



**Table 1 (continued)**

Title	Reference	Retracted by	DOI	Refcode
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$ )nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ $\mu$ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- $\mu$ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ $\mu$ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^1, O^6, O^6$ :2 $\kappa^4 O^1, N, N, O^1$ } (ethanol-1 $\kappa O$ )- $\mu$ -nitrate-1:2 $\kappa^2 O$ :O'-dinitrato-1 $\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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# {6,6'-Dimethoxy-2,2'-[ethane-1,2-diyl-bis(nitrilomethylidene)]diphenolato}-methanol- $\mu$ -nitrate-dinitratolutetium(III)-zinc(II)

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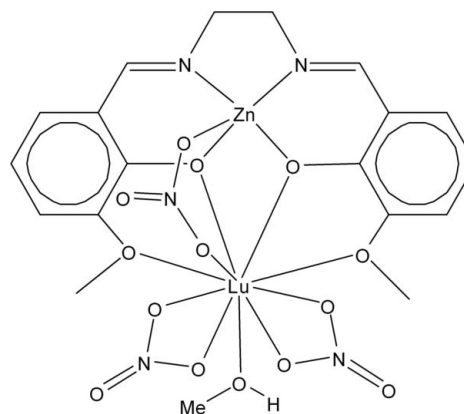
Received 24 July 2007; accepted 1 August 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.147; data-to-parameter ratio = 17.3.

In the title heteronuclear  $\text{Zn}^{\text{II}}-\text{Lu}^{\text{III}}$  complex (systematic name: {6,6'-dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato-1 $\kappa^4$ O<sup>1</sup>,O<sup>1'</sup>,O<sup>6</sup>,O<sup>6'</sup>:2 $\kappa^4$ O<sup>1</sup>,N,N',O<sup>1'</sup>}(methanol-1 $\kappa$ O)- $\mu$ -nitrate-1:2 $\kappa^2$ O:O'-dinitrato-1 $\kappa^4$ O,O'-lutetium(III)-zinc(II)),  $[\text{LuZn}(\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4)(\text{NO}_3)_3(\text{CH}_4\text{O})]$ , with the hexadentate Schiff base compartmental ligand  $N,N'$ -bis(3-methoxysalicylidene)ethylenediamine, the Lu and Zn atoms are triply bridged by two phenolate O atoms provided by the Schiff base ligand and one nitrate ion. The five-coordinated Zn is in a square-pyramidal geometry with the donor centers of two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Lu<sup>III</sup> center has a tenfold coordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, and two O atoms from two nitrate ions and one from the bridging nitrate ion. Weak intermolecular C—H...O interactions generate a two-dimensional layer structure.

## Related literature

For related literature, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005); Sui *et al.* (2006, 2007).



## Experimental

### Crystal data

$[\text{LuZn}(\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4)(\text{NO}_3)_3(\text{CH}_4\text{O})]$   
 $M_r = 784.76$   
 Monoclinic,  $P2_1/n$   
 $a = 9.6105$  (11) Å  
 $b = 13.7179$  (16) Å  
 $c = 19.851$  (2) Å  
 $\beta = 91.559$  (2)°  
 $V = 2616.2$  (5) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 4.75$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.22 \times 0.11 \times 0.06$  mm

### Data collection

Bruker APEX II area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2004)  
 $T_{\text{min}} = 0.422$ ,  $T_{\text{max}} = 0.764$   
 18694 measured reflections  
 6348 independent reflections  
 4676 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.147$   
 $S = 1.01$   
 6348 reflections  
 367 parameters  
 1 restraint  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.89$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.24$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C10}-\text{H10}\cdots\text{O12}^i$	0.93	2.53	3.443 (7)	168
$\text{C12}-\text{H12}\cdots\text{O9}^j$	0.93	2.58	3.445 (8)	154

Symmetry code: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: APEX2; software used to prepare material for publication: APEX2 and publCIF (Westrip, 2007).

We gratefully acknowledge financial support from the Department of Education, JiangXi Province (grant No. 2007317), and the Natural Science Foundation of JiangXi Province (grant No. 0620029).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2271).

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Article retracted

**supplementary materials**

**Article retracted**

*Acta Cryst.* (2007). E63, m2277-m2278 [ doi:10.1107/S1600536807037737 ]

**{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}methanol- $\mu$ -nitratodinitratolutetium(III)zinc(II)**

**Y. Sui, Y.-H. Sui, Q.-Y. Luo and Y.-D. Wang**

**Comment**

The potential applications of trivalent lanthanide complexes as contrast agent for magnetic resonance imaging and stains for fluorescence imaging have prompted considerable interest in the preparation, magnetic and optical properties of 3 d-4f heterometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). As part of our investigations into the structure and applications of 3 d-4f heterometallic Schiff base complexes (Sui *et al.*, 2006; Sui *et al.*, 2007), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Zn<sup>II</sup>—Lu<sup>III</sup> complex with salen-type Schiff base *N,N'*-bis(3-methoxysalicylidene) ethylenediamine (H<sub>2</sub>L).

