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[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)lutetium(III)–nitrate–water–ethyl acetate (1/1/0.5/0.25)

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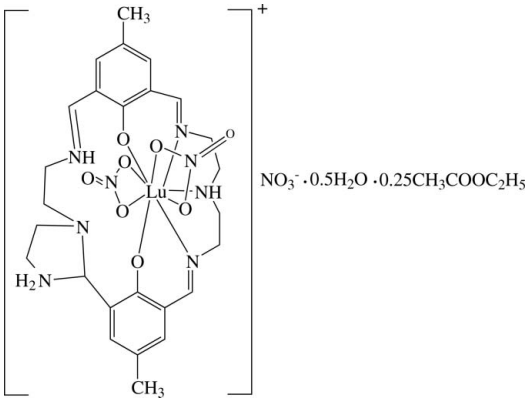
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.016 Å; disorder in solvent or counterion; R factor = 0.050; wR factor = 0.104; data-to-parameter ratio = 10.7.

In the asymmetric unit of the title compound, [Lu^{III}($C_{26}H_{34}N_6O_2$)(NO_3)$_2$]NO_3·0.5H_2O·0.25$C_4H_8O_2$, there are two cations and two anions of the title complex, together with a water molecule and half a molecule of ethyl acetate. The Lu atom exhibits a nine-coordinate distorted tricapped trigonal-prismatic coordination geometry. The water molecule is disordered, with occupation factors of 0.4 and 0.6.

Related literature

For related literature, see: Alexander (1995); Hu *et al.* (2003, 2004, 2007); Spodine *et al.* (2000).



Experimental

Crystal data

[Lu($C_{26}H_{34}N_6O_2$)(NO_3)$_2$]NO_3·0.5H_2O·0.25$C_4H_8O_2$
M_r = 854.63
Monoclinic, *Cc*
a = 24.649 (3) Å
b = 14.0182 (11) Å
c = 21.4453 (17) Å
β = 102.307 (2)°
V = 7239.8 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.80 mm^{-1}
T = 291 (2) K
0.32 × 0.26 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.42, T_{max} = 0.51
20514 measured reflections
9791 independent reflections
8284 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.104
S = 0.98
9791 reflections
913 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −1.58 e Å^{-3}
Absolute structure: Flack (1983), with 2678 Friedel pairs
Flack parameter: 0.016 (10)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2	0.90	2.07	2.765 (13)	133
N4—H4B···O22	0.90	1.94	2.826 (13)	166
N4—H4B···O20	0.90	2.45	3.108 (14)	130
N4—H4B···N18	0.90	2.59	3.435 (15)	156
N6—H6A···O1	0.86	1.99	2.635 (11)	131
N6—H6A···O6	0.86	2.63	3.407 (14)	151
N10—H10···O15	0.91	2.35	2.810 (13)	111
N12—H12D···O10	0.90	1.90	2.641 (12)	138
N14—H14A···O9	0.86	1.86	2.560 (10)	137
O25—H25F···O8	0.85	2.53	3.007 (19)	116
O25—H25C···O5^{i}	0.85	2.32	2.992 (19)	137
N2—H2···O19^{i}	0.91	2.08	2.959 (11)	163
N10—H10···O20^{ii}	0.91	2.24	3.112 (14)	161
N12—H12C···O18^{iii}	0.90	1.92	2.810 (13)	170
N12—H12C···O19^{iii}	0.90	2.53	3.126 (12)	124
N12—H12C···N17^{iii}	0.90	2.59	3.413 (14)	152

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HG2233).

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supplementary materials

Acta Cryst. (2007). E**63**, m1668-m1669 [**doi:10.1107/S1600536807022350**]

[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)lutetium(III)-nitrate-water-ethyl acetate (1/1/0.5/0.25)

X.-L. Hu, Z. Chen, L. Qiu and Z.-Q. Pan

Comment

Lanthanide macrocyclic complexes are of particular interest because they have many possible applications in biological systems, material science and chemical processes (Alexander, 1995). Our research is focused on the syntheses, crystal structures and properties of lanthanide(III) complexes with macrocyclic Schiff bases (Hu *et al.*, 2003; Hu *et al.*, 2004). Recently, we have reported the crystal structure of a gadolinium(III) complex with the macrocyclic ligand dervided from 2,6-diformyl-4-methylphenol and 1,5-diamino-3-azapentane ($[Gd(III)(C_{26}H_{34}N_6O_2)(NO_3)_2]^+\cdot(NO_3)^-\cdot H_20$), in which the central ion is nine-coordinate, being bound to five donor atoms from the cyclic polydentate ligand and to four O atoms of two bidentae nitrates (Hu *et al.*, 2007). As a part of a continuing study, herein we report a new lutecium analogue $[Lu(III)(C_{26}H_{34}N_6O_2)(NO_3)_2]^+.\ (NO_3)^-.\ 0.5H_20.\ 0.25CH_3COOC_2H_5$ (I), but which is a different solvate, belonging to a different space group (space group *Cc*, compared with *C2/c*).

In the asymmetric unit (Fig. 1), there are two molecules of the title complex (I) which exhibit a similar coordinate geometry with the previous complex (Hu *et al.*, 2007)(Fig. 2). Lu1 is encapsulated within the macrocyclic ligand which provided five donor atoms (the two O atoms O1,O2 from the phenolates and the three N atoms N1, N2, N3 from one end of the macrocycle). The ninefold coordination is completed around Lu1 by two bidentate nitrates which locate on the opposite sides of the bisphenoidal positions. The third nitrate is ionic. At the free end of the macrocycle, a five-membered imidazole rings is formed. The coordination polyhedron can be described as a distorted tricapped trigonal prism in which N2, O3 and O6 are located at capped sites, as shown in Fig.2. When the phenol oxygen atoms coordinate to the lanthanide ion, the phenol H atoms dissociate and are transferred to the neigbouring imidazole nitrogen to give a zwitterionic structure. This proton transfer has been conformed by NMR study of the tetraiminodiphenol analogue (Spodine *et al.*, 2000).

Experimental

To a methanolic solution (20 ml) of 2,6-diformyl-4-methylphenol(1 mmol) and $Lu(NO_3)_3\cdot 6H_2O$ (0.5 mmol), 1,5-diamino-3-azapentane (1 mmol) was added dropwise. After refluxing 3 h, the solvent was removed. The resultant yellow solid was recrystallized in methanol/ethyl acetate (4/1,*v*/*v*) to yield yellow crystals suitable for X-ray analysis.

Refinement

The carbon-bound H atoms were generated geometrically (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The nitrogen H were located in a difference Fourier map, and were refined with an N—H distance restraint of 0.90 (1) Å for the sp^3-N and 0.86 (1) Å for the sp^2-N, their temperature

factors were set to $1.2U_{eq}$(C). The water H atoms were also located in a difference Fourier map, and was refined with an O—H distance restraint of 0.85 (1) Å.

Figures

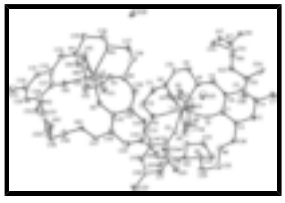

Fig. 1. Thermal ellipsoid plot of (I). Displacement ellipsoids are drawn at the 30% probability level.

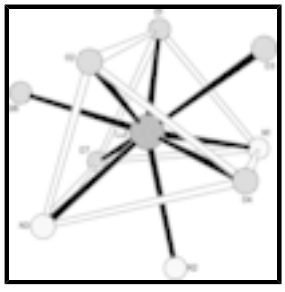

Fig. 2. Coordination polyhedron in (I).

