 (15)	0.0219 (12)	0.0286 (13)	0.0047 (11)	0.0038 (11)	-0.0028 (10)
C11	0.0173 (9)	0.0198 (10)	0.0145 (10)	-0.0015 (8)	0.0039 (8)	0.0043 (8)
C12	0.0174 (10)	0.0181 (10)	0.0152 (10)	-0.0014 (8)	0.0039 (8)	0.0033 (8)
C13	0.0255 (11)	0.0185 (10)	0.0173 (10)	0.0017 (8)	0.0039 (9)	0.0019 (8)
C14	0.0363 (13)	0.0183 (11)	0.0201 (11)	-0.0044 (9)	0.0034 (10)	0.0015 (9)
C15	0.0342 (13)	0.0251 (12)	0.0222 (12)	-0.0117 (10)	0.0064 (10)	0.0048 (9)
C16	0.0212 (10)	0.0288 (12)	0.0150 (10)	-0.0074 (9)	0.0039 (8)	0.0051 (9)
C17	0.0233 (11)	0.0429 (15)	0.0236 (12)	-0.0098 (10)	0.0107 (10)	0.0055 (11)
C18	0.0227 (11)	0.0450 (15)	0.0234 (12)	-0.0038 (10)	0.0145 (10)	0.0028 (11)
C19	0.0192 (10)	0.0338 (13)	0.0162 (11)	0.0014 (9)	0.0069 (8)	0.0020 (9)
C20	0.0282 (12)	0.0333 (13)	0.0263 (13)	0.0037 (10)	0.0148 (10)	0.0003 (10)

Geometric parameters (\AA , $^\circ$)

La1—O2	2.3308 (15)	C4—C5	1.364 (4)
La1—O1 ⁱ	2.4704 (15)	C4—H4	0.9500
La1—O1	2.4953 (15)	C5—C6	1.413 (4)
La1—O9	2.5553 (17)	C5—H5	0.9500

La1—O6	2.5759 (17)	C6—C7	1.422 (3)
La1—O3	2.5932 (16)	C7—C8	1.356 (4)
La1—O7	2.6267 (16)	C7—H7	0.9500
La1—O10	2.6365 (18)	C8—C9	1.404 (4)
La1—O4	2.6499 (16)	C8—H8	0.9500
O1—C2	1.340 (2)	C9—C10	1.482 (4)
O1—La1 ⁱ	2.4704 (15)	C10—H10A	0.9800
O2—C12	1.312 (3)	C10—H10B	0.9800
O3—N3	1.282 (3)	C10—H10C	0.9800
O4—N3	1.269 (3)	C11—C16	1.409 (3)
O5—N3	1.214 (3)	C11—C12	1.431 (3)
O6—N4	1.271 (3)	C12—C13	1.395 (3)
O7—N4	1.271 (3)	C13—C14	1.403 (3)
O8—N4	1.222 (3)	C13—H13	0.9500
O9—N5	1.268 (3)	C14—C15	1.373 (4)
O10—N5	1.276 (3)	C14—H14	0.9500
O11—N5	1.212 (3)	C15—C16	1.409 (4)
N1—C9	1.332 (3)	C15—H15	0.9500
N1—C1	1.374 (3)	C16—C17	1.416 (3)
N1—H1	0.875 (10)	C17—C18	1.369 (4)
N2—C19	1.332 (3)	C17—H17	0.9500
N2—C11	1.369 (3)	C18—C19	1.410 (3)
N2—H2	0.873 (10)	C18—H18	0.9500
C1—C6	1.407 (3)	C19—C20	1.489 (3)
C1—C2	1.414 (3)	C20—H20A	0.9800
C2—C3	1.384 (3)	C20—H20B	0.9800
C3—C4	1.408 (3)	C20—H20C	0.9800
C3—H3	0.9500		
O2—La1—O1 ⁱ	147.09 (5)	O1—C2—C3	123.8 (2)
O2—La1—O1	85.68 (5)	O1—C2—C1	118.82 (19)
O1 ⁱ —La1—O1	66.36 (6)	C3—C2—C1	117.34 (19)
O2—La1—O9	79.43 (5)	C2—C3—C4	121.2 (2)
O1 ⁱ —La1—O9	105.44 (5)	C2—C3—H3	119.4
O1—La1—O9	131.04 (5)	C4—C3—H3	119.4
O2—La1—O6	90.03 (6)	C5—C4—C3	121.3 (2)
O1 ⁱ —La1—O6	122.78 (5)	C5—C4—H4	119.4
O1—La1—O6	152.87 (5)	C3—C4—H4	119.4
O9—La1—O6	73.96 (6)	C4—C5—C6	119.5 (2)
O2—La1—O3	71.61 (5)	C4—C5—H5	120.2
O1 ⁱ —La1—O3	118.10 (5)	C6—C5—H5	120.2
O1—La1—O3	81.59 (5)	C1—C6—C5	118.8 (2)
O9—La1—O3	134.40 (6)	C1—C6—C7	117.2 (2)
O6—La1—O3	71.66 (6)	C5—C6—C7	124.0 (2)
O2—La1—O7	136.33 (5)	C8—C7—C6	120.4 (2)
O1 ⁱ —La1—O7	74.72 (5)	C8—C7—H7	119.8
O1—La1—O7	137.50 (5)	C6—C7—H7	119.8
O9—La1—O7	74.71 (6)	C7—C8—C9	121.5 (2)