Complex (I) crystallizes in the space group *P*2<sub>1</sub>/*n*, with zinc and lutetium triply bridged by two phenolate O atoms provided by a salen-type Schiff base ligand and one nitrate. The inner salen-type cavity is occupied by zinc(II), while lutetium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand.

The Lu<sup>III</sup> center has a decacoordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, two O atoms from two nitrates and one from the bridging nitrate. The five kinds of Lu—O bond distances are significantly different, the longest being the Lu—O(methoxy) separations and the shortest being the Lu—O(phenolate) and Lu—O6(bridging nitrate).

The Zn<sup>II</sup> is in a square-pyramidal geometry and is five-coordinated by two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Zn atom is 0.5813 (3) Å above the mean N<sub>2</sub>O<sub>2</sub> plane with an average deviation from the plane of 0.0951 (4) Å, which construct the bottom of square-pyramid. The Zn—O7(bridging nitrate) separation is 2.001 (4) Å and the angles of this Zn—O vector with the Zn—N or Zn—O bonds lie between 103.1 (5)° and 115.7 (6)°, which suggesting that the Zn<sup>II</sup> is in a slightly distorted square-pyramidal conformation.

Adjacent molecules are held together by weak interactions (C10—H10<sup>i</sup>⋯O12<sup>i</sup>=3.443 (7) and C12—H12<sup>i</sup>⋯O9<sup>i</sup>=3.445 (8); symmetry codes: (i) 1/2 + x, 1/2 - y, 1/2 + z). these link the molecules into a two-dimensional layer structure (Fig 2).

**Experimental**

H<sub>2</sub>L was prepared by the 2:1 condensation of 3-methoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of zinc(II) acetate dihydrate (0.188 g, 1 mmol) with H<sub>2</sub>L (0.328 g, 1 mmol) in methanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of lutetium(III) nitrate hexahydrate (0.469 g, 1 mmol). The reaction mixture was cooled and the resulting precipitate was filtered off, washed with diethyl ether and dried *in vacuo*. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol solution. Analysis calculated for C<sub>19</sub>H<sub>22</sub>LuN<sub>5</sub>O<sub>14</sub>Zn: C 29.08, H 2.83, Lu 22.30, N 8.92, Zn 8.33%; found: C 30.01, H 2.85, Lu 22.39, N 8.98, Zn 8.38%. IR (KBr, cm<sup>-1</sup>): 1640 (C=N), 1386, 1490 (nitrate).

## Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.97 Å (methylene) and 0.96 Å (methyl), and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms and  $1.2U_{\text{eq}}(\text{C})$  for other H atoms. The methyl group of methanol was constrained as idealized non-rotating CH<sub>3</sub> group. The hydroxyl H atom, H1, was located in a difference Fourier map and refined with the O1—H1 distance restrained to 0.9 Å

## Figures

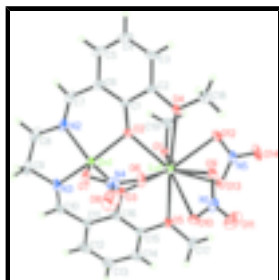


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

Fig. 2. The packing diagram of (I), viewed along the *c* axis; hydrogen bonds are shown as dashed lines.

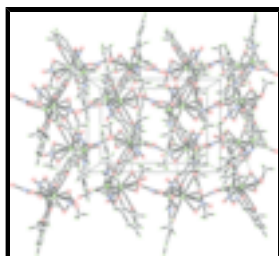


Table 1. Selected geometric parameters (Å).  
Table 2. Hydrogen-bonding geometry (Å, °).

