Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis(μ-anthracene-9-carboxylato)-bis[(anthracene-9-carboxylato)-(2,2′-bipyridyl)lanthanum(III)]

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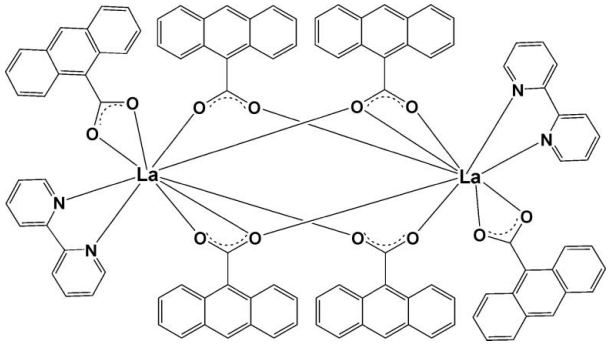
Received 16 November 2007; accepted 22 November 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.075; data-to-parameter ratio = 12.9.

The title complex, $[La_2(C_{15}H_9O_2)_6(C_{10}H_8N_2)_2]$, has a centrosymmetric binuclear cage structure in which two La^{III} atoms are both nine-coordinated and bridged by four anthracene-9-carboxylate ligands, with an La···La separation of 4.0880 (4) Å. The remaining coordination sites are occupied by two N atoms of a 2,2′-bipyridine (bipy) and two O atoms of an anthracene-9-carboxylate ligand. The six anthracene-9-carboxylate groups coordinate each La^{III} atom in three different ways. Adjacent discrete dinuclear units are arranged into a one-dimensional chain along the [111] direction by intermolecular π–π stacking interactions, with a centroid–centroid separation of 3.704 (7) Å.

Related literature

For related literature, see: Bünzli (2006); Fu *et al.* (2005); Janiak (2000); Roh *et al.* (2005); Shi *et al.* (2001); Suárez *et al.* (2004); Wan *et al.* (2003); Wang *et al.* (1999, 2006); Ye *et al.* (2005).



Experimental

Crystal data

$[La_2(C_{15}H_9O_2)_6(C_{10}H_8N_2)_2]$
M_r = 1917.52
Triclinic, $P\overline{1}$
a = 12.1038 (7) Å
b = 13.4887 (8) Å
c = 15.4568 (14) Å
α = 113.036 (4)°
β = 103.257 (4)°
γ = 102.913 (3)°
V = 2117.7 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 273 (2) K
0.20 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.815, T_{max} = 0.883
32552 measured reflections
7432 independent reflections
6474 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.05
7432 reflections
577 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—O2	2.4561 (18)	La1—O2^{i}	2.6750 (19)
La1—O5	2.4574 (19)	La1—O3^{i}	2.687 (2)
La1—O1	2.4974 (18)	La1—N1	2.730 (2)
La1—O6	2.522 (2)	La1—N2	2.741 (2)
La1—O4	2.535 (2)		
O2—La1—O5	73.16 (7)	O6—La1—O3^{i}	75.51 (8)
O2—La1—O1	73.15 (6)	O4—La1—O3^{i}	70.62 (7)
O5—La1—O1	135.97 (6)	O2^{i}—La1—O3^{i}	47.91 (6)
O2—La1—O6	151.98 (7)	O2—La1—N1	91.57 (7)
O5—La1—O6	90.68 (7)	O5—La1—N1	134.60 (7)
O1—La1—O6	130.65 (7)	O1—La1—N1	73.52 (7)
O2—La1—O4	151.37 (7)	O6—La1—N1	83.64 (8)
O5—La1—O4	135.00 (7)	O4—La1—N1	71.68 (7)
O1—La1—O4	79.76 (6)	O2^{i}—La1—N1	145.95 (7)
O6—La1—O4	51.39 (7)	O3^{i}—La1—N1	142.16 (7)
O2—La1—O2^{i}	74.44 (6)	O2—La1—N2	78.12 (7)
O5—La1—O2^{i}	71.53 (6)	O5—La1—N2	75.60 (7)
O1—La1—O2^{i}	72.74 (6)	O1—La1—N2	123.19 (7)
O6—La1—O2^{i}	122.70 (7)	O6—La1—N2	75.71 (7)
O4—La1—O2^{i}	106.39 (7)	O4—La1—N2	110.34 (7)
O2—La1—O3^{i}	121.09 (6)	O2^{i}—La1—N2	141.93 (7)
O5—La1—O3^{i}	77.60 (8)	O3^{i}—La1—N2	140.02 (8)
O1—La1—O3^{i}	96.65 (8)	N1—La1—N2	59.30 (7)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

This work was supported by the Startup Fund for PhDs in Natural Scientific Research of Zhengzhou University of Light Industry (grant No. 2008 to CSL). The authors also gratefully thank Nankai University and Henan Provincial Key Laboratory of Surface and Interface Science for supporting this research.

 doi:10.1107/S1600536807062241

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2026).

References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Bünzli, J.-C. G. (2006). *Acc. Chem. Res.* **39**, 53–61.

Fu, L.-M., Wen, X.-F., Ai, X.-C., Sun, Y., Wu, Y.-S., Zhang, J.-P. & Wang, Y. (2005). *Angew. Chem. Int. Ed.* **44**, 747–750.

Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.

Roh, S.-G., Nah, M.-K., Oh, J. B., Baek, N. S., Park, K.-M. & Kim, H. K. (2005). *Polyhedron*, **24,** 137–142.

Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

Shi, Q., Hu, M., Cao, R., Liang, Y. & Hong, M. (2001). *Acta Cryst.* E**57**, m122–m123.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Suárez, S., Imbert, D., Gumy, F., Piguet, C. & Bünzli, J.-C. G. (2004). *Chem. Mater.* **16**, 3257–3266.

Wan, Y., Zhang, L., Jin, L., Gao, S. & Lu, S. (2003). *Inorg. Chem.* **42**, 4985–4994.

Wang, S.-P., Gao, Z.-H., Xu, L.-J. & Wang, R.-F. (2006). *Acta Cryst.* E**62**, m1853–m1855.

Wang, R., Jin, L., Li, L., Lu, S. & Zhang, J. (1999). *J. Coord. Chem.* **47**, 279–287.

Ye, B. H., Tong, M. L. & Chen, X. M. (2005). *Coord. Chem. Rev.* **249**, 545–565.

supporting information

Acta Cryst. (2008). E**64**, m15–m16 [https://doi.org/10.1107/S1600536807062241]

Tetrakis(μ-anthracene-9-carboxylato)bis[(anthracene-9-carboxylato)(2,2′-bipyridyl)lanthanum(III)]

Chun-Sen Liu, Li-Fen Yan, Ze Chang and Jun-Jie Wang

S1. Comment

In recent years, the rational design and synthesis of functional rare-earth (RE) coordination complexes with various N– and/or O-donor ligands has attracted great interest not only because of their fascinating structural diversities but also becasue of their potential applications as functional materials, for example, optical materials, electronic materials, catalytic materials, and molecular-based magnets (Bünzli, 2006; Fu *et al.*, 2005; Suárez *et al.*, 2004). The effective and facile approach for the synthesis of such complexes is still the appropriate choice of well designed organic ligands as bridges or terminal groups (building blocks), with metal ions or metal clusters as nodes (Ye *et al.*, 2005). Among such ligands, versatile carboxylic acids exhibiting diverse coordination modes have been well used in the preparations of various functional rare-earth (RE) complexes (Roh *et al.*, 2005; Shi *et al.*, 2001; Wan *et al.*, 2003; Wang *et al.*, 1999; Wang *et al.*, 2006). Besides, the introduction of 2,2′-bipyridyl-like bidentate chelating molecules (2,2′-bipyridine or 1,10-phenanthroline) into the reaction systems, the use of various carboxylic acid ligands, as auxiliary ligands, can generate some interesting coordination architectures (Ye *et al.*, 2005). We report here the crystal structure of the title complex (I), a La^{III} complex with anthracene-9-carboxylate (*L*) and chelating 2,2′-bipyridine (bipy) as ligands.