supplementary materials

O6—La1—O7	49.33 (5)	C7—C8—H8	119.3
O3—La1—O7	103.20 (5)	C9—C8—H8	119.3
O2—La1—O10	76.14 (6)	N1—C9—C8	117.6 (2)
O1 ⁱ —La1—O10	82.77 (5)	N1—C9—C10	118.0 (2)
O1—La1—O10	81.90 (5)	C8—C9—C10	124.4 (2)
O9—La1—O10	49.32 (6)	C9—C10—H10A	109.5
O6—La1—O10	122.99 (6)	C9—C10—H10B	109.5
O3—La1—O10	144.64 (6)	H10A—C10—H10B	109.5
O7—La1—O10	110.09 (6)	C9—C10—H10C	109.5
O2—La1—O4	120.22 (5)	H10A—C10—H10C	109.5
O1 ⁱ —La1—O4	74.90 (5)	H10B—C10—H10C	109.5
O1—La1—O4	82.87 (5)	N2—C11—C16	119.0 (2)
O9—La1—O4	144.12 (6)	N2—C11—C12	118.05 (19)
O6—La1—O4	76.23 (6)	C16—C11—C12	122.9 (2)
O3—La1—O4	48.71 (5)	O2—C12—C13	125.5 (2)
O7—La1—O4	70.83 (5)	O2—C12—C11	118.66 (19)
O10—La1—O4	156.62 (5)	C13—C12—C11	115.9 (2)
C2—O1—La1 ⁱ	123.42 (12)	C12—C13—C14	121.5 (2)
C2—O1—La1	122.24 (12)	C12—C13—H13	119.3
La1 ⁱ —O1—La1	113.64 (6)	C14—C13—H13	119.3
C12—O2—La1	163.94 (14)	C15—C14—C13	121.9 (2)
N3—O3—La1	98.69 (13)	C15—C14—H14	119.0
N3—O4—La1	96.33 (12)	C13—C14—H14	119.0
N4—O6—La1	97.65 (13)	C14—C15—C16	119.4 (2)
N4—O7—La1	95.21 (12)	C14—C15—H15	120.3
N5—O9—La1	97.36 (13)	C16—C15—H15	120.3
N5—O10—La1	93.33 (13)	C11—C16—C15	118.4 (2)
C9—N1—C1	124.0 (2)	C11—C16—C17	117.0 (2)
C9—N1—H1	116.9 (19)	C15—C16—C17	124.5 (2)
C1—N1—H1	119.0 (19)	C18—C17—C16	121.5 (2)
C19—N2—C11	124.5 (2)	C18—C17—H17	119.3
C19—N2—H2	118.1 (18)	C16—C17—H17	119.3
C11—N2—H2	117.4 (18)	C17—C18—C19	119.8 (2)
O5—N3—O4	122.9 (2)	C17—C18—H18	120.1
O5—N3—O3	121.1 (2)	C19—C18—H18	120.1
O4—N3—O3	115.96 (18)	N2—C19—C18	118.1 (2)
O8—N4—O6	121.1 (2)	N2—C19—C20	118.2 (2)
O8—N4—O7	121.5 (2)	C18—C19—C20	123.7 (2)
O6—N4—O7	117.34 (18)	C19—C20—H20A	109.5
O11—N5—O9	121.4 (2)	C19—C20—H20B	109.5
O11—N5—O10	121.7 (3)	H20A—C20—H20B	109.5
O9—N5—O10	116.9 (2)	C19—C20—H20C	109.5
N1—C1—C6	119.2 (2)	H20A—C20—H20C	109.5
N1—C1—C2	119.01 (18)	H20B—C20—H20C	109.5
C6—C1—C2	121.8 (2)		
O2—La1—O1—C2	27.09 (15)	O6—La1—O10—N5	2.99 (16)
O1 ⁱ —La1—O1—C2	-170.71 (18)	O3—La1—O10—N5	-102.47 (16)
O9—La1—O1—C2	99.05 (15)	O7—La1—O10—N5	56.84 (15)