{6,6'-dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato- $1\kappa^4\text{O}^1, \text{O}^{1'}, \text{O}^6, \text{O}^{6'}$ : $2\kappa^4\text{O}^1, \text{N}, \text{N}', \text{O}^{1'}$ }(methanol- $1\kappa\text{O}$ )- $\mu$ -nitrate- $1$ : $2\kappa^2\text{O}:\text{O}'$ -dinitrate- $1\kappa^4\text{O}, \text{O}'$ -lutetium(III)\ zinc(II)

### Crystal data

[LuZn(C<sub>18</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>)(NO<sub>3</sub>)<sub>3</sub>(CH<sub>4</sub>O)]

$M_r = 784.76$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 9.6105$  (11) Å

$b = 13.7179$  (16) Å

$c = 19.851$  (2) Å

$\beta = 91.559$  (2)°

$V = 2616.2$  (5) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1536$

$D_x = 1.992$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 6963 reflections

$\theta = 2.1$ – $28.3$ °

$\mu = 4.75$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, yellow

$0.22 \times 0.11 \times 0.06$  mm

### Data collection

Bruker APEX II area-detector

6348 independent reflections

diffractometer	
Radiation source: fine-focus sealed tube	4676 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.036$
$T = 293(2)$ K	$\theta_{\text{max}} = 28.3^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.422$ , $T_{\text{max}} = 0.764$	$k = -16 \rightarrow 18$
18694 measured reflections	$l = -26 \rightarrow 26$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.1008P)^2]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
6348 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
367 parameters	$\Delta\rho_{\text{max}} = 1.89 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -1.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Lu1	0.71866 (3)	0.27793 (2)	0.115439 (12)	0.03144 (12)
Zn1	0.68616 (7)	0.37139 (5)	0.27269 (3)	0.02574 (17)
O9	0.7326 (5)	0.3589 (3)	0.0042 (2)	0.0345 (10)
C16	0.9327 (6)	0.2406 (4)	0.2552 (3)	0.0233 (11)
N3	0.7914 (6)	0.3541 (4)	0.3614 (3)	0.0358 (12)
C1	0.4254 (6)	0.3545 (4)	0.1936 (3)	0.0269 (12)
C15	1.0143 (6)	0.1820 (5)	0.2139 (3)	0.0278 (12)



## supplementary materials

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O10	0.9304 (4)	0.3295 (4)	0.0530 (2)	0.0362 (10)
N1	0.8632 (7)	0.3645 (4)	0.0027 (3)	0.0417 (14)
O4	0.4598 (4)	0.3571 (4)	0.0784 (2)	0.0382 (11)
N2	0.5204 (6)	0.3680 (4)	0.3370 (2)	0.0347 (12)
C2	0.3668 (6)	0.3698 (5)	0.1290 (3)	0.0302 (13)
C12	1.0935 (7)	0.1994 (6)	0.3476 (4)	0.0429 (18)
H12	1.1202	0.2044	0.3928	0.051*
C6	0.3432 (6)	0.3723 (5)	0.2495 (4)	0.0338 (14)
C11	0.9745 (7)	0.2492 (5)	0.3237 (3)	0.0316 (13)
C3	0.2275 (6)	0.3960 (6)	0.1195 (4)	0.0422 (17)
H3	0.1902	0.4059	0.0763	0.051*
C14	1.1308 (7)	0.1341 (5)	0.2382 (3)	0.0372 (15)
H14	1.1825	0.0954	0.2097	0.045*
O11	0.9235 (7)	0.3988 (6)	-0.0447 (3)	0.081 (2)
C5	0.2012 (7)	0.3978 (5)	0.2378 (4)	0.0437 (18)
H5	0.1451	0.4082	0.2745	0.052*
C10	0.8999 (7)	0.3033 (5)	0.3734 (3)	0.0341 (14)
H10	0.9337	0.3007	0.4177	0.041*
C7	0.3935 (7)	0.3673 (5)	0.3192 (3)	0.0382 (15)
H7	0.3280	0.3634	0.3527	0.046*
C13	1.1710 (7)	0.1434 (6)	0.3053 (4)	0.0457 (18)
H13	1.2505	0.1118	0.3217	0.055*
C17	1.0623 (7)	0.1394 (6)	0.1013 (3)	0.0463 (18)
H17A	1.1524	0.1677	0.1101	0.069*
H17B	1.0312	0.1553	0.0563	0.069*
H17C	1.0682	0.0699	0.1061	0.069*
C18	0.4098 (8)	0.3814 (7)	0.0115 (4)	0.053 (2)
H18A	0.3271	0.3446	0.0010	0.080*
H18B	0.4799	0.3661	-0.0203	0.080*
H18C	0.3888	0.4498	0.0092	0.080*
C4	0.1453 (7)	0.4072 (5)	0.1753 (4)	0.0483 (19)
H4	0.0510	0.4213	0.1695	0.058*
O3	0.8215 (4)	0.2822 (3)	0.22720 (19)	0.0252 (9)
O2	0.5557 (4)	0.3227 (3)	0.1980 (2)	0.0277 (9)
O7	0.7422 (4)	0.5038 (3)	0.24088 (19)	0.0299 (9)
O5	0.9661 (4)	0.1771 (3)	0.1480 (2)	0.0305 (9)
O1	0.6452 (4)	0.1208 (3)	0.1631 (2)	0.0312 (9)
O6	0.7588 (5)	0.4461 (3)	0.1366 (2)	0.0372 (10)
O12	0.5672 (5)	0.1831 (4)	0.0287 (2)	0.0362 (10)
O13	0.7842 (5)	0.1475 (3)	0.0300 (2)	0.0366 (10)
N5	0.6642 (6)	0.1335 (4)	0.0041 (2)	0.0341 (12)
N4	0.7731 (6)	0.5131 (4)	0.1793 (3)	0.0411 (13)
C9	0.7120 (8)	0.3983 (5)	0.4171 (3)	0.0416 (16)
H9A	0.7151	0.4689	0.4144	0.050*
H9B	0.7509	0.3782	0.4605	0.050*
C8	0.5620 (8)	0.3619 (6)	0.4081 (3)	0.0459 (18)
H8A	0.5556	0.2949	0.4234	0.055*
H8B	0.5005	0.4014	0.4347	0.055*
C19	0.5051 (8)	0.0893 (6)	0.1656 (4)	0.052 (2)