[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta- 1(29),2,9,11,13,15 (30),16,23,25,27-decaene-29,30-diol- κ^5*N*^{3},*N*^{6},*N*^{9},*O*^{29},*O*^{30}]bis(nitrato-κ^2*O*,*O*')lutetium(III)– nitrate–water–ethyl acetate (1/1/0.5/0.25)

Crystal data

$[Lu(C_{26}H_{34}N_6O_2)(NO_3)_2]NO_3{\cdot}0.5H_2O{\cdot}0.25C_4H_8O_2$	F_{000} = 3432
M_r = 854.63	D_x = 1.568 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 5188 reflections
a = 24.649 (3) Å	θ = 2.7–25.6º
b = 14.0182 (11) Å	μ = 2.80 mm^{-1}
c = 21.4453 (17) Å	*T* = 291 (2) K
β = 102.307 (2)º	Block, yellow
V = 7239.8 (11) Å^3	0.32 × 0.26 × 0.24 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	9791 independent reflections
Radiation source: sealed tube	8284 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan	*h* = −28→30

(SADABS; Bruker, 2000)
T_{min} = 0.42, T_{max} = 0.51
20514 measured reflections
k = −17→17
l = −26→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.104
S = 0.98
9791 reflections
913 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 1.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −1.58 e Å^{-3}
Extinction correction: none
Absolute structure: Flack (1983), with 2678 Friedel pairs
Flack parameter: 0.016 (10)

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}	Occ. (<1)
C1	0.9197 (4)	0.6393 (7)	0.5542 (6)	0.043 (2)	
C2	0.9711 (4)	0.6880 (7)	0.5549 (6)	0.040 (2)	
C3	0.9722 (5)	0.7835 (6)	0.5339 (6)	0.045 (3)	
H3	1.0062	0.8125	0.5342	0.054*	
C4	0.9244 (5)	0.8340 (7)	0.5132 (6)	0.050 (3)	
C5	0.8765 (5)	0.7906 (8)	0.5130 (6)	0.055 (3)	
H5	0.8442	0.8258	0.4995	0.066*	
C6	0.8709 (4)	0.6956 (8)	0.5316 (6)	0.045 (3)	
C7	0.9282 (5)	0.9340 (7)	0.4926 (6)	0.054 (3)	
H7A	0.8916	0.9582	0.4757	0.080*	
H7B	0.9497	0.9367	0.4602	0.080*	
H7C	0.9458	0.9720	0.5284	0.080*	

C8	0.8162 (5)	0.6599 (8)	0.5362 (6)	0.049 (3)
H8	0.7878	0.7049	0.5283	0.059*
C9	0.7438 (5)	0.5612 (9)	0.5532 (7)	0.052 (3)
H9A	0.7247	0.5244	0.5168	0.063*
H9B	0.7251	0.6222	0.5528	0.063*
C10	0.7423 (5)	0.5092 (8)	0.6134 (6)	0.049 (3)
H10A	0.7599	0.5470	0.6500	0.059*
H10B	0.7042	0.4971	0.6163	0.059*
C11	0.7781 (5)	0.3693 (8)	0.6744 (6)	0.052 (3)
H11A	0.7420	0.3599	0.6846	0.062*
H11B	0.8007	0.4071	0.7080	0.062*
C12	0.8055 (5)	0.2746 (9)	0.6691 (6)	0.057 (3)
H12A	0.8178	0.2472	0.7112	0.069*
H12B	0.7789	0.2312	0.6438	0.069*
C13	0.8871 (5)	0.2180 (9)	0.6469 (5)	0.051 (3)
H13	0.8802	0.1712	0.6749	0.062*
C14	0.9349 (3)	0.2014 (5)	0.6188 (3)	0.040 (3)
C15	0.9667 (3)	0.1209 (4)	0.6392 (3)	0.054 (4)
H15	0.9573	0.0813	0.6701	0.065*
C16	1.0125 (3)	0.0996 (4)	0.6135 (4)	0.059 (4)
C17	1.0265 (3)	0.1588 (6)	0.5674 (4)	0.056 (3)
H17	1.0571	0.1446	0.5502	0.067*
C18	0.9947 (3)	0.2393 (5)	0.5470 (3)	0.054 (3)
C19	0.9489 (3)	0.2606 (4)	0.5727 (3)	0.046 (3)
C20	1.0465 (5)	0.0076 (8)	0.6313 (6)	0.058 (3)
H20A	1.0267	−0.0345	0.6539	0.088*
H20B	1.0818	0.0232	0.6580	0.088*
H20C	1.0520	−0.0231	0.5932	0.088*
C21	1.0143 (6)	0.3040 (10)	0.4989 (7)	0.065 (4)
H21	1.0444	0.2733	0.4831	0.078*
C22	0.9861 (6)	0.4177 (8)	0.4176 (7)	0.062 (3)
H22A	0.9938	0.4066	0.3757	0.074*
H22B	0.9578	0.4667	0.4142	0.074*
C23	1.0382 (5)	0.4466 (8)	0.4648 (6)	0.049 (3)
H23A	1.0713	0.4243	0.4516	0.059*
H23B	1.0404	0.5153	0.4705	0.059*
C24	1.0743 (5)	0.4001 (9)	0.5807 (6)	0.061 (3)
H24A	1.1089	0.3773	0.5714	0.073*
H24B	1.0640	0.3578	0.6121	0.073*
C25	1.0821 (5)	0.5007 (8)	0.6073 (7)	0.054 (3)
H25A	1.0968	0.4984	0.6530	0.064*
H25B	1.1083	0.5350	0.5877	0.064*
C26	1.0234 (4)	0.6374 (7)	0.5722 (5)	0.043 (2)
H26	1.0555	0.6687	0.5675	0.052*
C27	0.6628 (5)	−0.0607 (8)	0.8491 (6)	0.051 (3)
C28	0.6884 (4)	−0.1463 (7)	0.8727 (5)	0.043 (2)
C29	0.6701 (4)	−0.2323 (7)	0.8434 (7)	0.051 (3)
H29	0.6879	−0.2880	0.8604	0.061*
C30	0.6263 (5)	−0.2399 (7)	0.7895 (7)	0.056 (3)

C31	0.5985 (5)	−0.1562 (7)	0.7699 (6)	0.050 (3)
H31	0.5670	−0.1592	0.7372	0.060*
C32	0.6154 (5)	−0.0653 (7)	0.7970 (5)	0.042 (2)
C33	0.6069 (5)	−0.3341 (8)	0.7597 (7)	0.062 (4)
H33A	0.6329	−0.3568	0.7355	0.093*
H33B	0.5711	−0.3265	0.7319	0.093*
H33C	0.6044	−0.3793	0.7926	0.093*
C34	0.5814 (4)	0.0168 (8)	0.7729 (6)	0.049 (3)
H34	0.5461	0.0044	0.7486	0.059*
C35	0.5516 (4)	0.1746 (8)	0.7561 (6)	0.050 (3)
H35A	0.5271	0.1493	0.7182	0.060*
H35B	0.5295	0.1873	0.7876	0.060*
C36	0.5767 (5)	0.2641 (8)	0.7401 (6)	0.049 (3)
H36A	0.5938	0.2546	0.7038	0.059*
H36B	0.5486	0.3133	0.7293	0.059*
C37	0.6478 (5)	0.3853 (7)	0.7905 (6)	0.050 (3)
H37A	0.6624	0.3846	0.7519	0.060*
H37B	0.6213	0.4372	0.7871	0.060*
C38	0.6937 (4)	0.4018 (9)	0.8460 (6)	0.051 (3)
H38A	0.6797	0.4046	0.8850	0.061*
H38B	0.7123	0.4615	0.8412	0.061*
C39	0.7845 (5)	0.3431 (8)	0.8509 (6)	0.049 (3)
H39	0.7936	0.4075	0.8555	0.059*
C40	0.8274 (5)	0.2798 (8)	0.8475 (6)	0.053 (3)
C41	0.8802 (5)	0.3194 (8)	0.8479 (6)	0.051 (3)
H41	0.8848	0.3850	0.8531	0.061*
C42	0.9261 (5)	0.2645 (9)	0.8407 (7)	0.059 (3)
C43	0.9177 (5)	0.1680 (9)	0.8314 (6)	0.056 (3)
H43	0.9469	0.1308	0.8241	0.067*
C44	0.8659 (5)	0.1219 (8)	0.8326 (6)	0.050 (3)
C45	0.8203 (4)	0.1779 (6)	0.8436 (5)	0.038 (2)
C46	0.9822 (5)	0.3050 (9)	0.8427 (7)	0.058 (3)
H46A	1.0025	0.2634	0.8204	0.088*
H46B	1.0018	0.3111	0.8863	0.088*
H46C	0.9786	0.3666	0.8227	0.088*
C47	0.8622 (4)	0.0231 (7)	0.8258 (6)	0.045 (3)
H47	0.8922	−0.0100	0.8166	0.054*
C48	0.8125 (6)	−0.1293 (8)	0.8313 (7)	0.056 (3)
H48A	0.8399	−0.1581	0.8107	0.068*
H48B	0.7759	−0.1466	0.8071	0.068*
C49	0.8200 (6)	−0.1655 (8)	0.8978 (7)	0.057 (3)
H49A	0.8088	−0.2320	0.8968	0.068*
H49B	0.8589	−0.1619	0.9186	0.068*
C50	0.8126 (5)	−0.1082 (9)	1.0030 (6)	0.053 (3)
H50A	0.8464	−0.0707	1.0113	0.064*
H50B	0.8206	−0.1718	1.0202	0.064*
C51	0.7663 (5)	−0.0596 (10)	1.0305 (6)	0.058 (3)
H51A	0.7636	−0.0869	1.0713	0.070*
H51B	0.7722	0.0086	1.0353	0.070*