O6—La1—O1—C2	-54.5 (2)	O4—La1—O10—N5	144.81 (15)
O3—La1—O1—C2	-44.94 (15)	La1—O4—N3—O5	-173.9 (2)
O7—La1—O1—C2	-145.33 (14)	La1—O4—N3—O3	5.5 (2)
O10—La1—O1—C2	103.68 (15)	La1—O3—N3—O5	173.8 (2)
O4—La1—O1—C2	-94.12 (15)	La1—O3—N3—O4	-5.7 (2)
O2—La1—O1—La1 ⁱ	-162.20 (7)	La1—O6—N4—O8	172.3 (2)
O1 ⁱ —La1—O1—La1 ⁱ	0.0	La1—O6—N4—O7	-7.0 (2)
O9—La1—O1—La1 ⁱ	-90.24 (8)	La1—O7—N4—O8	-172.5 (2)
O6—La1—O1—La1 ⁱ	116.21 (11)	La1—O7—N4—O6	6.8 (2)
O3—La1—O1—La1 ⁱ	125.77 (6)	La1—O9—N5—O11	-160.3 (2)
O7—La1—O1—La1 ⁱ	25.38 (10)	La1—O9—N5—O10	18.1 (2)
O10—La1—O1—La1 ⁱ	-85.61 (7)	La1—O10—N5—O11	161.0 (3)
O4—La1—O1—La1 ⁱ	76.59 (6)	La1—O10—N5—O9	-17.4 (2)
O1 ⁱ —La1—O2—C12	-2.5 (6)	C9—N1—C1—C6	-2.5 (3)
O1—La1—O2—C12	28.6 (5)	C9—N1—C1—C2	177.0 (2)
O9—La1—O2—C12	-104.6 (5)	La1 ⁱ —O1—C2—C3	-79.0 (2)
O6—La1—O2—C12	-178.2 (5)	La1—O1—C2—C3	90.8 (2)
O3—La1—O2—C12	111.1 (5)	La1 ⁱ —O1—C2—C1	100.81 (19)
O7—La1—O2—C12	-158.8 (5)	La1—O1—C2—C1	-89.4 (2)
O10—La1—O2—C12	-54.1 (5)	N1—C1—C2—O1	-3.6 (3)
O4—La1—O2—C12	107.7 (5)	C6—C1—C2—O1	175.98 (19)
O2—La1—O3—N3	-172.85 (14)	N1—C1—C2—C3	176.21 (19)
O1 ⁱ —La1—O3—N3	-27.22 (14)	C6—C1—C2—C3	-4.2 (3)
O1—La1—O3—N3	-84.63 (13)	O1—C2—C3—C4	-178.2 (2)
O9—La1—O3—N3	133.73 (13)	C1—C2—C3—C4	2.1 (3)
O6—La1—O3—N3	90.79 (13)	C2—C3—C4—C5	1.0 (4)
O7—La1—O3—N3	52.32 (14)	C3—C4—C5—C6	-2.0 (4)
O10—La1—O3—N3	-147.60 (12)	N1—C1—C6—C5	-177.14 (19)
O4—La1—O3—N3	3.24 (12)	C2—C1—C6—C5	3.3 (3)
O2—La1—O4—N3	1.05 (15)	N1—C1—C6—C7	3.6 (3)
O1 ⁱ —La1—O4—N3	149.16 (13)	C2—C1—C6—C7	-176.0 (2)
O1—La1—O4—N3	81.80 (13)	C4—C5—C6—C1	-0.1 (3)
O9—La1—O4—N3	-115.25 (14)	C4—C5—C6—C7	179.1 (2)
O6—La1—O4—N3	-80.79 (13)	C1—C6—C7—C8	-1.8 (3)
O3—La1—O4—N3	-3.25 (12)	C5—C6—C7—C8	178.9 (2)
O7—La1—O4—N3	-132.09 (14)	C6—C7—C8—C9	-1.1 (4)
O10—La1—O4—N3	131.47 (16)	C1—N1—C9—C8	-0.5 (3)
O2—La1—O6—N4	166.36 (14)	C1—N1—C9—C10	179.4 (2)
O1 ⁱ —La1—O6—N4	-10.92 (16)	C7—C8—C9—N1	2.3 (3)
O1—La1—O6—N4	-113.08 (15)	C7—C8—C9—C10	-177.6 (2)
O9—La1—O6—N4	87.38 (14)	C19—N2—C11—C16	-0.9 (3)
O3—La1—O6—N4	-123.06 (15)	C19—N2—C11—C12	178.4 (2)
O7—La1—O6—N4	3.96 (12)	La1—O2—C12—C13	75.9 (6)
O10—La1—O6—N4	92.94 (15)	La1—O2—C12—C11	-103.9 (5)
O4—La1—O6—N4	-72.44 (14)	N2—C11—C12—O2	-0.3 (3)
O2—La1—O7—N4	-29.91 (17)	C16—C11—C12—O2	178.99 (19)