The structure of complex (I) consists of a centrosymmetric dinuclear unit $[La_2(L)_6(bipy)_2]$ with central La^{III} ions nine-coordinated by two N-atom donors from one chelating bipy ligand and seven O atoms from five distinct *L* ligands (Fig. 1). The La–O distances are in the range of 2.4561 (18) - 2.687 (2) Å, which are normal and in agreement with those found in other carboxylato-containing La^{III} complexes (Shi *et al.*, 2001). The ligand bipy acts as a typical chelating ligand coordinating to the La^{III} ion with La–N bond distances of 2.730 (2) and 2.741 (2) Å, and an N–La–N angle of 59.30 (7)°. For *L*, there exists three different kinds of carboxylic coordination modes with the La^{III} center, namely *syn-syn* bridging (μ_2-η^1:η^1-bridging), symmetric bidentate chelate ((μ_1-η^1:η^1-chelating), and tridentate chelating/bridging (η-O,*O*′-μ-O,*O*). In this manner two La^{III} ions are connected to form an eight-membered ring [La(1)–O(1)–C(31)–O(5 A)–La(1 A)–O(1 A)–C(31 A)–O(5)], as well as a four-membered ring [La(1)–O(2)–La(1 A)–O(2 A)]. The non-bonding La(1)···La(1 A) separation is 4.0880 (4) Å (symmetry operation (A) = 1 - *x*, 1 - *y*, 1 - *z*).

In the crystal adjacent dinuclear $[La_2(L)_6(bipy)_2]$ units are arranged into one-dimensional chains, along the [111] direction, by the intermolecular $\pi\cdots\pi$ stacking interactions (symmetry operation: 2 - *x*, 2 - *y*, 2 - *z*; dashed solid lines in Fig. 2) between the completely parallel anthracene rings of different *L* ligands, with a centroid-centroid separation of 3.704 (7) Å (Janiak *et al.*, 2000).

S2. Experimental

A mixed solution of anthracene-9-carboxylic acid (0.05 mmol) and 2,2′-bipyridine (0.05 mmol) in CH_3OH (10 ml) in the presence of excess 2,6-dimethylpyridine (*ca* 0.05 ml for adjusting the pH value to basic condition) was carefully layered on top of a H_2O solution (15 ml) of $La(NO_3)_3$ (0.1 mmol) in a test tube. Yellow single crystals suitable for X-ray analysis

of the title complex (I) appeared at the tube wall after *ca* two weeks at room temperature. Yield: ~40% based on anthracene-9-carboxylic acid. Elemental analysis calculated for $C_{110}H_{70}La_2O_{12}N_4$: C 68.90, H 3.68, N 2.92%; found: C 68.69, H 3.77, N 3.03%.

S3. Refinement

H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93 Å (aromatic) and U_{iso}(H) = 1.2U_{eq}(C).

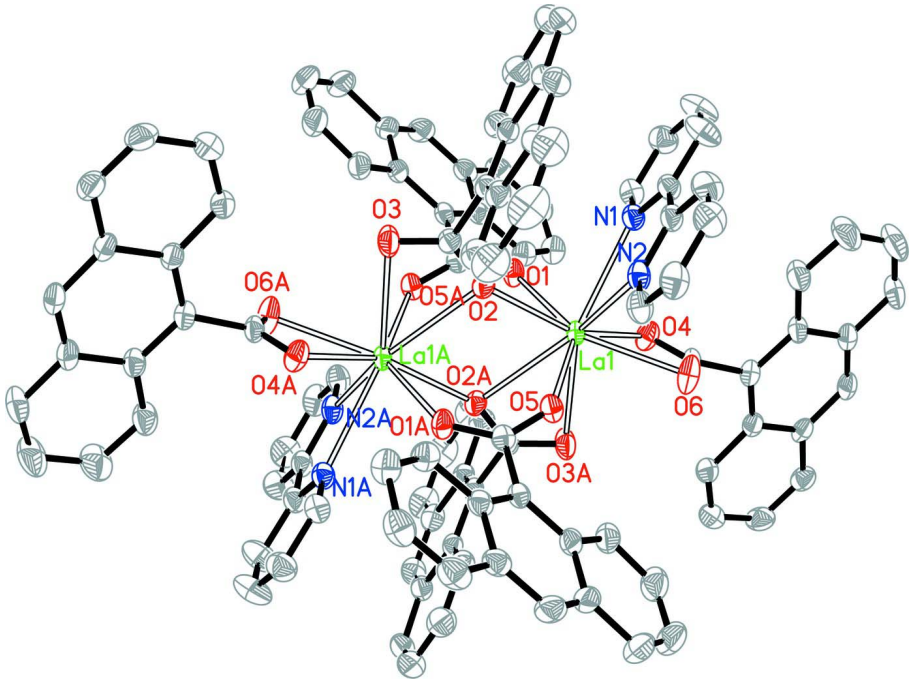


Figure 1

The molecular structure of complex (I). Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffix A are generated by the symmetry operation (1 - *x*, 1 - *y*, 1 - *z*). For the sake of clarity, all H atoms have been omitted.

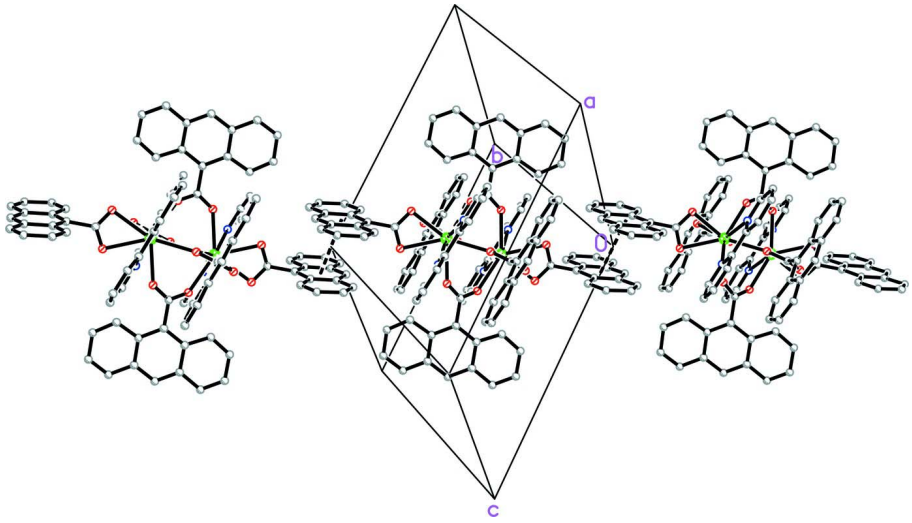


Figure 2

Part of the crystal packing in complex (I), showing a $\pi\cdots\pi$ stacking (dashed solid lines) chain. All H atoms have been omitted for clarity.