C52	0.7310 (5)	−0.1478 (7)	0.9330 (6)	0.045 (3)	
H52	0.7338	−0.2126	0.9505	0.054*	
C53	0.7210 (8)	0.7880 (17)	0.6733 (11)	0.048 (5)	0.50
H53A	0.7306	0.7770	0.7185	0.072*	0.50
H53B	0.7231	0.7290	0.6512	0.072*	0.50
H53C	0.6839	0.8128	0.6617	0.072*	0.50
C54	0.7593 (9)	0.8558 (15)	0.6559 (9)	0.041 (5)	0.50
H54A	0.7586	0.9148	0.6793	0.049*	0.50
H54B	0.7488	0.8699	0.6106	0.049*	0.50
C55	0.8599 (8)	0.8684 (18)	0.6700 (14)	0.054 (7)	0.50
C56	0.9091 (9)	0.8130 (16)	0.6889 (11)	0.048 (5)	0.50
H56A	0.9384	0.8525	0.7120	0.072*	0.50
H56B	0.9198	0.7875	0.6518	0.072*	0.50
H56C	0.9023	0.7615	0.7158	0.072*	0.50
Lu1	0.861690 (18)	0.43572 (3)	0.58012 (2)	0.04135 (12)	
Lu2	0.686348 (16)	0.16395 (2)	0.834229 (18)	0.03540 (10)	
N1	0.8014 (4)	0.5761 (6)	0.5494 (5)	0.046 (2)	
N2	0.7720 (4)	0.4191 (6)	0.6124 (5)	0.046 (2)	
H2	0.7502	0.3815	0.5827	0.055*	
N3	0.8538 (4)	0.2866 (6)	0.6385 (4)	0.045 (2)	
N4	0.9676 (5)	0.3261 (7)	0.4451 (5)	0.057 (3)	
H4A	0.9359	0.3351	0.4588	0.069*	
H4B	0.9625	0.2790	0.4159	0.069*	
N5	1.0309 (4)	0.3991 (6)	0.5223 (5)	0.055 (2)	
N6	1.0278 (4)	0.5506 (6)	0.5939 (5)	0.052 (2)	
H6A	0.9988	0.5216	0.6006	0.062*	
N7	0.8102 (5)	0.4138 (7)	0.4465 (6)	0.056 (3)	
N8	0.9215 (4)	0.4878 (8)	0.7090 (5)	0.057 (3)	
N9	0.7326 (4)	0.3201 (6)	0.8481 (6)	0.051 (3)	
N10	0.6186 (4)	0.2922 (6)	0.7962 (5)	0.048 (2)	
H10	0.5997	0.3011	0.8279	0.058*	
N11	0.5950 (3)	0.1032 (6)	0.7817 (4)	0.042 (2)	
N12	0.7163 (4)	−0.0818 (6)	0.9802 (5)	0.050 (2)	
H12C	0.6901	−0.1084	0.9981	0.061*	
H12D	0.7024	−0.0275	0.9607	0.061*	
N13	0.7873 (3)	−0.1108 (6)	0.9349 (4)	0.041 (2)	
N14	0.8188 (4)	−0.0240 (6)	0.8319 (4)	0.042 (2)	
H14A	0.7905	0.0089	0.8368	0.050*	
N15	0.7020 (4)	0.1155 (7)	0.7101 (5)	0.049 (2)	
N16	0.6773 (5)	0.2001 (7)	0.9653 (6)	0.057 (3)	
N17	0.6489 (4)	0.7472 (7)	0.0480 (5)	0.056 (2)	
N18	0.9898 (5)	0.1321 (8)	0.3560 (5)	0.059 (3)	
O1	0.9185 (3)	0.5520 (5)	0.5724 (4)	0.0416 (17)	
O2	0.9172 (3)	0.3362 (5)	0.5484 (4)	0.0427 (17)	
O3	0.8551 (4)	0.4623 (6)	0.4596 (4)	0.057 (2)	
O4	0.7950 (4)	0.3748 (6)	0.4930 (4)	0.060 (2)	
O5	0.7842 (4)	0.4060 (6)	0.3895 (5)	0.070 (3)	
O6	0.9455 (4)	0.4326 (6)	0.6774 (4)	0.059 (2)	
O7	0.8713 (3)	0.5109 (5)	0.6807 (4)	0.051 (2)	

O8	0.9429 (4)	0.5204 (6)	0.7596 (4)	0.066 (2)	
O9	0.7745 (3)	0.1369 (5)	0.8477 (4)	0.0429 (17)	
O10	0.6809 (3)	0.0204 (5)	0.8760 (3)	0.0414 (17)	
O11	0.6952 (3)	0.1997 (5)	0.7290 (4)	0.050 (2)	
O12	0.7000 (4)	0.0487 (6)	0.7474 (4)	0.054 (2)	
O13	0.7098 (4)	0.1021 (6)	0.6571 (4)	0.056 (2)	
O14	0.7238 (4)	0.1754 (6)	0.9538 (4)	0.052 (2)	
O15	0.6371 (4)	0.2078 (6)	0.9178 (4)	0.054 (2)	
O16	0.6708 (3)	0.2150 (6)	1.0200 (4)	0.056 (2)	
O17	0.6216 (3)	0.6988 (5)	0.0788 (4)	0.052 (2)	
O18	0.6296 (3)	0.8255 (6)	0.0222 (4)	0.054 (2)	
O19	0.6943 (3)	0.7219 (6)	0.0393 (4)	0.054 (2)	
O20	1.0301 (4)	0.1780 (6)	0.3784 (4)	0.060 (2)	
O21	0.9908 (3)	0.0624 (6)	0.3228 (5)	0.059 (2)	
O22	0.9461 (3)	0.1601 (5)	0.3690 (4)	0.055 (2)	
O23	0.8155 (6)	0.8141 (9)	0.6712 (7)	0.039 (3)	0.50
O24	0.8546 (6)	0.9498 (14)	0.6541 (10)	0.065 (5)	0.50
O25	0.8703 (6)	0.6513 (10)	0.8171 (8)	0.066 (4)	0.60
H25F	0.8771	0.6497	0.7799	0.079*	0.60
H25C	0.8395	0.6238	0.8167	0.079*	0.60
O26	0.5948 (7)	0.5428 (14)	0.9459 (10)	0.056 (5)	0.40
H26A	0.6012	0.5507	0.9861	0.067*	0.40
H26B	0.5846	0.4856	0.9370	0.067*	0.40