H19A	0.4583	0.1248	0.1999	0.079*
H19B	0.5028	0.0209	0.1756	0.079*
H19C	0.4593	0.1008	0.1227	0.079*
O14	0.6430 (6)	0.0768 (4)	-0.0412 (3)	0.0619 (16)
O8	0.8349 (9)	0.6088 (5)	0.1561 (4)	0.086 (2)
H1	0.699 (6)	0.151 (5)	0.132 (3)	0.037 (19)*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Lu1	0.03498 (17)	0.03647 (19)	0.02275 (15)	-0.00013 (11)	-0.00161 (11)	-0.00127 (10)
Zn1	0.0316 (4)	0.0291 (4)	0.0166 (3)	-0.0008 (3)	0.0017 (3)	-0.0009 (3)
O9	0.034 (2)	0.049 (3)	0.020 (2)	0.003 (2)	-0.0042 (17)	0.0029 (18)
C16	0.024 (3)	0.027 (3)	0.019 (3)	-0.003 (2)	-0.009 (2)	0.006 (2)
N3	0.051 (3)	0.039 (3)	0.017 (2)	-0.005 (3)	-0.002 (2)	-0.007 (2)
C1	0.018 (3)	0.027 (3)	0.036 (3)	-0.001 (2)	0.001 (2)	-0.006 (2)
C15	0.028 (3)	0.030 (3)	0.025 (3)	-0.001 (2)	-0.004 (2)	0.003 (2)
O10	0.026 (2)	0.046 (3)	0.037 (2)	-0.0026 (19)	-0.0018 (18)	0.005 (2)
N1	0.052 (4)	0.045 (4)	0.028 (3)	0.001 (3)	0.009 (3)	0.002 (2)
O4	0.031 (2)	0.056 (3)	0.028 (2)	0.009 (2)	-0.0102 (18)	-0.008 (2)
N2	0.045 (3)	0.041 (3)	0.018 (2)	-0.001 (2)	0.009 (2)	-0.001 (2)
C2	0.021 (3)	0.027 (3)	0.042 (3)	0.003 (2)	0.000 (2)	-0.009 (3)
C12	0.040 (4)	0.058 (5)	0.030 (3)	-0.006 (3)	-0.017 (3)	0.014 (3)
C6	0.027 (3)	0.025 (3)	0.050 (4)	-0.001 (2)	0.013 (3)	-0.001 (3)
C11	0.034 (3)	0.041 (4)	0.020 (3)	-0.006 (3)	-0.011 (2)	0.005 (3)
C3	0.022 (3)	0.040 (4)	0.064 (5)	0.005 (3)	-0.010 (3)	-0.008 (3)
C14	0.031 (3)	0.039 (4)	0.041 (4)	0.008 (3)	-0.008 (3)	0.004 (3)
O11	0.074 (4)	0.112 (6)	0.059 (4)	-0.004 (4)	0.030 (3)	0.041 (4)
C5	0.029 (3)	0.032 (4)	0.070 (5)	0.002 (3)	0.018 (3)	-0.007 (4)
C10	0.039 (4)	0.046 (4)	0.016 (3)	-0.012 (3)	-0.007 (2)	0.002 (3)
C7	0.043 (4)	0.034 (4)	0.039 (3)	0.004 (3)	0.019 (3)	0.000 (3)
C13	0.034 (4)	0.054 (5)	0.048 (4)	0.012 (3)	-0.012 (3)	0.016 (4)
C17	0.043 (4)	0.061 (5)	0.034 (4)	0.017 (3)	0.003 (3)	-0.005 (3)
C18	0.049 (4)	0.073 (6)	0.038 (4)	0.013 (4)	-0.011 (3)	-0.002 (4)
C4	0.020 (3)	0.042 (4)	0.083 (6)	0.005 (3)	0.007 (3)	-0.003 (4)
O3	0.024 (2)	0.036 (2)	0.0158 (18)	0.0032 (16)	-0.0046 (15)	-0.0008 (15)
O2	0.0231 (19)	0.035 (2)	0.025 (2)	0.0036 (17)	-0.0015 (16)	-0.0048 (18)
O7	0.044 (2)	0.023 (2)	0.023 (2)	0.0001 (17)	0.0051 (18)	-0.0026 (16)
O5	0.029 (2)	0.039 (3)	0.023 (2)	0.0060 (18)	-0.0043 (16)	-0.0035 (18)
O1	0.031 (2)	0.027 (2)	0.036 (2)	-0.0040 (17)	-0.0015 (18)	0.0063 (19)
O6	0.059 (3)	0.029 (3)	0.023 (2)	-0.005 (2)	0.004 (2)	-0.0032 (18)
O12	0.038 (2)	0.041 (3)	0.028 (2)	0.000 (2)	-0.0088 (19)	-0.003 (2)
O13	0.035 (2)	0.045 (3)	0.030 (2)	0.001 (2)	-0.0026 (19)	-0.007 (2)
N5	0.051 (3)	0.029 (3)	0.021 (2)	-0.002 (2)	-0.005 (2)	0.000 (2)
N4	0.041 (3)	0.039 (3)	0.044 (3)	0.005 (3)	0.002 (3)	0.008 (3)
C9	0.067 (5)	0.040 (4)	0.018 (3)	0.005 (3)	0.006 (3)	-0.003 (3)
C8	0.069 (5)	0.045 (4)	0.025 (3)	0.010 (4)	0.021 (3)	0.008 (3)
C19	0.039 (4)	0.061 (5)	0.057 (5)	-0.017 (4)	0.006 (3)	0.014 (4)