Tetrakis(μ-anthracene-9-carboxylato)bis[(anthracene-9- carboxylato)(2,2′-bipyridyl)lanthanum(III)]

Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 12.1038\ (7)$ Å
$b = 13.4887\ (8)$ Å
$c = 15.4568\ (14)$ Å
$\alpha = 113.036\ (4)°$
$\beta = 103.257\ (4)°$
$\gamma = 102.913\ (3)°$
$V = 2117.7\ (3)$ Å^3
$Z = 1$
$F(000) = 968$
$D_x = 1.504$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6220 reflections
$\theta = 2.4–28.2°$
$\mu = 1.07$ mm^{-1}
$T = 273$ K
Block, yellow
0.20 × 0.14 × 0.12 mm

Data collection

CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.815$, $T_{max} = 0.883$
32552 measured reflections
7432 independent reflections
6474 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -14\rightarrow14$
$k = -16\rightarrow13$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.076$
$S = 1.05$
7432 reflections
577 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.7206P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.86$ e Å^{-3}

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	0.676202 (12)	0.570648 (12)	0.595266 (10)	0.03410 (7)
C1	0.4637 (3)	0.2753 (2)	0.4356 (2)	0.0417 (6)
C2	0.5386 (2)	0.2008 (2)	0.4404 (2)	0.0413 (6)
C3	0.5804 (3)	0.1540 (2)	0.3612 (2)	0.0470 (7)
C4	0.5564 (3)	0.1751 (3)	0.2769 (3)	0.0621 (9)
H4A	0.5098	0.2204	0.2724	0.074*
C5	0.6003 (4)	0.1301 (4)	0.2026 (3)	0.0801 (12)
H5A	0.5845	0.1455	0.1483	0.096*
C6	0.6698 (4)	0.0602 (4)	0.2080 (3)	0.0879 (14)
H6A	0.6992	0.0295	0.1567	0.105*
C7	0.6943 (4)	0.0371 (3)	0.2856 (3)	0.0772 (11)
H7A	0.7398	−0.0098	0.2869	0.093*
C8	0.6519 (3)	0.0833 (3)	0.3665 (3)	0.0553 (8)
C9	0.6768 (3)	0.0623 (3)	0.4482 (3)	0.0614 (9)
H9A	0.7222	0.0155	0.4504	0.074*
C10	0.6364 (3)	0.1086 (3)	0.5273 (3)	0.0524 (8)
C11	0.6596 (3)	0.0849 (3)	0.6105 (3)	0.0678 (10)
H11A	0.7037	0.0372	0.6129	0.081*
C12	0.6187 (4)	0.1304 (4)	0.6856 (3)	0.0742 (11)
H12A	0.6346	0.1137	0.7392	0.089*
C13	0.5520 (4)	0.2029 (3)	0.6833 (3)	0.0685 (10)
H13A	0.5254	0.2350	0.7361	0.082*
C14	0.5261 (3)	0.2266 (3)	0.6052 (2)	0.0549 (8)
H14A	0.4811	0.2742	0.6051	0.066*
C15	0.5660 (2)	0.1803 (2)	0.5236 (2)	0.0438 (7)
C16	0.8859 (2)	0.7626 (2)	0.7512 (2)	0.0419 (7)
C17	0.9949 (3)	0.8618 (2)	0.8350 (2)	0.0442 (7)
C18	1.0854 (3)	0.8381 (3)	0.8901 (2)	0.0494 (7)
C19	1.0865 (3)	0.7256 (3)	0.8641 (3)	0.0663 (10)
H19A	1.0251	0.6636	0.8079	0.080*
C20	1.1754 (4)	0.7066 (4)	0.9198 (4)	0.0891 (13)
H20A	1.1752	0.6320	0.9005	0.107*

C21	1.2676 (4)	0.7984 (4)	1.0063 (4)	0.0918 (14)
H21A	1.3272	0.7840	1.0445	0.110*
C22	1.2707 (3)	0.9062 (4)	1.0342 (3)	0.0714 (11)
H22A	1.3328	0.9658	1.0916	0.086*
C23	1.1809 (3)	0.9318 (3)	0.9780 (2)	0.0505 (8)
C24	1.1819 (3)	1.0422 (3)	1.0058 (2)	0.0502 (8)
H24A	1.2421	1.1020	1.0644	0.060*
C25	1.0950 (3)	1.0675 (2)	0.9486 (2)	0.0449 (7)
C26	1.0969 (3)	1.1815 (3)	0.9768 (2)	0.0562 (8)
H26A	1.1579	1.2422	1.0344	0.067*
C27	1.0122 (4)	1.2028 (3)	0.9217 (3)	0.0664 (10)
H27A	1.0144	1.2781	0.9418	0.080*
C28	0.9189 (3)	1.1124 (3)	0.8327 (3)	0.0662 (9)
H28A	0.8623	1.1293	0.7942	0.079*
C29	0.9114 (3)	1.0020 (3)	0.8034 (2)	0.0518 (8)
H29A	0.8488	0.9434	0.7458	0.062*
C30	0.9994 (3)	0.9749 (2)	0.8606 (2)	0.0441 (7)
C31	0.4199 (3)	0.4836 (2)	0.6572 (2)	0.0398 (6)
C32	0.3754 (2)	0.4597 (2)	0.7333 (2)	0.0405 (6)
C33	0.4244 (3)	0.5438 (3)	0.8357 (2)	0.0432 (7)
C34	0.5145 (3)	0.6538 (3)	0.8742 (2)	0.0510 (7)
H34A	0.5438	0.6736	0.8304	0.061*
C35	0.5585 (3)	0.7305 (3)	0.9737 (2)	0.0606 (9)
H35A	0.6169	0.8017	0.9963	0.073*
C36	0.5174 (3)	0.7041 (3)	1.0432 (3)	0.0646 (9)
H36A	0.5497	0.7566	1.1112	0.078*
C37	0.4315 (3)	0.6030 (3)	1.0101 (3)	0.0620 (9)
H37A	0.4040	0.5864	1.0560	0.074*
C38	0.3804 (3)	0.5196 (3)	0.9068 (2)	0.0506 (7)
C39	0.2918 (3)	0.4143 (3)	0.8735 (3)	0.0610 (9)
H39A	0.2636	0.3992	0.9198	0.073*
C40	0.2441 (3)	0.3311 (3)	0.7739 (3)	0.0548 (8)
C41	0.1542 (4)	0.2229 (4)	0.7433 (4)	0.0769 (11)
H41A	0.1273	0.2088	0.7905	0.092*
C42	0.1084 (4)	0.1412 (4)	0.6463 (4)	0.0841 (13)
H42A	0.0496	0.0714	0.6269	0.101*
C43	0.1487 (3)	0.1611 (3)	0.5753 (3)	0.0732 (11)
H43A	0.1166	0.1035	0.5090	0.088*
C44	0.2334 (3)	0.2621 (3)	0.6001 (3)	0.0572 (8)
H44A	0.2581	0.2723	0.5505	0.069*
C45	0.2853 (3)	0.3533 (3)	0.7012 (2)	0.0466 (7)
C46	0.8254 (3)	0.4121 (3)	0.4462 (2)	0.0567 (8)
H46A	0.7874	0.4405	0.4067	0.068*
C47	0.8931 (3)	0.3470 (3)	0.4104 (3)	0.0637 (9)
H47A	0.8997	0.3313	0.3480	0.076*
C48	0.9498 (4)	0.3063 (3)	0.4680 (3)	0.0731 (11)
H48A	0.9977	0.2637	0.4464	0.088*
C49	0.9358 (3)	0.3287 (3)	0.5586 (3)	0.0682 (10)