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.046 (6)	0.027 (5)	0.053 (7)	−0.003 (4)	0.006 (5)	−0.004 (5)
C2	0.031 (5)	0.038 (5)	0.057 (7)	−0.012 (4)	0.019 (4)	−0.010 (5)
C3	0.057 (6)	0.024 (5)	0.057 (7)	−0.004 (4)	0.018 (5)	−0.006 (5)
C4	0.058 (7)	0.032 (5)	0.053 (7)	−0.006 (5)	−0.004 (5)	−0.009 (5)
C5	0.061 (7)	0.036 (6)	0.065 (8)	0.020 (5)	0.009 (6)	0.007 (6)
C6	0.041 (6)	0.043 (6)	0.053 (7)	0.014 (5)	0.015 (5)	−0.004 (5)
C7	0.063 (7)	0.038 (6)	0.049 (7)	0.007 (5)	−0.010 (6)	0.002 (5)
C8	0.044 (6)	0.051 (6)	0.050 (7)	0.013 (5)	0.005 (5)	−0.014 (5)
C9	0.037 (6)	0.057 (7)	0.061 (9)	0.007 (5)	0.007 (6)	0.001 (6)
C10	0.048 (6)	0.041 (6)	0.058 (8)	0.004 (5)	0.013 (5)	0.006 (5)
C11	0.067 (8)	0.044 (6)	0.055 (7)	−0.019 (5)	0.037 (6)	−0.016 (5)
C12	0.056 (7)	0.062 (7)	0.055 (8)	−0.027 (6)	0.015 (6)	−0.002 (6)
C13	0.054 (7)	0.061 (7)	0.033 (6)	−0.018 (6)	−0.006 (5)	0.007 (5)
C14	0.056 (7)	0.018 (4)	0.039 (6)	0.002 (4)	−0.005 (5)	0.009 (4)
C15	0.066 (8)	0.028 (5)	0.055 (7)	−0.003 (5)	−0.020 (6)	0.011 (5)
C16	0.068 (8)	0.053 (7)	0.046 (7)	0.010 (6)	−0.013 (6)	−0.025 (6)
C17	0.039 (6)	0.058 (7)	0.062 (8)	0.008 (5)	−0.009 (5)	−0.016 (6)
C18	0.065 (8)	0.052 (7)	0.040 (6)	0.007 (5)	−0.003 (6)	−0.014 (5)
C19	0.049 (7)	0.040 (6)	0.040 (6)	−0.002 (5)	−0.010 (5)	−0.008 (5)
C20	0.064 (8)	0.046 (6)	0.052 (8)	0.017 (5)	−0.015 (6)	−0.011 (6)
C21	0.057 (8)	0.066 (8)	0.068 (9)	0.024 (6)	0.005 (7)	−0.006 (7)

C22	0.073 (9)	0.052 (7)	0.066 (9)	0.015 (6)	0.032 (7)	0.014 (6)
C23	0.048 (6)	0.050 (6)	0.055 (7)	0.010 (5)	0.027 (5)	−0.020 (5)
C24	0.056 (7)	0.065 (7)	0.054 (8)	0.019 (6)	−0.003 (6)	−0.015 (6)
C25	0.040 (6)	0.048 (6)	0.070 (9)	0.006 (5)	0.007 (5)	0.006 (6)
C26	0.032 (5)	0.046 (6)	0.051 (7)	−0.002 (4)	0.010 (5)	0.008 (5)
C27	0.047 (6)	0.047 (6)	0.058 (8)	−0.012 (5)	0.015 (6)	0.019 (6)
C28	0.044 (6)	0.042 (6)	0.045 (6)	−0.007 (4)	0.014 (5)	−0.012 (5)
C29	0.049 (6)	0.022 (4)	0.078 (9)	0.002 (4)	0.007 (6)	0.011 (5)
C30	0.066 (7)	0.019 (5)	0.077 (9)	−0.010 (4)	0.006 (6)	−0.013 (5)
C31	0.037 (6)	0.040 (6)	0.070 (8)	−0.004 (4)	0.007 (5)	0.007 (6)
C32	0.044 (6)	0.041 (5)	0.039 (6)	−0.001 (4)	0.002 (5)	−0.003 (5)
C33	0.057 (7)	0.046 (6)	0.070 (9)	−0.014 (5)	−0.015 (6)	−0.018 (6)
C34	0.031 (5)	0.058 (7)	0.051 (7)	−0.011 (5)	−0.009 (5)	−0.013 (6)
C35	0.038 (5)	0.050 (6)	0.057 (7)	0.008 (4)	0.003 (5)	0.020 (6)
C36	0.055 (7)	0.043 (6)	0.048 (7)	0.010 (5)	0.009 (5)	−0.003 (5)
C37	0.071 (8)	0.034 (5)	0.050 (7)	0.009 (5)	0.026 (6)	0.018 (5)
C38	0.032 (6)	0.067 (7)	0.055 (8)	−0.002 (5)	0.011 (5)	−0.003 (6)
C39	0.060 (7)	0.039 (6)	0.054 (8)	−0.007 (5)	0.022 (6)	−0.014 (5)
C40	0.051 (7)	0.049 (6)	0.057 (8)	−0.009 (5)	0.007 (6)	−0.004 (6)
C41	0.061 (7)	0.039 (6)	0.049 (7)	−0.016 (5)	0.005 (6)	0.016 (5)
C42	0.040 (6)	0.062 (7)	0.078 (9)	−0.013 (5)	0.018 (6)	0.023 (7)
C43	0.055 (7)	0.062 (7)	0.057 (8)	0.001 (6)	0.026 (6)	0.002 (6)
C44	0.053 (7)	0.042 (6)	0.054 (7)	−0.006 (5)	0.006 (5)	−0.002 (5)
C45	0.038 (5)	0.030 (5)	0.048 (6)	−0.010 (4)	0.018 (4)	−0.006 (4)
C46	0.053 (7)	0.048 (6)	0.072 (9)	−0.020 (5)	0.008 (6)	0.020 (6)
C47	0.034 (5)	0.047 (6)	0.053 (7)	0.016 (5)	0.008 (4)	0.016 (6)
C48	0.066 (8)	0.037 (6)	0.074 (9)	−0.011 (5)	0.031 (7)	0.003 (6)
C49	0.059 (8)	0.048 (6)	0.069 (9)	0.011 (5)	0.027 (7)	0.025 (6)
C50	0.043 (6)	0.052 (7)	0.059 (8)	−0.005 (5)	−0.001 (5)	0.002 (6)
C51	0.056 (7)	0.074 (9)	0.045 (7)	−0.016 (6)	0.010 (6)	−0.003 (6)
C52	0.051 (6)	0.039 (6)	0.049 (7)	0.001 (4)	0.019 (5)	0.014 (5)
C53	0.033 (10)	0.067 (14)	0.044 (12)	−0.009 (9)	0.007 (9)	−0.022 (11)
C54	0.060 (14)	0.044 (11)	0.023 (10)	0.030 (10)	0.018 (9)	0.013 (8)
C55	0.026 (10)	0.053 (13)	0.082 (19)	0.015 (9)	0.011 (11)	−0.023 (13)
C56	0.037 (11)	0.060 (13)	0.049 (13)	0.027 (10)	0.011 (9)	0.001 (11)
Lu1	0.0338 (2)	0.0395 (2)	0.0515 (3)	−0.00315 (19)	0.01054 (18)	−0.0019 (2)
Lu2	0.0344 (2)	0.02812 (18)	0.0447 (2)	−0.00110 (17)	0.01064 (16)	0.0027 (2)
N1	0.035 (5)	0.045 (5)	0.056 (6)	0.005 (4)	0.004 (4)	−0.001 (4)
N2	0.042 (5)	0.035 (4)	0.062 (6)	−0.010 (4)	0.016 (4)	−0.006 (4)
N3	0.045 (5)	0.050 (5)	0.038 (5)	−0.015 (4)	0.008 (4)	0.009 (4)
N4	0.062 (6)	0.070 (7)	0.039 (6)	0.004 (5)	0.009 (5)	0.000 (5)
N5	0.062 (6)	0.042 (5)	0.058 (6)	0.004 (4)	0.007 (5)	0.000 (5)
N6	0.033 (5)	0.044 (5)	0.079 (7)	−0.005 (4)	0.011 (5)	−0.002 (5)
N7	0.071 (7)	0.040 (5)	0.051 (7)	0.001 (5)	−0.001 (6)	0.006 (5)
N8	0.041 (5)	0.069 (6)	0.059 (7)	−0.018 (5)	0.005 (5)	−0.021 (6)
N9	0.046 (5)	0.025 (4)	0.080 (8)	−0.008 (4)	0.008 (5)	−0.013 (5)
N10	0.033 (4)	0.042 (5)	0.069 (7)	0.005 (4)	0.008 (4)	0.015 (5)
N11	0.030 (4)	0.047 (5)	0.043 (5)	0.006 (4)	−0.001 (4)	0.009 (4)
N12	0.042 (5)	0.035 (5)	0.073 (7)	0.003 (4)	0.010 (5)	0.002 (5)