## supplementary materials

O14	0.083 (4)	0.058 (4)	0.043 (3)	0.002 (3)	-0.022 (3)	-0.030 (3)
O8	0.116 (6)	0.060 (4)	0.083 (5)	-0.010 (4)	0.030 (4)	0.003 (4)

### Geometric parameters (Å, °)

Lu1—O1	2.465 (4)	C6—C5	1.421 (9)
Lu1—O2	2.378 (4)	C6—C7	1.456 (10)
Lu1—O3	2.405 (4)	C11—C10	1.442 (10)
Lu1—O4	2.794 (4)	C3—C4	1.387 (10)
Lu1—O5	2.812 (4)	C3—H3	0.9300
Lu1—O6	2.374 (5)	C14—C13	1.382 (10)
Lu1—O9	2.479 (4)	C14—H14	0.9300
Lu1—O10	2.513 (4)	C5—C4	1.344 (11)
Lu1—O12	2.577 (4)	C5—H5	0.9300
Lu1—O13	2.556 (4)	C10—H10	0.9300
Zn1—O2	2.029 (4)	C7—H7	0.9300
Zn1—O3	2.017 (4)	C13—H13	0.9300
Zn1—O7	2.001 (4)	C17—O5	1.424 (8)
Zn1—N2	2.069 (5)	C17—H17A	0.9600
Zn1—N3	2.021 (5)	C17—H17B	0.9600
Lu1—H1	1.79 (6)	C17—H17C	0.9600
O9—N1	1.259 (7)	C18—H18A	0.9600
C16—O3	1.321 (6)	C18—H18B	0.9600
C16—C15	1.403 (8)	C18—H18C	0.9600
C16—C11	1.412 (7)	C4—H4	0.9300
N3—C10	1.271 (9)	O7—N4	1.272 (7)
N3—C9	1.489 (8)	O1—C19	1.416 (8)
C1—O2	1.327 (7)	O1—H1	0.91 (2)
C1—C6	1.400 (8)	O6—N4	1.257 (7)
C1—C2	1.402 (9)	O12—N5	1.264 (7)
C15—C14	1.375 (8)	O13—N5	1.264 (7)
C15—O5	1.376 (7)	N5—O14	1.202 (7)
O10—N1	1.269 (7)	N4—O8	1.517 (9)
N1—O11	1.213 (7)	C9—C8	1.531 (11)
O4—C2	1.374 (8)	C9—H9A	0.9700
O4—C18	1.440 (8)	C9—H9B	0.9700
N2—C7	1.260 (9)	C8—H8A	0.9700
N2—C8	1.459 (8)	C8—H8B	0.9700
C2—C3	1.394 (8)	C19—H19A	0.9600
C12—C13	1.372 (11)	C19—H19B	0.9600
C12—C11	1.404 (9)	C19—H19C	0.9600
C12—H12	0.9300		
O6—Lu1—O2	74.58 (15)	C8—N2—Zn1	113.7 (4)
O6—Lu1—O3	75.68 (14)	O4—C2—C3	125.1 (6)
O2—Lu1—O3	67.64 (13)	O4—C2—C1	113.4 (5)
O6—Lu1—O1	145.94 (14)	C3—C2—C1	121.5 (6)
O2—Lu1—O1	76.13 (15)	C13—C12—C11	121.1 (6)
O3—Lu1—O1	77.39 (14)	C13—C12—H12	119.5
O6—Lu1—O9	73.13 (15)	C11—C12—H12	119.5