H49A	0.9728	0.2999	0.5982	0.082*
C50	0.8664 (3)	0.3944 (2)	0.5909 (2)	0.0478 (7)
C51	0.8494 (3)	0.4215 (2)	0.6884 (2)	0.0482 (7)
C52	0.9075 (4)	0.3890 (4)	0.7559 (3)	0.0806 (12)
H52A	0.9579	0.3472	0.7400	0.097*
C53	0.8904 (4)	0.4186 (4)	0.8458 (3)	0.0865 (13)
H53A	0.9299	0.3979	0.8915	0.104*
C54	0.8158 (4)	0.4782 (3)	0.8680 (3)	0.0648 (9)
H54A	0.8026	0.4985	0.9286	0.078*
C55	0.7601 (3)	0.5081 (3)	0.7987 (2)	0.0530 (8)
H55A	0.7089	0.5492	0.8140	0.064*
N1	0.7758 (2)	0.4809 (2)	0.71062 (18)	0.0458 (6)
N2	0.8112 (2)	0.4367 (2)	0.53454 (18)	0.0477 (6)
O1	0.53299 (17)	0.53114 (18)	0.68098 (14)	0.0478 (5)
O2	0.51838 (17)	0.38292 (15)	0.47574 (14)	0.0429 (5)
O3	0.3521 (2)	0.23338 (18)	0.3940 (2)	0.0691 (7)
O4	0.79298 (19)	0.73251 (18)	0.77239 (15)	0.0539 (5)
O5	0.65790 (17)	0.54654 (17)	0.42597 (14)	0.0463 (5)
O6	0.88922 (19)	0.7120 (2)	0.66595 (16)	0.0647 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.02422 (9)	0.03431 (10)	0.03495 (10)	0.00919 (7)	0.00716 (7)	0.01018 (7)
C1	0.0407 (16)	0.0328 (14)	0.0416 (15)	0.0117 (13)	0.0086 (13)	0.0118 (12)
C2	0.0337 (15)	0.0296 (13)	0.0490 (16)	0.0089 (11)	0.0086 (13)	0.0120 (12)
C3	0.0426 (16)	0.0338 (14)	0.0514 (17)	0.0087 (13)	0.0115 (14)	0.0127 (13)
C4	0.064 (2)	0.056 (2)	0.057 (2)	0.0152 (17)	0.0173 (17)	0.0218 (17)
C5	0.090 (3)	0.077 (3)	0.062 (2)	0.018 (2)	0.032 (2)	0.025 (2)
C6	0.097 (3)	0.075 (3)	0.080 (3)	0.025 (3)	0.052 (3)	0.016 (2)
C7	0.075 (3)	0.065 (2)	0.093 (3)	0.035 (2)	0.046 (2)	0.023 (2)
C8	0.0467 (18)	0.0410 (16)	0.070 (2)	0.0174 (14)	0.0216 (16)	0.0167 (15)
C9	0.0497 (19)	0.0471 (18)	0.086 (3)	0.0260 (16)	0.0185 (18)	0.0275 (18)
C10	0.0399 (17)	0.0426 (16)	0.066 (2)	0.0122 (14)	0.0061 (15)	0.0253 (15)
C11	0.053 (2)	0.062 (2)	0.081 (3)	0.0163 (18)	0.0016 (19)	0.040 (2)
C12	0.069 (3)	0.078 (3)	0.065 (2)	0.009 (2)	0.005 (2)	0.042 (2)
C13	0.070 (2)	0.068 (2)	0.055 (2)	0.012 (2)	0.0168 (18)	0.0258 (18)
C14	0.0515 (19)	0.0472 (17)	0.0571 (19)	0.0133 (15)	0.0149 (16)	0.0205 (15)
C15	0.0345 (15)	0.0336 (14)	0.0507 (17)	0.0076 (12)	0.0062 (13)	0.0148 (13)
C16	0.0257 (14)	0.0412 (15)	0.0504 (17)	0.0108 (12)	0.0085 (12)	0.0166 (13)
C17	0.0319 (15)	0.0437 (16)	0.0445 (16)	0.0089 (12)	0.0115 (13)	0.0123 (13)
C18	0.0317 (15)	0.0540 (18)	0.0555 (18)	0.0139 (14)	0.0116 (14)	0.0216 (15)
C19	0.0448 (19)	0.056 (2)	0.079 (2)	0.0209 (16)	0.0081 (17)	0.0194 (18)
C20	0.074 (3)	0.080 (3)	0.110 (3)	0.048 (2)	0.018 (3)	0.038 (3)
C21	0.061 (3)	0.097 (3)	0.101 (3)	0.046 (2)	0.005 (2)	0.034 (3)
C22	0.0365 (18)	0.086 (3)	0.069 (2)	0.0188 (18)	−0.0009 (17)	0.027 (2)
C23	0.0316 (15)	0.059 (2)	0.0506 (17)	0.0093 (14)	0.0103 (13)	0.0217 (15)
C24	0.0334 (15)	0.0551 (19)	0.0411 (16)	0.0009 (14)	0.0056 (13)	0.0144 (14)

C25	0.0396 (16)	0.0440 (16)	0.0381 (15)	0.0003 (13)	0.0121 (13)	0.0155 (13)
C26	0.057 (2)	0.0443 (17)	0.0518 (18)	0.0040 (15)	0.0138 (16)	0.0183 (15)
C27	0.080 (3)	0.0425 (18)	0.070 (2)	0.0149 (18)	0.019 (2)	0.0273 (17)
C28	0.062 (2)	0.066 (2)	0.071 (2)	0.0210 (18)	0.0108 (19)	0.0391 (19)
C29	0.0437 (17)	0.0533 (18)	0.0469 (17)	0.0085 (14)	0.0063 (14)	0.0225 (15)
C30	0.0372 (15)	0.0477 (16)	0.0400 (15)	0.0062 (13)	0.0111 (13)	0.0195 (13)
C31	0.0392 (16)	0.0403 (15)	0.0402 (15)	0.0177 (13)	0.0162 (13)	0.0157 (12)
C32	0.0314 (14)	0.0476 (16)	0.0484 (16)	0.0188 (13)	0.0147 (13)	0.0250 (13)
C33	0.0378 (15)	0.0534 (17)	0.0501 (16)	0.0233 (14)	0.0197 (13)	0.0288 (14)
C34	0.0517 (18)	0.0562 (18)	0.0481 (17)	0.0194 (15)	0.0232 (15)	0.0239 (15)
C35	0.055 (2)	0.064 (2)	0.0520 (19)	0.0182 (17)	0.0194 (16)	0.0186 (16)
C36	0.063 (2)	0.080 (3)	0.0449 (18)	0.031 (2)	0.0173 (17)	0.0215 (18)
C37	0.067 (2)	0.086 (3)	0.0514 (19)	0.036 (2)	0.0290 (18)	0.0400 (19)
C38	0.0497 (18)	0.064 (2)	0.0537 (18)	0.0286 (16)	0.0238 (15)	0.0348 (16)
C39	0.062 (2)	0.076 (2)	0.070 (2)	0.0271 (19)	0.0358 (18)	0.050 (2)
C40	0.0447 (17)	0.0577 (19)	0.076 (2)	0.0205 (15)	0.0251 (17)	0.0416 (18)
C41	0.063 (2)	0.073 (3)	0.108 (3)	0.015 (2)	0.036 (2)	0.057 (3)
C42	0.064 (3)	0.058 (2)	0.117 (4)	0.003 (2)	0.022 (3)	0.042 (3)
C43	0.056 (2)	0.054 (2)	0.082 (3)	0.0096 (18)	0.008 (2)	0.0211 (19)
C44	0.0427 (18)	0.0528 (19)	0.068 (2)	0.0162 (15)	0.0133 (16)	0.0241 (16)
C45	0.0339 (15)	0.0495 (17)	0.0608 (18)	0.0194 (13)	0.0159 (14)	0.0276 (15)
C46	0.0452 (18)	0.067 (2)	0.0551 (19)	0.0247 (16)	0.0202 (15)	0.0216 (16)
C47	0.053 (2)	0.069 (2)	0.065 (2)	0.0260 (18)	0.0319 (18)	0.0183 (18)
C48	0.065 (2)	0.075 (2)	0.099 (3)	0.046 (2)	0.048 (2)	0.037 (2)
C49	0.066 (2)	0.073 (2)	0.090 (3)	0.047 (2)	0.042 (2)	0.041 (2)
C50	0.0342 (15)	0.0405 (16)	0.0613 (19)	0.0153 (13)	0.0123 (14)	0.0181 (14)
C51	0.0399 (16)	0.0421 (16)	0.0556 (18)	0.0166 (13)	0.0095 (14)	0.0193 (14)
C52	0.097 (3)	0.090 (3)	0.077 (3)	0.066 (3)	0.029 (2)	0.043 (2)
C53	0.113 (4)	0.097 (3)	0.072 (3)	0.064 (3)	0.025 (3)	0.051 (2)
C54	0.072 (2)	0.068 (2)	0.0527 (19)	0.0237 (19)	0.0171 (18)	0.0290 (17)
C55	0.0466 (18)	0.0565 (19)	0.0508 (18)	0.0193 (15)	0.0131 (15)	0.0218 (15)
N1	0.0374 (13)	0.0460 (14)	0.0504 (14)	0.0164 (11)	0.0131 (11)	0.0195 (11)
N2	0.0338 (13)	0.0489 (14)	0.0506 (14)	0.0163 (11)	0.0147 (11)	0.0129 (12)
O1	0.0324 (11)	0.0619 (13)	0.0439 (11)	0.0120 (9)	0.0152 (9)	0.0212 (10)
O2	0.0362 (10)	0.0302 (10)	0.0521 (11)	0.0110 (8)	0.0116 (9)	0.0120 (9)
O3	0.0373 (13)	0.0405 (12)	0.0923 (18)	0.0074 (10)	−0.0081 (12)	0.0162 (12)
O4	0.0465 (12)	0.0508 (12)	0.0424 (11)	0.0008 (10)	0.0138 (10)	0.0106 (9)
O5	0.0364 (11)	0.0573 (12)	0.0421 (11)	0.0165 (9)	0.0117 (9)	0.0214 (10)
O6	0.0363 (12)	0.0677 (14)	0.0507 (13)	0.0010 (10)	0.0174 (10)	−0.0016 (11)