N13	0.040 (5)	0.036 (4)	0.045 (5)	−0.003 (3)	0.002 (4)	0.001 (4)
N14	0.039 (5)	0.031 (4)	0.054 (6)	0.009 (3)	0.008 (4)	−0.002 (4)
N15	0.034 (5)	0.069 (7)	0.045 (6)	−0.005 (4)	0.014 (4)	0.000 (5)
N16	0.070 (7)	0.042 (5)	0.063 (8)	−0.024 (5)	0.021 (6)	0.005 (5)
N17	0.058 (6)	0.062 (6)	0.055 (6)	0.010 (5)	0.026 (5)	0.007 (5)
N18	0.062 (7)	0.062 (6)	0.056 (7)	−0.011 (5)	0.022 (5)	−0.012 (6)
O1	0.033 (3)	0.041 (4)	0.052 (5)	−0.003 (3)	0.011 (3)	0.002 (3)
O2	0.053 (4)	0.035 (4)	0.041 (4)	0.012 (3)	0.011 (3)	0.005 (3)
O3	0.055 (5)	0.054 (5)	0.059 (6)	−0.007 (4)	0.007 (4)	−0.001 (4)
O4	0.062 (5)	0.058 (5)	0.054 (5)	−0.007 (4)	0.001 (4)	0.002 (4)
O5	0.056 (5)	0.066 (5)	0.072 (7)	0.005 (4)	−0.020 (5)	0.012 (5)
O6	0.059 (5)	0.066 (5)	0.051 (5)	−0.005 (4)	0.010 (4)	0.000 (4)
O7	0.035 (4)	0.055 (5)	0.064 (5)	−0.018 (3)	0.011 (4)	−0.018 (4)
O8	0.068 (6)	0.063 (5)	0.057 (6)	−0.009 (4)	−0.007 (4)	−0.031 (5)
O9	0.046 (4)	0.033 (3)	0.053 (5)	0.003 (3)	0.017 (4)	0.001 (3)
O10	0.044 (4)	0.035 (3)	0.041 (4)	−0.012 (3)	−0.001 (3)	0.004 (3)
O11	0.052 (5)	0.035 (4)	0.068 (6)	0.011 (3)	0.021 (4)	0.008 (4)
O12	0.060 (5)	0.051 (5)	0.056 (5)	−0.002 (4)	0.022 (4)	0.004 (4)
O13	0.066 (5)	0.062 (5)	0.054 (5)	−0.014 (4)	0.044 (4)	−0.011 (4)
O14	0.048 (5)	0.056 (5)	0.053 (5)	−0.023 (4)	0.012 (4)	−0.014 (4)
O15	0.058 (5)	0.052 (5)	0.052 (5)	0.002 (4)	0.014 (4)	−0.003 (4)
O16	0.054 (5)	0.056 (5)	0.057 (6)	−0.012 (4)	0.013 (4)	−0.012 (4)
O17	0.054 (5)	0.049 (4)	0.057 (5)	−0.010 (4)	0.018 (4)	0.017 (4)
O18	0.049 (5)	0.053 (5)	0.067 (6)	0.015 (4)	0.027 (4)	0.027 (4)
O19	0.046 (4)	0.063 (5)	0.055 (5)	0.013 (4)	0.012 (4)	0.022 (4)
O20	0.058 (5)	0.065 (5)	0.059 (6)	−0.025 (4)	0.015 (4)	−0.023 (4)
O21	0.049 (5)	0.058 (5)	0.070 (6)	−0.004 (4)	0.015 (4)	−0.009 (5)
O22	0.049 (5)	0.054 (4)	0.064 (6)	−0.015 (4)	0.014 (4)	−0.016 (4)
O23	0.035 (7)	0.036 (7)	0.041 (8)	0.011 (5)	−0.006 (6)	0.001 (6)
O24	0.031 (8)	0.081 (13)	0.082 (14)	−0.011 (8)	0.011 (8)	0.008 (10)
O25	0.068 (10)	0.061 (9)	0.075 (11)	−0.009 (7)	0.028 (8)	0.020 (8)
O26	0.034 (9)	0.072 (13)	0.061 (13)	−0.028 (9)	0.009 (9)	−0.027 (11)

Geometric parameters (Å, °)

C1—O1	1.286 (12)	C39—C40	1.394 (17)
C1—C6	1.434 (14)	C39—H39	0.9300
C1—C2	1.436 (14)	C40—C41	1.414 (17)
C2—C3	1.416 (14)	C40—C45	1.439 (14)
C2—C26	1.449 (14)	C41—C42	1.404 (18)
C3—C4	1.365 (15)	C41—H41	0.9300
C3—H3	0.9300	C42—C43	1.376 (18)
C4—C5	1.328 (18)	C42—C46	1.488 (15)
C4—C7	1.479 (15)	C43—C44	1.434 (17)
C5—C6	1.405 (16)	C43—H43	0.9300
C5—H5	0.9300	C44—C47	1.393 (15)
C6—C8	1.460 (17)	C44—C45	1.432 (16)
C7—H7A	0.9600	C45—O9	1.287 (12)
C7—H7B	0.9600	C46—H46A	0.9600