O2—Lu1—O9	123.42 (15)	C1—C6—C5	118.2 (7)
O3—Lu1—O9	141.30 (14)	C1—C6—C7	124.4 (6)
O1—Lu1—O9	139.19 (14)	C5—C6—C7	117.4 (6)
O6—Lu1—O10	71.59 (16)	C12—C11—C16	119.5 (6)
O2—Lu1—O10	145.56 (16)	C12—C11—C10	115.7 (6)
O3—Lu1—O10	97.50 (14)	C16—C11—C10	124.7 (6)
O1—Lu1—O10	132.82 (15)	C4—C3—C2	119.1 (7)
O9—Lu1—O10	50.98 (14)	C4—C3—H3	120.5
O6—Lu1—O13	139.06 (15)	C2—C3—H3	120.5
O2—Lu1—O13	144.78 (15)	C15—C14—C13	119.9 (6)
O3—Lu1—O13	121.81 (14)	C15—C14—H14	120.1
O1—Lu1—O13	73.83 (15)	C13—C14—H14	120.1
O9—Lu1—O13	72.64 (15)	C4—C5—C6	122.2 (7)
O10—Lu1—O13	69.62 (16)	C4—C5—H5	118.9
O6—Lu1—O12	133.99 (16)	C6—C5—H5	118.9
O2—Lu1—O12	102.71 (14)	N3—C10—C11	125.0 (5)
O3—Lu1—O12	147.06 (14)	N3—C10—H10	117.5
O1—Lu1—O12	69.69 (15)	C11—C10—H10	117.5
O9—Lu1—O12	70.97 (15)	N2—C7—C6	124.0 (6)
O10—Lu1—O12	105.23 (15)	N2—C7—H7	118.0
O13—Lu1—O12	49.32 (14)	C6—C7—H7	118.0
O6—Lu1—O4	78.92 (16)	C12—C13—C14	119.9 (6)
O2—Lu1—O4	58.84 (13)	C12—C13—H13	120.0
O3—Lu1—O4	125.00 (13)	C14—C13—H13	120.0
O1—Lu1—O4	100.30 (15)	O5—C17—H17A	109.5
O9—Lu1—O4	70.16 (14)	O5—C17—H17B	109.5
O10—Lu1—O4	119.20 (15)	H17A—C17—H17B	109.5
O13—Lu1—O4	109.33 (13)	O5—C17—H17C	109.5
O12—Lu1—O4	62.46 (14)	H17A—C17—H17C	109.5
O6—Lu1—O5	107.77 (15)	H17B—C17—H17C	109.5
O2—Lu1—O5	122.51 (12)	O4—C18—H18A	109.5
O3—Lu1—O5	58.40 (12)	O4—C18—H18B	109.5
O1—Lu1—O5	74.38 (14)	H18A—C18—H18B	109.5
O9—Lu1—O5	111.08 (13)	O4—C18—H18C	109.5
O10—Lu1—O5	63.94 (14)	H18A—C18—H18C	109.5
O13—Lu1—O5	65.56 (13)	H18B—C18—H18C	109.5
O12—Lu1—O5	111.37 (14)	C5—C4—C3	120.3 (6)
O4—Lu1—O5	173.31 (13)	C5—C4—H4	119.9
O6—Lu1—H1	159 (2)	C3—C4—H4	119.9
O2—Lu1—H1	92.7 (16)	C16—O3—Zn1	126.7 (3)
O3—Lu1—H1	84 (2)	C16—O3—Lu1	133.2 (3)
O1—Lu1—H1	16.5 (16)	Zn1—O3—Lu1	100.03 (15)
O9—Lu1—H1	127.8 (19)	C1—O2—Zn1	120.2 (4)
O10—Lu1—H1	117.4 (17)	C1—O2—Lu1	132.7 (4)
O13—Lu1—H1	58.1 (17)	Zn1—O2—Lu1	100.56 (15)
O12—Lu1—H1	65 (2)	N4—O7—Zn1	117.8 (4)
O4—Lu1—H1	109 (2)	C15—O5—C17	115.4 (5)
O5—Lu1—H1	65 (2)	C15—O5—Lu1	117.0 (3)
O7—Zn1—O3	103.10 (17)	C17—O5—Lu1	126.1 (4)