supplementary materials

O1 ⁱ —La1—O7—N4	163.12 (14)	N2—C11—C12—C13	179.88 (19)
O1—La1—O7—N4	139.10 (12)	C16—C11—C12—C13	-0.8 (3)
O9—La1—O7—N4	-85.73 (14)	O2—C12—C13—C14	179.9 (2)
O6—La1—O7—N4	-3.94 (13)	C11—C12—C13—C14	-0.3 (3)
O3—La1—O7—N4	47.18 (14)	C12—C13—C14—C15	0.8 (4)
O10—La1—O7—N4	-120.70 (13)	C13—C14—C15—C16	-0.1 (4)
O4—La1—O7—N4	84.13 (13)	N2—C11—C16—C15	-179.2 (2)
O2—La1—O9—N5	70.58 (14)	C12—C11—C16—C15	1.4 (3)
O1 ⁱ —La1—O9—N5	-75.98 (14)	N2—C11—C16—C17	2.4 (3)
O1—La1—O9—N5	-4.11 (16)	C12—C11—C16—C17	-176.9 (2)
O6—La1—O9—N5	163.69 (15)	C14—C15—C16—C11	-1.0 (3)
O3—La1—O9—N5	121.40 (14)	C14—C15—C16—C17	177.2 (2)
O7—La1—O9—N5	-144.95 (14)	C11—C16—C17—C18	-2.3 (4)
O10—La1—O9—N5	-10.16 (13)	C15—C16—C17—C18	179.4 (2)
O4—La1—O9—N5	-161.43 (13)	C16—C17—C18—C19	0.7 (4)
O2—La1—O10—N5	-77.84 (14)	C11—N2—C19—C18	-0.8 (3)
O1 ⁱ —La1—O10—N5	127.61 (14)	C11—N2—C19—C20	178.9 (2)
O1—La1—O10—N5	-165.36 (14)	C17—C18—C19—N2	0.9 (4)
O9—La1—O10—N5	10.04 (13)	C17—C18—C19—C20	-178.8 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O4 ⁱ	0.88 (1)	2.39 (2)	3.115 (3)	140 (2)
N2—H2 \cdots O3	0.87 (1)	2.08 (1)	2.950 (2)	173 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Fig. 1

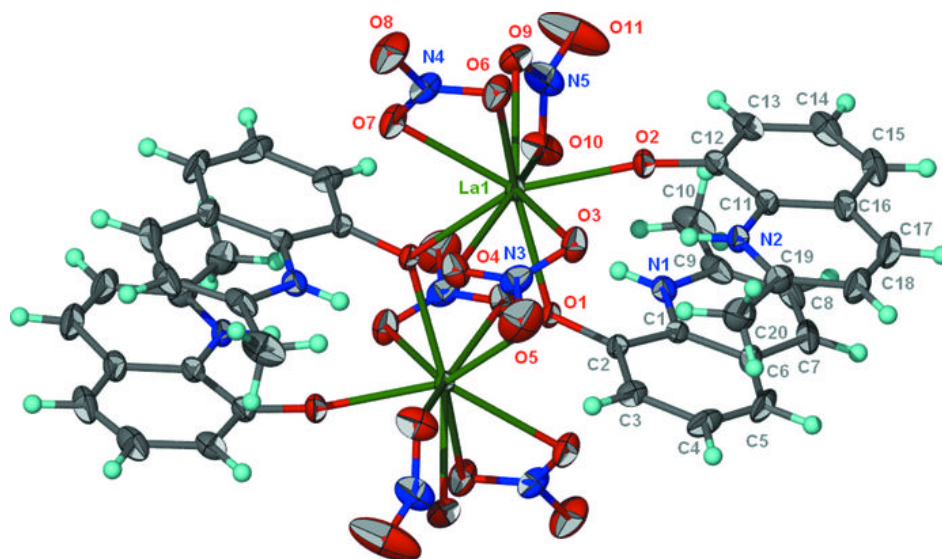


Fig. 2