C7—H7C	0.9600	C46—H46B	0.9600
C8—N1	1.279 (15)	C46—H46C	0.9600
C8—H8	0.9300	C47—N14	1.287 (14)
C9—N1	1.456 (15)	C47—H47	0.9300
C9—C10	1.489 (18)	C48—N14	1.483 (13)
C9—H9A	0.9700	C48—C49	1.489 (18)
C9—H9B	0.9700	C48—H48A	0.9700
C10—N2	1.462 (13)	C48—H48B	0.9700
C10—H10A	0.9700	C49—N13	1.464 (15)
C10—H10B	0.9700	C49—H49A	0.9700
C11—N2	1.479 (15)	C49—H49B	0.9700
C11—C12	1.504 (17)	C50—N13	1.461 (15)
C11—H11A	0.9700	C50—C51	1.550 (19)
C11—H11B	0.9700	C50—H50A	0.9700
C12—N3	1.486 (15)	C50—H50B	0.9700
C12—H12A	0.9700	C51—N12	1.486 (15)
C12—H12B	0.9700	C51—H51A	0.9700
C13—N3	1.252 (15)	C51—H51B	0.9700
C13—C14	1.452 (14)	C52—N13	1.472 (13)
C13—H13	0.9300	C52—N12	1.474 (15)
C14—C15	1.3900	C52—H52	0.9800
C14—C19	1.3900	C53—C54	1.44 (3)
C15—C16	1.3900	C53—H53A	0.9600
C15—H15	0.9300	C53—H53B	0.9600
C16—C17	1.3900	C53—H53C	0.9600
C16—C20	1.541 (11)	C54—O23	1.47 (2)
C17—C18	1.3900	C54—H54A	0.9700
C17—H17	0.9300	C54—H54B	0.9700
C18—C19	1.3900	C55—O24	1.19 (3)
C18—C21	1.526 (17)	C55—O23	1.34 (3)
C19—O2	1.353 (8)	C55—C56	1.43 (3)
C20—H20A	0.9600	C56—H56A	0.9600
C20—H20B	0.9600	C56—H56B	0.9600
C20—H20C	0.9600	C56—H56C	0.9600
C21—N5	1.452 (17)	Lu1—O2	2.163 (7)
C21—N4	1.478 (16)	Lu1—O1	2.178 (7)
C21—H21	0.9800	Lu1—O7	2.366 (8)
C22—C23	1.512 (18)	Lu1—O4	2.368 (8)
C22—N4	1.522 (15)	Lu1—N2	2.465 (9)
C22—H22A	0.9700	Lu1—N3	2.466 (9)
C22—H22B	0.9700	Lu1—N1	2.469 (9)
C23—N5	1.446 (16)	Lu1—O3	2.582 (9)
C23—H23A	0.9700	Lu1—O6	2.605 (8)
C23—H23B	0.9700	Lu1—N7	2.892 (11)
C24—N5	1.462 (14)	Lu2—O9	2.163 (7)
C24—C25	1.519 (16)	Lu2—O10	2.218 (7)
C24—H24A	0.9700	Lu2—O11	2.366 (9)
C24—H24B	0.9700	Lu2—N11	2.446 (8)
C25—N6	1.482 (13)	Lu2—O15	2.447 (9)

C25—H25A	0.9700	Lu2—N9	2.457 (8)
C25—H25B	0.9700	Lu2—N10	2.471 (8)
C26—N6	1.299 (13)	Lu2—O14	2.539 (9)
C26—H26	0.9300	Lu2—O12	2.542 (9)
C27—O10	1.310 (13)	Lu2—N15	2.852 (10)
C27—C28	1.399 (15)	Lu2—N16	2.912 (12)
C27—C32	1.436 (16)	N2—H2	0.9100
C28—C29	1.389 (14)	N4—H4A	0.9000
C28—C52	1.482 (15)	N4—H4B	0.9000
C29—C30	1.408 (16)	N6—H6A	0.8600
C29—H29	0.9300	N7—O5	1.258 (14)
C30—C31	1.378 (15)	N7—O4	1.263 (14)
C30—C33	1.500 (13)	N7—O3	1.277 (13)
C31—C32	1.425 (15)	N8—O8	1.191 (12)
C31—H31	0.9300	N8—O6	1.257 (13)
C32—C34	1.453 (15)	N8—O7	1.298 (12)
C33—H33A	0.9600	N10—H10	0.9100
C33—H33B	0.9600	N12—H12C	0.9000
C33—H33C	0.9600	N12—H12D	0.9000
C34—N11	1.260 (14)	N14—H14A	0.8600
C34—H34	0.9300	N15—O13	1.209 (12)
C35—C36	1.472 (16)	N15—O12	1.239 (12)
C35—N11	1.483 (12)	N15—O11	1.271 (12)
C35—H35A	0.9700	N16—O16	1.234 (14)
C35—H35B	0.9700	N16—O15	1.265 (14)
C36—N10	1.462 (14)	N16—O14	1.271 (14)
C36—H36A	0.9700	N17—O19	1.224 (12)
C36—H36B	0.9700	N17—O17	1.241 (12)
C37—C38	1.476 (16)	N17—O18	1.275 (12)
C37—N10	1.508 (14)	N18—O20	1.194 (12)
C37—H37A	0.9700	N18—O21	1.211 (13)
C37—H37B	0.9700	N18—O22	1.234 (13)
C38—N9	1.489 (15)	O25—H25F	0.8499
C38—H38A	0.9700	O25—H25C	0.8500
C38—H38B	0.9700	O26—H26A	0.8499
C39—N9	1.309 (15)	O26—H26B	0.8500
O1—C1—C6	123.7 (10)	N13—C52—C28	120.6 (9)
O1—C1—C2	121.7 (9)	N12—C52—C28	110.9 (9)
C6—C1—C2	114.6 (9)	N13—C52—H52	109.1
C3—C2—C1	121.6 (10)	N12—C52—H52	109.1
C3—C2—C26	117.9 (9)	C28—C52—H52	109.1
C1—C2—C26	120.3 (9)	C54—C53—H53A	109.5
C4—C3—C2	121.3 (10)	C54—C53—H53B	109.5
C4—C3—H3	119.4	H53A—C53—H53B	109.5
C2—C3—H3	119.4	C54—C53—H53C	109.5
C5—C4—C3	118.0 (10)	H53A—C53—H53C	109.5
C5—C4—C7	123.1 (11)	H53B—C53—H53C	109.5
C3—C4—C7	118.9 (11)	C53—C54—O23	108.4 (16)
C4—C5—C6	125.2 (11)	C53—C54—H54A	110.0

C4—C5—H5	117.4	O23—C54—H54A	110.0
C6—C5—H5	117.4	C53—C54—H54B	110.0
C5—C6—C1	119.4 (10)	O23—C54—H54B	110.0
C5—C6—C8	119.6 (10)	H54A—C54—H54B	108.4
C1—C6—C8	120.5 (10)	O24—C55—O23	120.7 (18)
C4—C7—H7A	109.5	O24—C55—C56	130 (2)
C4—C7—H7B	109.5	O23—C55—C56	110 (2)
H7A—C7—H7B	109.5	C55—C56—H56A	109.5
C4—C7—H7C	109.5	C55—C56—H56B	109.5
H7A—C7—H7C	109.5	H56A—C56—H56B	109.5
H7B—C7—H7C	109.5	C55—C56—H56C	109.5
N1—C8—C6	129.8 (10)	H56A—C56—H56C	109.5
N1—C8—H8	115.1	H56B—C56—H56C	109.5
C6—C8—H8	115.1	O2—Lu1—O1	90.0 (3)
N1—C9—C10	108.9 (10)	O2—Lu1—O7	128.8 (3)
N1—C9—H9A	109.9	O1—Lu1—O7	78.1 (3)
C10—C9—H9A	109.9	O2—Lu1—O4	84.2 (3)
N1—C9—H9B	109.9	O1—Lu1—O4	124.0 (3)
C10—C9—H9B	109.9	O7—Lu1—O4	142.9 (3)
H9A—C9—H9B	108.3	O2—Lu1—N2	133.9 (3)
N2—C10—C9	107.8 (10)	O1—Lu1—N2	136.2 (3)
N2—C10—H10A	110.1	O7—Lu1—N2	73.0 (3)
C9—C10—H10A	110.1	O4—Lu1—N2	71.0 (3)
N2—C10—H10B	110.1	O2—Lu1—N3	74.7 (3)
C9—C10—H10B	110.1	O1—Lu1—N3	142.6 (3)
H10A—C10—H10B	108.5	O7—Lu1—N3	85.3 (3)
N2—C11—C12	108.1 (9)	O4—Lu1—N3	88.7 (3)
N2—C11—H11A	110.1	N2—Lu1—N3	66.7 (3)
C12—C11—H11A	110.1	O2—Lu1—N1	144.6 (3)
N2—C11—H11B	110.1	O1—Lu1—N1	75.1 (3)
C12—C11—H11B	110.1	O7—Lu1—N1	80.0 (3)
H11A—C11—H11B	108.4	O4—Lu1—N1	78.5 (3)
N3—C12—C11	110.3 (9)	N2—Lu1—N1	68.0 (3)
N3—C12—H12A	109.6	N3—Lu1—N1	134.7 (3)
C11—C12—H12A	109.6	O2—Lu1—O3	71.8 (3)
N3—C12—H12B	109.6	O1—Lu1—O3	73.8 (3)
C11—C12—H12B	109.6	O7—Lu1—O3	145.2 (3)
H12A—C12—H12B	108.1	O4—Lu1—O3	51.5 (3)
N3—C13—C14	129.0 (10)	N2—Lu1—O3	115.2 (3)
N3—C13—H13	115.5	N3—Lu1—O3	129.5 (3)
C14—C13—H13	115.5	N1—Lu1—O3	73.2 (3)
C15—C14—C19	120.0	O2—Lu1—O6	78.1 (3)
C15—C14—C13	116.9 (6)	O1—Lu1—O6	70.2 (3)
C19—C14—C13	123.1 (6)	O7—Lu1—O6	50.9 (3)
C14—C15—C16	120.0	O4—Lu1—O6	157.5 (3)
C14—C15—H15	120.0	N2—Lu1—O6	112.3 (3)
C16—C15—H15	120.0	N3—Lu1—O6	73.4 (3)
C17—C16—C15	120.0	N1—Lu1—O6	123.8 (3)
C17—C16—C20	118.2 (8)	O3—Lu1—O6	132.4 (3)