Geometric parameters (Å, º)

La1—O2	2.4561 (18)	C26—C27	1.335 (5)
La1—O5	2.4574 (19)	C26—H26A	0.9300
La1—O1	2.4974 (18)	C27—C28	1.419 (5)
La1—O6	2.522 (2)	C27—H27A	0.9300
La1—O4	2.535 (2)	C28—C29	1.350 (5)
La1—O2^{i}	2.6750 (19)	C28—H28A	0.9300

La1—O3^{i}	2.687 (2)	C29—C30	1.429 (4)
La1—N1	2.730 (2)	C29—H29A	0.9300
La1—N2	2.741 (2)	C31—O5^{i}	1.254 (3)
La1—C16	2.886 (3)	C31—O1	1.270 (3)
La1—C1^{i}	3.064 (3)	C31—C32	1.512 (4)
La1—La1^{i}	4.0880 (4)	C32—C45	1.411 (4)
C1—O3	1.238 (3)	C32—C33	1.416 (4)
C1—O2	1.268 (3)	C33—C34	1.426 (4)
C1—C2	1.508 (4)	C33—C38	1.439 (4)
C1—La1^{i}	3.064 (3)	C34—C35	1.360 (4)
C2—C15	1.400 (4)	C34—H34A	0.9300
C2—C3	1.406 (4)	C35—C36	1.413 (5)
C3—C4	1.421 (5)	C35—H35A	0.9300
C3—C8	1.435 (4)	C36—C37	1.334 (5)
C4—C5	1.358 (5)	C36—H36A	0.9300
C4—H4A	0.9300	C37—C38	1.423 (5)
C5—C6	1.411 (7)	C37—H37A	0.9300
C5—H5A	0.9300	C38—C39	1.388 (5)
C6—C7	1.339 (6)	C39—C40	1.383 (5)
C6—H6A	0.9300	C39—H39A	0.9300
C7—C8	1.430 (5)	C40—C41	1.432 (5)
C7—H7A	0.9300	C40—C45	1.433 (4)
C8—C9	1.382 (5)	C41—C42	1.350 (6)
C9—C10	1.392 (5)	C41—H41A	0.9300
C9—H9A	0.9300	C42—C43	1.389 (6)
C10—C11	1.423 (5)	C42—H42A	0.9300
C10—C15	1.434 (4)	C43—C44	1.358 (5)
C11—C12	1.345 (6)	C43—H43A	0.9300
C11—H11A	0.9300	C44—C45	1.432 (4)
C12—C13	1.406 (6)	C44—H44A	0.9300
C12—H12A	0.9300	C46—N2	1.334 (4)
C13—C14	1.352 (5)	C46—C47	1.378 (5)
C13—H13A	0.9300	C46—H46A	0.9300
C14—C15	1.419 (4)	C47—C48	1.355 (5)
C14—H14A	0.9300	C47—H47A	0.9300
C16—O6	1.240 (3)	C48—C49	1.371 (5)
C16—O4	1.267 (3)	C48—H48A	0.9300
C16—C17	1.510 (4)	C49—C50	1.386 (4)
C17—C18	1.403 (4)	C49—H49A	0.9300
C17—C30	1.403 (4)	C50—N2	1.350 (4)
C18—C19	1.414 (5)	C50—C51	1.481 (4)
C18—C23	1.436 (4)	C51—N1	1.341 (4)
C19—C20	1.355 (5)	C51—C52	1.391 (5)
C19—H19A	0.9300	C52—C53	1.366 (6)
C20—C21	1.403 (6)	C52—H52A	0.9300
C20—H20A	0.9300	C53—C54	1.353 (6)
C21—C22	1.333 (6)	C53—H53A	0.9300
C21—H21A	0.9300	C54—C55	1.376 (5)

C22—C23	1.424 (5)	C54—H54A	0.9300
C22—H22A	0.9300	C55—N1	1.336 (4)
C23—C24	1.375 (5)	C55—H55A	0.9300
C24—C25	1.405 (4)	O2—La1^{i}	2.6750 (19)
C24—H24A	0.9300	O3—La1^{i}	2.687 (2)
C25—C26	1.418 (4)	O5—C31^{i}	1.254 (3)
C25—C30	1.433 (4)		

O2—La1—O5	73.16 (7)	C20—C19—C18	121.2 (3)
O2—La1—O1	73.15 (6)	C20—C19—H19A	119.4
O5—La1—O1	135.97 (6)	C18—C19—H19A	119.4
O2—La1—O6	151.98 (7)	C19—C20—C21	120.6 (4)
O5—La1—O6	90.68 (7)	C19—C20—H20A	119.7
O1—La1—O6	130.65 (7)	C21—C20—H20A	119.7
O2—La1—O4	151.37 (7)	C22—C21—C20	120.7 (4)
O5—La1—O4	135.00 (7)	C22—C21—H21A	119.7
O1—La1—O4	79.76 (6)	C20—C21—H21A	119.7
O6—La1—O4	51.39 (7)	C21—C22—C23	121.4 (4)
O2—La1—O2^{i}	74.44 (6)	C21—C22—H22A	119.3
O5—La1—O2^{i}	71.53 (6)	C23—C22—H22A	119.3
O1—La1—O2^{i}	72.74 (6)	C24—C23—C22	122.3 (3)
O6—La1—O2^{i}	122.70 (7)	C24—C23—C18	119.4 (3)
O4—La1—O2^{i}	106.39 (7)	C22—C23—C18	118.2 (3)
O2—La1—O3^{i}	121.09 (6)	C23—C24—C25	122.2 (3)
O5—La1—O3^{i}	77.60 (8)	C23—C24—H24A	118.9
O1—La1—O3^{i}	96.65 (8)	C25—C24—H24A	118.9
O6—La1—O3^{i}	75.51 (8)	C24—C25—C26	122.1 (3)
O4—La1—O3^{i}	70.62 (7)	C24—C25—C30	119.0 (3)
O2^{i}—La1—O3^{i}	47.91 (6)	C26—C25—C30	118.9 (3)
O2—La1—N1	91.57 (7)	C27—C26—C25	120.8 (3)
O5—La1—N1	134.60 (7)	C27—C26—H26A	119.6
O1—La1—N1	73.52 (7)	C25—C26—H26A	119.6
O6—La1—N1	83.64 (8)	C26—C27—C28	121.0 (3)
O4—La1—N1	71.68 (7)	C26—C27—H27A	119.5
O2^{i}—La1—N1	145.95 (7)	C28—C27—H27A	119.5
O3^{i}—La1—N1	142.16 (7)	C29—C28—C27	120.7 (3)
O2—La1—N2	78.12 (7)	C29—C28—H28A	119.7
O5—La1—N2	75.60 (7)	C27—C28—H28A	119.7
O1—La1—N2	123.19 (7)	C28—C29—C30	120.3 (3)
O6—La1—N2	75.71 (7)	C28—C29—H29A	119.8
O4—La1—N2	110.34 (7)	C30—C29—H29A	119.8
O2^{i}—La1—N2	141.93 (7)	C17—C30—C29	122.9 (3)
O3^{i}—La1—N2	140.02 (8)	C17—C30—C25	118.8 (3)
N1—La1—N2	59.30 (7)	C29—C30—C25	118.3 (3)
O2—La1—C16	167.67 (7)	O5^{i}—C31—O1	124.4 (3)
O5—La1—C16	113.22 (8)	O5^{i}—C31—C32	117.3 (2)
O1—La1—C16	105.56 (7)	O1—C31—C32	118.3 (2)
O6—La1—C16	25.37 (7)	C45—C32—C33	120.7 (3)