## supplementary materials

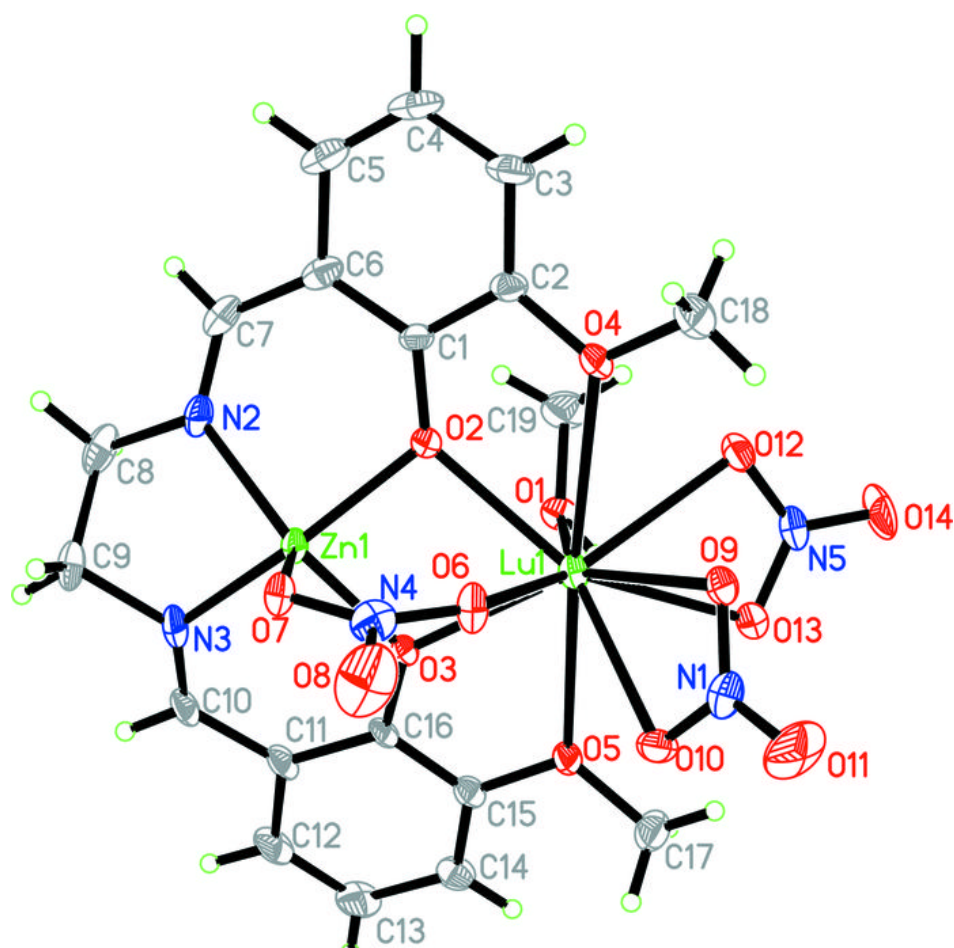
O7—Zn1—N3	104.4 (2)	C19—O1—Lu1	124.2 (4)
O3—Zn1—N3	90.3 (2)	C19—O1—H1	136 (4)
O7—Zn1—O2	103.56 (17)	Lu1—O1—H1	34 (5)
O3—Zn1—O2	82.30 (16)	N4—O6—Lu1	147.7 (4)
N3—Zn1—O2	152.0 (2)	N5—O12—Lu1	96.9 (3)
O7—Zn1—N2	115.71 (19)	N5—O13—Lu1	97.9 (3)
O3—Zn1—N2	141.2 (2)	O14—N5—O12	121.7 (6)
N3—Zn1—N2	80.5 (2)	O14—N5—O13	122.4 (6)
O2—Zn1—N2	88.42 (19)	O12—N5—O13	115.8 (5)
N1—O9—Lu1	97.3 (3)	O6—N4—O7	123.4 (5)
O3—C16—C15	117.4 (5)	O6—N4—O8	117.7 (5)
O3—C16—C11	125.1 (6)	O7—N4—O8	118.8 (6)
C15—C16—C11	117.5 (5)	N3—C9—C8	106.3 (5)
C10—N3—C9	121.3 (5)	N3—C9—H9A	110.5
C10—N3—Zn1	128.0 (4)	C8—C9—H9A	110.5
C9—N3—Zn1	110.1 (4)	N3—C9—H9B	110.5
O2—C1—C6	123.9 (6)	C8—C9—H9B	110.5
O2—C1—C2	117.6 (5)	H9A—C9—H9B	108.7
C6—C1—C2	118.5 (5)	N2—C8—C9	109.1 (5)
C14—C15—O5	124.1 (6)	N2—C8—H8A	109.9
C14—C15—C16	122.1 (6)	C9—C8—H8A	109.9
O5—C15—C16	113.9 (5)	N2—C8—H8B	109.9
N1—O10—Lu1	95.3 (3)	C9—C8—H8B	109.9
O11—N1—O9	122.7 (6)	H8A—C8—H8B	108.3
O11—N1—O10	120.9 (6)	O1—C19—H19A	109.5
O9—N1—O10	116.4 (5)	O1—C19—H19B	109.5
C2—O4—C18	115.9 (5)	H19A—C19—H19B	109.5
C2—O4—Lu1	116.7 (3)	O1—C19—H19C	109.5
C18—O4—Lu1	127.3 (4)	H19A—C19—H19C	109.5
C7—N2—C8	120.5 (6)	H19B—C19—H19C	109.5
C7—N2—Zn1	125.7 (4)		

### Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C10—H10...O12 <sup>i</sup>	0.93	2.53	3.443 (7)	168
C12—H12...O9 <sup>i</sup>	0.93	2.58	3.445 (8)	154
C17—H17B...O10	0.96	2.58	3.043 (9)	110
C17—H17B...O13	0.96	2.42	2.993 (8)	118
C18—H18B...O9	0.96	2.47	3.125 (9)	126
C19—H19C...O12	0.96	2.44	3.079 (9)	124

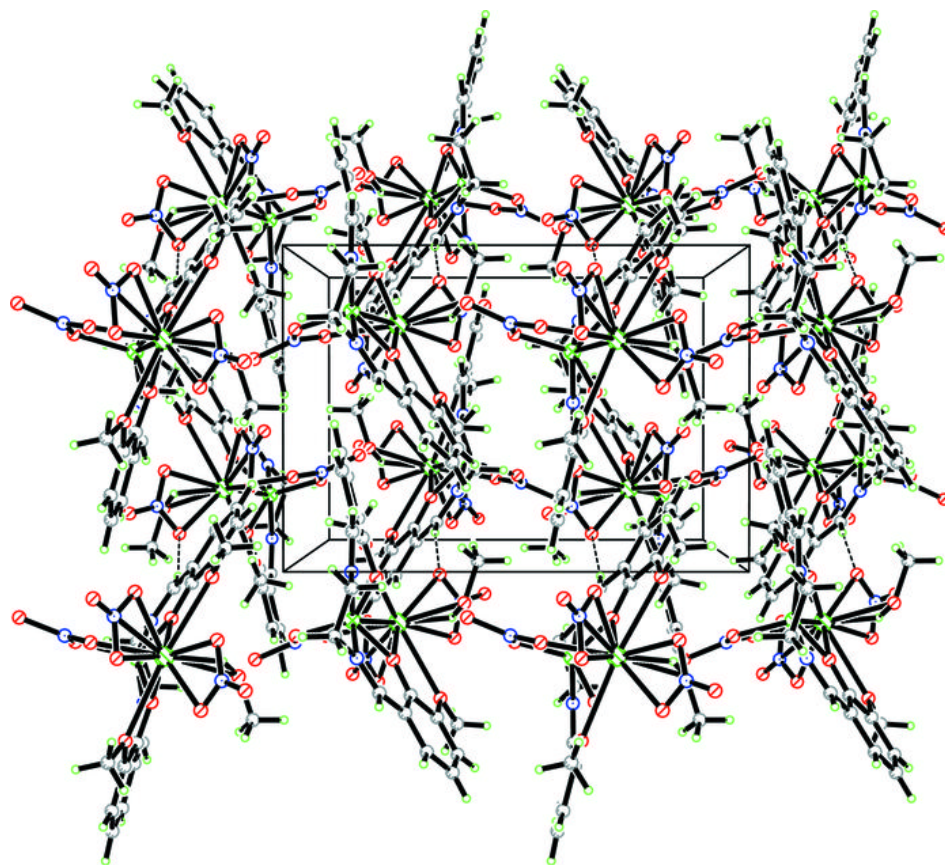
Symmetry codes: (i)  $x+1/2, -y+1/2, z+1/2$ .

Fig. 1



Article

Fig. 2



Article