C15—C16—C20	121.7 (8)	O2—Lu1—N7	78.1 (3)
C18—C17—C16	120.0	O1—Lu1—N7	99.1 (3)
C18—C17—H17	120.0	O7—Lu1—N7	152.6 (3)
C16—C17—H17	120.0	O4—Lu1—N7	25.4 (3)
C19—C18—C17	120.0	N2—Lu1—N7	92.2 (3)
C19—C18—C21	122.7 (7)	N3—Lu1—N7	110.4 (3)
C17—C18—C21	117.2 (7)	N1—Lu1—N7	73.0 (3)
O2—C19—C18	117.8 (6)	O3—Lu1—N7	26.2 (3)
O2—C19—C14	122.1 (6)	O6—Lu1—N7	153.8 (3)
C18—C19—C14	120.0	O9—Lu2—O10	86.1 (3)
C16—C20—H20A	109.5	O9—Lu2—O11	82.6 (3)
C16—C20—H20B	109.5	O10—Lu2—O11	127.1 (3)
H20A—C20—H20B	109.5	O9—Lu2—N11	143.1 (3)
C16—C20—H20C	109.5	O10—Lu2—N11	75.0 (3)
H20A—C20—H20C	109.5	O11—Lu2—N11	84.1 (3)
H20B—C20—H20C	109.5	O9—Lu2—O15	125.9 (3)
N5—C21—N4	101.2 (10)	O10—Lu2—O15	81.4 (3)
N5—C21—C18	114.8 (11)	O11—Lu2—O15	143.7 (3)
N4—C21—C18	110.3 (11)	N11—Lu2—O15	82.7 (3)
N5—C21—H21	110.1	O9—Lu2—N9	73.3 (3)
N4—C21—H21	110.1	O10—Lu2—N9	145.6 (3)
C18—C21—H21	110.1	O11—Lu2—N9	78.0 (3)
C23—C22—N4	104.4 (10)	N11—Lu2—N9	136.4 (3)
C23—C22—H22A	110.9	O15—Lu2—N9	88.7 (3)
N4—C22—H22A	110.9	O9—Lu2—N10	139.5 (3)
C23—C22—H22B	110.9	O10—Lu2—N10	134.3 (3)
N4—C22—H22B	110.9	O11—Lu2—N10	74.0 (3)
H22A—C22—H22B	108.9	N11—Lu2—N10	67.1 (3)
N5—C23—C22	101.8 (10)	O15—Lu2—N10	69.7 (3)
N5—C23—H23A	111.4	N9—Lu2—N10	69.9 (3)
C22—C23—H23A	111.4	O9—Lu2—O14	74.8 (3)
N5—C23—H23B	111.4	O10—Lu2—O14	71.9 (3)
C22—C23—H23B	111.4	O11—Lu2—O14	149.6 (3)
H23A—C23—H23B	109.3	N11—Lu2—O14	126.0 (3)
N5—C24—C25	110.0 (10)	O15—Lu2—O14	51.3 (3)
N5—C24—H24A	109.7	N9—Lu2—O14	76.2 (3)
C25—C24—H24A	109.7	N10—Lu2—O14	111.2 (3)
N5—C24—H24B	109.7	O9—Lu2—O12	72.6 (3)
C25—C24—H24B	109.7	O10—Lu2—O12	75.4 (3)
H24A—C24—H24B	108.2	O11—Lu2—O12	51.9 (3)
N6—C25—C24	109.2 (9)	N11—Lu2—O12	72.2 (3)
N6—C25—H25A	109.8	O15—Lu2—O12	149.3 (3)
C24—C25—H25A	109.8	N9—Lu2—O12	121.7 (3)
N6—C25—H25B	109.8	N10—Lu2—O12	114.0 (3)
C24—C25—H25B	109.8	O14—Lu2—O12	134.8 (3)
H25A—C25—H25B	108.3	O9—Lu2—N15	75.6 (3)
N6—C26—C2	123.6 (9)	O10—Lu2—N15	101.1 (3)
N6—C26—H26	118.2	O11—Lu2—N15	26.1 (3)
C2—C26—H26	118.2	N11—Lu2—N15	77.4 (3)