O4—La1—C16	26.01 (7)	C45—C32—C31	119.4 (3)
O2^{i}—La1—C16	117.24 (7)	C33—C32—C31	119.9 (2)
O3^{i}—La1—C16	71.17 (7)	C32—C33—C34	124.3 (3)
N1—La1—C16	76.45 (8)	C32—C33—C38	119.1 (3)
N2—La1—C16	93.00 (8)	C34—C33—C38	116.6 (3)
O2—La1—C1^{i}	98.51 (7)	C35—C34—C33	121.4 (3)
O5—La1—C1^{i}	74.95 (7)	C35—C34—H34A	119.3
O1—La1—C1^{i}	82.90 (7)	C33—C34—H34A	119.3
O6—La1—C1^{i}	99.13 (8)	C34—C35—C36	121.4 (3)
O4—La1—C1^{i}	87.00 (8)	C34—C35—H35A	119.3
O2^{i}—La1—C1^{i}	24.33 (6)	C36—C35—H35A	119.3
O3^{i}—La1—C1^{i}	23.71 (7)	C37—C36—C35	119.1 (3)
N1—La1—C1^{i}	150.44 (7)	C37—C36—H36A	120.4
N2—La1—C1^{i}	150.03 (8)	C35—C36—H36A	120.4
C16—La1—C1^{i}	93.44 (8)	C36—C37—C38	122.3 (3)
O2—La1—La1^{i}	39.08 (4)	C36—C37—H37A	118.8
O5—La1—La1^{i}	67.58 (5)	C38—C37—H37A	118.8
O1—La1—La1^{i}	68.39 (4)	C39—C38—C37	121.7 (3)
O6—La1—La1^{i}	152.12 (6)	C39—C38—C33	119.2 (3)
O4—La1—La1^{i}	135.40 (5)	C37—C38—C33	119.1 (3)
O2^{i}—La1—La1^{i}	35.37 (4)	C40—C39—C38	122.3 (3)
O3^{i}—La1—La1^{i}	82.63 (4)	C40—C39—H39A	118.9
N1—La1—La1^{i}	123.96 (5)	C38—C39—H39A	118.9
N2—La1—La1^{i}	113.04 (5)	C39—C40—C41	120.3 (3)
C16—La1—La1^{i}	152.43 (6)	C39—C40—C45	119.7 (3)
C1^{i}—La1—La1^{i}	59.52 (5)	C41—C40—C45	119.9 (3)
O3—C1—O2	120.6 (3)	C42—C41—C40	120.4 (4)
O3—C1—C2	121.4 (2)	C42—C41—H41A	119.8
O2—C1—C2	118.0 (2)	C40—C41—H41A	119.8
O3—C1—La1^{i}	60.80 (16)	C41—C42—C43	120.2 (4)
O2—C1—La1^{i}	60.37 (14)	C41—C42—H42A	119.9
C2—C1—La1^{i}	172.5 (2)	C43—C42—H42A	119.9
C15—C2—C3	121.4 (3)	C44—C43—C42	121.9 (4)
C15—C2—C1	119.7 (3)	C44—C43—H43A	119.1
C3—C2—C1	119.0 (3)	C42—C43—H43A	119.1
C2—C3—C4	122.8 (3)	C43—C44—C45	121.1 (3)
C2—C3—C8	118.6 (3)	C43—C44—H44A	119.5
C4—C3—C8	118.6 (3)	C45—C44—H44A	119.5
C5—C4—C3	121.1 (4)	C32—C45—C44	124.5 (3)
C5—C4—H4A	119.4	C32—C45—C40	119.0 (3)
C3—C4—H4A	119.4	C44—C45—C40	116.5 (3)
C4—C5—C6	120.0 (4)	N2—C46—C47	123.7 (3)
C4—C5—H5A	120.0	N2—C46—H46A	118.2
C6—C5—H5A	120.0	C47—C46—H46A	118.2
C7—C6—C5	121.2 (4)	C48—C47—C46	118.6 (3)
C7—C6—H6A	119.4	C48—C47—H47A	120.7
C5—C6—H6A	119.4	C46—C47—H47A	120.7
C6—C7—C8	121.2 (4)	C47—C48—C49	119.2 (3)

C6—C7—H7A	119.4	C47—C48—H48A	120.4
C8—C7—H7A	119.4	C49—C48—H48A	120.4
C9—C8—C7	122.7 (3)	C48—C49—C50	119.8 (4)
C9—C8—C3	119.5 (3)	C48—C49—H49A	120.1
C7—C8—C3	117.9 (3)	C50—C49—H49A	120.1
C8—C9—C10	122.5 (3)	N2—C50—C49	121.2 (3)
C8—C9—H9A	118.8	N2—C50—C51	117.1 (3)
C10—C9—H9A	118.8	C49—C50—C51	121.7 (3)
C9—C10—C11	122.6 (3)	N1—C51—C52	120.4 (3)
C9—C10—C15	118.6 (3)	N1—C51—C50	117.1 (3)
C11—C10—C15	118.8 (3)	C52—C51—C50	122.5 (3)
C12—C11—C10	121.2 (4)	C53—C52—C51	119.9 (4)
C12—C11—H11A	119.4	C53—C52—H52A	120.1
C10—C11—H11A	119.4	C51—C52—H52A	120.1
C11—C12—C13	120.2 (4)	C54—C53—C52	119.7 (4)
C11—C12—H12A	119.9	C54—C53—H53A	120.2
C13—C12—H12A	119.9	C52—C53—H53A	120.2
C14—C13—C12	120.9 (4)	C53—C54—C55	118.3 (4)
C14—C13—H13A	119.6	C53—C54—H54A	120.8
C12—C13—H13A	119.6	C55—C54—H54A	120.8
C13—C14—C15	121.4 (3)	N1—C55—C54	123.2 (3)
C13—C14—H14A	119.3	N1—C55—H55A	118.4
C15—C14—H14A	119.3	C54—C55—H55A	118.4
C2—C15—C14	123.0 (3)	C55—N1—C51	118.5 (3)
C2—C15—C10	119.4 (3)	C55—N1—La1	117.7 (2)
C14—C15—C10	117.6 (3)	C51—N1—La1	123.5 (2)
O6—C16—O4	122.0 (2)	C46—N2—C50	117.5 (3)
O6—C16—C17	120.7 (3)	C46—N2—La1	119.7 (2)
O4—C16—C17	117.3 (3)	C50—N2—La1	122.81 (19)
O6—C16—La1	60.64 (14)	C31—O1—La1	137.62 (17)
O4—C16—La1	61.34 (14)	C1—O2—La1	157.44 (19)
C17—C16—La1	178.3 (2)	C1—O2—La1^{i}	95.30 (17)
C18—C17—C30	121.5 (3)	La1—O2—La1^{i}	105.56 (6)
C18—C17—C16	118.8 (3)	C1—O3—La1^{i}	95.49 (17)
C30—C17—C16	119.5 (3)	C16—O4—La1	92.64 (16)
C17—C18—C19	123.1 (3)	C31^{i}—O5—La1	141.40 (18)
C17—C18—C23	118.9 (3)	C16—O6—La1	93.99 (16)
C19—C18—C23	118.0 (3)		

O3—C1—C2—C15	−92.3 (4)	C49—C50—C51—N1	−176.9 (3)
O2—C1—C2—C15	87.7 (3)	N2—C50—C51—C52	−175.9 (3)
O3—C1—C2—C3	88.3 (4)	C49—C50—C51—C52	4.0 (5)
O2—C1—C2—C3	−91.8 (3)	N1—C51—C52—C53	−0.5 (6)
C15—C2—C3—C4	−178.7 (3)	C50—C51—C52—C53	178.5 (4)
C1—C2—C3—C4	0.8 (4)	C51—C52—C53—C54	0.7 (7)
C15—C2—C3—C8	0.4 (4)	C52—C53—C54—C55	−0.6 (7)
C1—C2—C3—C8	179.9 (3)	C53—C54—C55—N1	0.1 (6)
C2—C3—C4—C5	178.7 (3)	C54—C55—N1—C51	0.1 (5)

C8—C3—C4—C5	−0.4 (5)	C54—C55—N1—La1	−173.1 (3)
C3—C4—C5—C6	0.8 (6)	C52—C51—N1—C55	0.1 (5)
C4—C5—C6—C7	−0.3 (7)	C50—C51—N1—C55	−179.0 (3)
C5—C6—C7—C8	−0.6 (7)	C52—C51—N1—La1	172.9 (3)
C6—C7—C8—C9	−179.2 (4)	C50—C51—N1—La1	−6.2 (4)
C6—C7—C8—C3	0.9 (6)	O2—La1—N1—C55	−107.2 (2)
C2—C3—C8—C9	0.5 (4)	O5—La1—N1—C55	−174.87 (19)
C4—C3—C8—C9	179.7 (3)	O1—La1—N1—C55	−35.3 (2)
C2—C3—C8—C7	−179.6 (3)	O6—La1—N1—C55	100.5 (2)
C4—C3—C8—C7	−0.5 (4)	O4—La1—N1—C55	49.1 (2)
C7—C8—C9—C10	179.3 (3)	O2^{i}—La1—N1—C55	−43.2 (3)
C3—C8—C9—C10	−0.9 (5)	O3^{i}—La1—N1—C55	44.1 (3)
C8—C9—C10—C11	178.5 (3)	N2—La1—N1—C55	177.6 (2)
C8—C9—C10—C15	0.2 (5)	C16—La1—N1—C55	75.7 (2)
C9—C10—C11—C12	−179.6 (3)	C1^{i}—La1—N1—C55	3.2 (3)
C15—C10—C11—C12	−1.3 (5)	La1^{i}—La1—N1—C55	−83.8 (2)
C10—C11—C12—C13	−0.2 (6)	O2—La1—N1—C51	79.9 (2)
C11—C12—C13—C14	1.2 (6)	O5—La1—N1—C51	12.2 (3)
C12—C13—C14—C15	−0.6 (5)	O1—La1—N1—C51	151.8 (2)
C3—C2—C15—C14	179.6 (3)	O6—La1—N1—C51	−72.4 (2)
C1—C2—C15—C14	0.1 (4)	O4—La1—N1—C51	−123.8 (2)
C3—C2—C15—C10	−1.1 (4)	O2^{i}—La1—N1—C51	143.9 (2)
C1—C2—C15—C10	179.5 (2)	O3^{i}—La1—N1—C51	−128.8 (2)
C13—C14—C15—C2	178.5 (3)	N2—La1—N1—C51	4.7 (2)
C13—C14—C15—C10	−0.8 (4)	C16—La1—N1—C51	−97.2 (2)
C9—C10—C15—C2	0.8 (4)	C1^{i}—La1—N1—C51	−169.7 (2)
C11—C10—C15—C2	−177.6 (3)	La1^{i}—La1—N1—C51	103.3 (2)
C9—C10—C15—C14	−179.9 (3)	C47—C46—N2—C50	−0.3 (5)
C11—C10—C15—C14	1.8 (4)	C47—C46—N2—La1	179.0 (3)
O2—La1—C16—O6	90.1 (4)	C49—C50—N2—C46	0.5 (4)
O5—La1—C16—O6	−29.0 (2)	C51—C50—N2—C46	−179.6 (3)
O1—La1—C16—O6	172.30 (19)	C49—C50—N2—La1	−178.8 (2)
O4—La1—C16—O6	179.9 (3)	C51—C50—N2—La1	1.1 (3)
O2^{i}—La1—C16—O6	−109.4 (2)	O2—La1—N2—C46	78.9 (2)
O3^{i}—La1—C16—O6	−95.9 (2)	O5—La1—N2—C46	3.4 (2)
N1—La1—C16—O6	104.0 (2)	O1—La1—N2—C46	139.4 (2)
N2—La1—C16—O6	46.6 (2)	O6—La1—N2—C46	−91.0 (2)
C1^{i}—La1—C16—O6	−104.1 (2)	O4—La1—N2—C46	−129.7 (2)
La1^{i}—La1—C16—O6	−114.7 (2)	O2^{i}—La1—N2—C46	34.3 (3)
O2—La1—C16—O4	−89.8 (4)	O3^{i}—La1—N2—C46	−45.9 (3)
O5—La1—C16—O4	151.05 (17)	N1—La1—N2—C46	177.9 (2)
O1—La1—C16—O4	−7.62 (19)	C16—La1—N2—C46	−109.8 (2)
O6—La1—C16—O4	−179.9 (3)	C1^{i}—La1—N2—C46	−7.6 (3)
O2^{i}—La1—C16—O4	70.66 (19)	La1^{i}—La1—N2—C46	61.0 (2)
O3^{i}—La1—C16—O4	84.21 (18)	O2—La1—N2—C50	−101.9 (2)
N1—La1—C16—O4	−75.91 (18)	O5—La1—N2—C50	−177.3 (2)
N2—La1—C16—O4	−133.33 (18)	O1—La1—N2—C50	−41.3 (2)
C1^{i}—La1—C16—O4	75.96 (18)	O6—La1—N2—C50	88.2 (2)

La1^{i}—La1—C16—O4	65.3 (2)	O4—La1—N2—C50	49.6 (2)
O6—C16—C17—C18	−84.6 (4)	O2^{i}—La1—N2—C50	−146.37 (19)
O4—C16—C17—C18	94.2 (3)	O3^{i}—La1—N2—C50	133.4 (2)
O6—C16—C17—C30	99.8 (4)	N1—La1—N2—C50	−2.8 (2)
O4—C16—C17—C30	−81.4 (4)	C16—La1—N2—C50	69.5 (2)
C30—C17—C18—C19	−177.4 (3)	C1^{i}—La1—N2—C50	171.70 (19)
C16—C17—C18—C19	7.1 (5)	La1^{i}—La1—N2—C50	−119.8 (2)
C30—C17—C18—C23	3.7 (4)	O5^{i}—C31—O1—La1	−10.6 (5)
C16—C17—C18—C23	−171.8 (3)	C32—C31—O1—La1	168.53 (18)
C17—C18—C19—C20	−179.6 (4)	O2—La1—O1—C31	−35.7 (3)
C23—C18—C19—C20	−0.7 (6)	O5—La1—O1—C31	5.8 (3)
C18—C19—C20—C21	1.4 (7)	O6—La1—O1—C31	161.4 (3)
C19—C20—C21—C22	−1.2 (8)	O4—La1—O1—C31	153.7 (3)
C20—C21—C22—C23	0.2 (7)	O2^{i}—La1—O1—C31	42.8 (3)
C21—C22—C23—C24	179.6 (4)	O3^{i}—La1—O1—C31	84.8 (3)
C21—C22—C23—C18	0.5 (6)	N1—La1—O1—C31	−132.6 (3)
C17—C18—C23—C24	−0.4 (5)	N2—La1—O1—C31	−98.6 (3)
C19—C18—C23—C24	−179.4 (3)	C16—La1—O1—C31	157.1 (3)
C17—C18—C23—C22	178.7 (3)	C1^{i}—La1—O1—C31	65.4 (3)
C19—C18—C23—C22	−0.3 (5)	La1^{i}—La1—O1—C31	5.5 (3)
C22—C23—C24—C25	178.2 (3)	O3—C1—O2—La1	149.3 (4)
C18—C23—C24—C25	−2.7 (5)	C2—C1—O2—La1	−30.6 (6)
C23—C24—C25—C26	−179.3 (3)	La1^{i}—C1—O2—La1	157.7 (5)
C23—C24—C25—C30	2.6 (4)	O3—C1—O2—La1^{i}	−8.4 (3)
C24—C25—C26—C27	−179.1 (3)	C2—C1—O2—La1^{i}	171.7 (2)
C30—C25—C26—C27	−1.0 (5)	O5—La1—O2—C1	128.1 (5)
C25—C26—C27—C28	−0.8 (6)	O1—La1—O2—C1	−80.7 (5)
C26—C27—C28—C29	2.1 (6)	O6—La1—O2—C1	71.0 (5)
C27—C28—C29—C30	−1.4 (5)	O4—La1—O2—C1	−61.1 (5)
C18—C17—C30—C29	177.2 (3)	O2^{i}—La1—O2—C1	−156.9 (5)
C16—C17—C30—C29	−7.4 (4)	O3^{i}—La1—O2—C1	−168.3 (5)
C18—C17—C30—C25	−3.8 (4)	N1—La1—O2—C1	−8.4 (5)
C16—C17—C30—C25	171.7 (3)	N2—La1—O2—C1	49.7 (5)
C28—C29—C30—C17	178.7 (3)	C16—La1—O2—C1	5.1 (7)
C28—C29—C30—C25	−0.4 (5)	C1^{i}—La1—O2—C1	−160.5 (4)
C24—C25—C30—C17	0.6 (4)	La1^{i}—La1—O2—C1	−156.9 (5)
C26—C25—C30—C17	−177.5 (3)	O5—La1—O2—La1^{i}	−74.97 (7)
C24—C25—C30—C29	179.7 (3)	O1—La1—O2—La1^{i}	76.26 (7)
C26—C25—C30—C29	1.6 (4)	O6—La1—O2—La1^{i}	−132.12 (15)
O5^{i}—C31—C32—C45	42.2 (4)	O4—La1—O2—La1^{i}	95.82 (15)
O1—C31—C32—C45	−137.0 (3)	O2^{i}—La1—O2—La1^{i}	0.0
O5^{i}—C31—C32—C33	−138.0 (3)	O3^{i}—La1—O2—La1^{i}	−11.37 (11)
O1—C31—C32—C33	42.8 (4)	N1—La1—O2—La1^{i}	148.51 (8)
C45—C32—C33—C34	−179.2 (3)	N2—La1—O2—La1^{i}	−153.33 (9)
C31—C32—C33—C34	0.9 (4)	C16—La1—O2—La1^{i}	162.1 (3)
C45—C32—C33—C38	−0.4 (4)	C1^{i}—La1—O2—La1^{i}	−3.61 (8)
C31—C32—C33—C38	179.8 (3)	O2—C1—O3—La1^{i}	8.3 (3)
C32—C33—C34—C35	−179.5 (3)	C2—C1—O3—La1^{i}	−171.7 (2)

C38—C33—C34—C35	1.6 (5)	O6—C16—O4—La1	−0.1 (3)
C33—C34—C35—C36	0.4 (5)	C17—C16—O4—La1	−178.8 (2)
C34—C35—C36—C37	−1.6 (5)	O2—La1—O4—C16	153.53 (17)
C35—C36—C37—C38	0.8 (6)	O5—La1—O4—C16	−39.0 (2)
C36—C37—C38—C39	179.4 (3)	O1—La1—O4—C16	172.54 (19)
C36—C37—C38—C33	1.3 (5)	O6—La1—O4—C16	0.04 (17)
C32—C33—C38—C39	0.5 (4)	O2^{i}—La1—O4—C16	−119.02 (18)
C34—C33—C38—C39	179.4 (3)	O3^{i}—La1—O4—C16	−86.61 (18)
C32—C33—C38—C37	178.6 (3)	N1—La1—O4—C16	96.65 (18)
C34—C33—C38—C37	−2.4 (4)	N2—La1—O4—C16	50.78 (19)
C37—C38—C39—C40	−178.0 (3)	C1^{i}—La1—O4—C16	−104.14 (18)
C33—C38—C39—C40	0.1 (5)	La1^{i}—La1—O4—C16	−143.20 (15)
C38—C39—C40—C41	178.9 (3)	O2—La1—O5—C31^{i}	46.3 (3)
C38—C39—C40—C45	−0.8 (5)	O1—La1—O5—C31^{i}	4.8 (3)
C39—C40—C41—C42	−179.4 (4)	O6—La1—O5—C31^{i}	−156.9 (3)
C45—C40—C41—C42	0.3 (6)	O4—La1—O5—C31^{i}	−127.5 (3)
C40—C41—C42—C43	0.5 (7)	O2^{i}—La1—O5—C31^{i}	−32.5 (3)
C41—C42—C43—C44	−0.6 (7)	O3^{i}—La1—O5—C31^{i}	−81.9 (3)
C42—C43—C44—C45	0.0 (6)	N1—La1—O5—C31^{i}	121.3 (3)
C33—C32—C45—C44	−178.0 (3)	N2—La1—O5—C31^{i}	128.0 (3)
C31—C32—C45—C44	1.8 (4)	C16—La1—O5—C31^{i}	−144.9 (3)
C33—C32—C45—C40	−0.2 (4)	C1^{i}—La1—O5—C31^{i}	−57.7 (3)
C31—C32—C45—C40	179.6 (3)	La1^{i}—La1—O5—C31^{i}	5.1 (3)
C43—C44—C45—C32	178.6 (3)	O4—C16—O6—La1	0.1 (3)
C43—C44—C45—C40	0.8 (5)	C17—C16—O6—La1	178.8 (2)
C39—C40—C45—C32	0.8 (5)	O2—La1—O6—C16	−152.95 (17)
C41—C40—C45—C32	−178.9 (3)	O5—La1—O6—C16	153.5 (2)
C39—C40—C45—C44	178.8 (3)	O1—La1—O6—C16	−9.8 (2)
C41—C40—C45—C44	−0.9 (5)	O4—La1—O6—C16	−0.04 (17)
N2—C46—C47—C48	−0.7 (5)	O2^{i}—La1—O6—C16	85.2 (2)
C46—C47—C48—C49	1.5 (6)	O3^{i}—La1—O6—C16	76.5 (2)
C47—C48—C49—C50	−1.4 (6)	N1—La1—O6—C16	−71.6 (2)
C48—C49—C50—N2	0.3 (5)	N2—La1—O6—C16	−131.5 (2)
C48—C49—C50—C51	−179.6 (3)	C1^{i}—La1—O6—C16	78.7 (2)
N2—C50—C51—N1	3.2 (4)	La1^{i}—La1—O6—C16	115.99 (18)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.