O10—C27—C28	120.0 (10)	O15—Lu2—N15	158.4 (3)
O10—C27—C32	121.8 (10)	N9—Lu2—N15	100.0 (3)
C28—C27—C32	118.2 (10)	N10—Lu2—N15	94.7 (3)
C29—C28—C27	120.2 (10)	O14—Lu2—N15	150.0 (3)
C29—C28—C52	118.9 (10)	O12—Lu2—N15	25.7 (3)
C27—C28—C52	120.6 (9)	O9—Lu2—N16	100.5 (3)
C28—C29—C30	123.7 (9)	O10—Lu2—N16	75.1 (3)
C28—C29—H29	118.2	O11—Lu2—N16	157.7 (3)
C30—C29—H29	118.2	N11—Lu2—N16	104.6 (3)
C31—C30—C29	115.5 (9)	O15—Lu2—N16	25.5 (3)
C31—C30—C33	121.8 (11)	N9—Lu2—N16	81.8 (3)
C29—C30—C33	122.3 (10)	N10—Lu2—N16	90.4 (4)
C30—C31—C32	123.6 (10)	O14—Lu2—N16	25.8 (3)
C30—C31—H31	118.2	O12—Lu2—N16	150.2 (3)
C32—C31—H31	118.2	N15—Lu2—N16	175.0 (3)
C31—C32—C27	118.5 (10)	C8—N1—C9	118.1 (9)
C31—C32—C34	117.8 (9)	C8—N1—Lu1	127.4 (7)
C27—C32—C34	123.6 (9)	C9—N1—Lu1	114.2 (7)
C30—C33—H33A	109.5	C10—N2—C11	110.5 (9)
C30—C33—H33B	109.5	C10—N2—Lu1	113.8 (7)
H33A—C33—H33B	109.5	C11—N2—Lu1	111.7 (7)
C30—C33—H33C	109.5	C10—N2—H2	106.8
H33A—C33—H33C	109.5	C11—N2—H2	106.8
H33B—C33—H33C	109.5	Lu1—N2—H2	106.8
N11—C34—C32	126.3 (9)	C13—N3—C12	114.3 (10)
N11—C34—H34	116.8	C13—N3—Lu1	127.1 (8)
C32—C34—H34	116.8	C12—N3—Lu1	118.5 (7)
C36—C35—N11	110.8 (9)	C21—N4—C22	103.4 (11)
C36—C35—H35A	109.5	C21—N4—H4A	111.1
N11—C35—H35A	109.5	C22—N4—H4A	111.1
C36—C35—H35B	109.5	C21—N4—H4B	111.1
N11—C35—H35B	109.5	C22—N4—H4B	111.1
H35A—C35—H35B	108.1	H4A—N4—H4B	109.0
N10—C36—C35	107.2 (10)	C23—N5—C21	101.9 (10)
N10—C36—H36A	110.3	C23—N5—C24	121.6 (11)
C35—C36—H36A	110.3	C21—N5—C24	113.9 (9)
N10—C36—H36B	110.3	C26—N6—C25	121.0 (9)
C35—C36—H36B	110.3	C26—N6—H6A	119.5
H36A—C36—H36B	108.5	C25—N6—H6A	119.5
C38—C37—N10	111.6 (9)	O5—N7—O4	123.6 (11)
C38—C37—H37A	109.3	O5—N7—O3	119.9 (12)
N10—C37—H37A	109.3	O4—N7—O3	116.4 (10)
C38—C37—H37B	109.3	O5—N7—Lu1	175.4 (10)
N10—C37—H37B	109.3	O4—N7—Lu1	53.4 (5)
H37A—C37—H37B	108.0	O3—N7—Lu1	63.2 (6)
C37—C38—N9	106.4 (10)	O8—N8—O6	124.0 (11)
C37—C38—H38A	110.5	O8—N8—O7	121.6 (11)
N9—C38—H38A	110.5	O6—N8—O7	114.3 (9)
C37—C38—H38B	110.5	C39—N9—C38	115.4 (9)

N9—C38—H38B	110.5	C39—N9—Lu2	130.5 (7)
H38A—C38—H38B	108.6	C38—N9—Lu2	113.8 (7)
N9—C39—C40	125.8 (10)	C36—N10—C37	115.6 (9)
N9—C39—H39	117.1	C36—N10—Lu2	112.6 (7)
C40—C39—H39	117.1	C37—N10—Lu2	110.8 (6)
C39—C40—C41	117.2 (11)	C36—N10—H10	105.7
C39—C40—C45	123.4 (11)	C37—N10—H10	105.7
C41—C40—C45	119.4 (11)	Lu2—N10—H10	105.7
C42—C41—C40	123.1 (11)	C34—N11—C35	116.4 (9)
C42—C41—H41	118.5	C34—N11—Lu2	126.4 (7)
C40—C41—H41	118.5	C35—N11—Lu2	117.1 (6)
C43—C42—C41	117.0 (10)	C52—N12—C51	110.1 (9)
C43—C42—C46	119.4 (12)	C52—N12—H12C	109.6
C41—C42—C46	123.6 (11)	C51—N12—H12C	109.6
C42—C43—C44	123.2 (11)	C52—N12—H12D	109.6
C42—C43—H43	118.4	C51—N12—H12D	109.6
C44—C43—H43	118.4	H12C—N12—H12D	108.2
C47—C44—C45	121.6 (10)	C50—N13—C49	112.9 (9)
C47—C44—C43	119.1 (11)	C50—N13—C52	103.7 (9)
C45—C44—C43	119.2 (10)	C49—N13—C52	115.1 (9)
O9—C45—C44	119.8 (9)	C47—N14—C48	126.7 (9)
O9—C45—C40	122.5 (9)	C47—N14—H14A	116.6
C44—C45—C40	117.6 (9)	C48—N14—H14A	116.6
C42—C46—H46A	109.5	O13—N15—O12	121.7 (11)
C42—C46—H46B	109.5	O13—N15—O11	120.2 (10)
H46A—C46—H46B	109.5	O12—N15—O11	118.1 (10)
C42—C46—H46C	109.5	O13—N15—Lu2	175.0 (8)
H46A—C46—H46C	109.5	O12—N15—Lu2	63.0 (6)
H46B—C46—H46C	109.5	O11—N15—Lu2	55.1 (5)
N14—C47—C44	122.6 (10)	O16—N16—O15	120.9 (12)
N14—C47—H47	118.7	O16—N16—O14	122.3 (11)
C44—C47—H47	118.7	O15—N16—O14	116.8 (11)
N14—C48—C49	109.9 (11)	O16—N16—Lu2	177.0 (9)
N14—C48—H48A	109.7	O15—N16—Lu2	56.3 (6)
C49—C48—H48A	109.7	O14—N16—Lu2	60.5 (6)
N14—C48—H48B	109.7	O19—N17—O17	122.7 (10)
C49—C48—H48B	109.7	O19—N17—O18	116.9 (10)
H48A—C48—H48B	108.2	O17—N17—O18	120.4 (10)
N13—C49—C48	111.8 (10)	O20—N18—O21	123.6 (11)
N13—C49—H49A	109.3	O20—N18—O22	115.3 (10)
C48—C49—H49A	109.3	O21—N18—O22	121.2 (10)
N13—C49—H49B	109.3	C1—O1—Lu1	142.3 (7)
C48—C49—H49B	109.3	C19—O2—Lu1	137.4 (6)
H49A—C49—H49B	107.9	N7—O3—Lu1	90.6 (7)
N13—C50—C51	101.5 (9)	N7—O4—Lu1	101.2 (7)
N13—C50—H50A	111.5	N8—O6—Lu1	92.2 (6)
C51—C50—H50A	111.5	N8—O7—Lu1	102.5 (7)
N13—C50—H50B	111.5	C45—O9—Lu2	141.6 (6)
C51—C50—H50B	111.5	C27—O10—Lu2	130.8 (7)

H50A—C50—H50B	109.3	N15—O11—Lu2	98.8 (6)
N12—C51—C50	101.3 (10)	N15—O12—Lu2	91.2 (6)
N12—C51—H51A	111.5	N16—O14—Lu2	93.7 (7)
C50—C51—H51A	111.5	N16—O15—Lu2	98.2 (8)
N12—C51—H51B	111.5	C55—O23—C54	120.3 (16)
C50—C51—H51B	111.5	H25F—O25—H25C	109.5
H51A—C51—H51B	109.3	H26A—O26—H26B	109.5
N13—C52—N12	97.4 (8)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O2	0.90	2.07	2.765 (13)	133
N4—H4B···O22	0.90	1.94	2.826 (13)	166
N4—H4B···O20	0.90	2.45	3.108 (14)	130
N4—H4B···N18	0.90	2.59	3.435 (15)	156
N6—H6A···O1	0.86	1.99	2.635 (11)	131
N6—H6A···O6	0.86	2.63	3.407 (14)	151
N10—H10···O15	0.91	2.35	2.810 (13)	111
N12—H12D···O10	0.90	1.90	2.641 (12)	138
N14—H14A···O9	0.86	1.86	2.560 (10)	137
O25—H25F···O8	0.85	2.53	3.007 (19)	116
O25—H25C···O5^{i}	0.85	2.32	2.992 (19)	137
N2—H2···O19^{i}	0.91	2.08	2.959 (11)	163
N10—H10···O20^{ii}	0.91	2.24	3.112 (14)	161
N12—H12C···O18^{iii}	0.90	1.92	2.810 (13)	170
N12—H12C···O19^{iii}	0.90	2.53	3.126 (12)	124
N12—H12C···N17^{iii}	0.90	2.59	3.413 (14)	152

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*+1/2; (iii) *x*, *y*−1, *z*+1.

Fig. 1

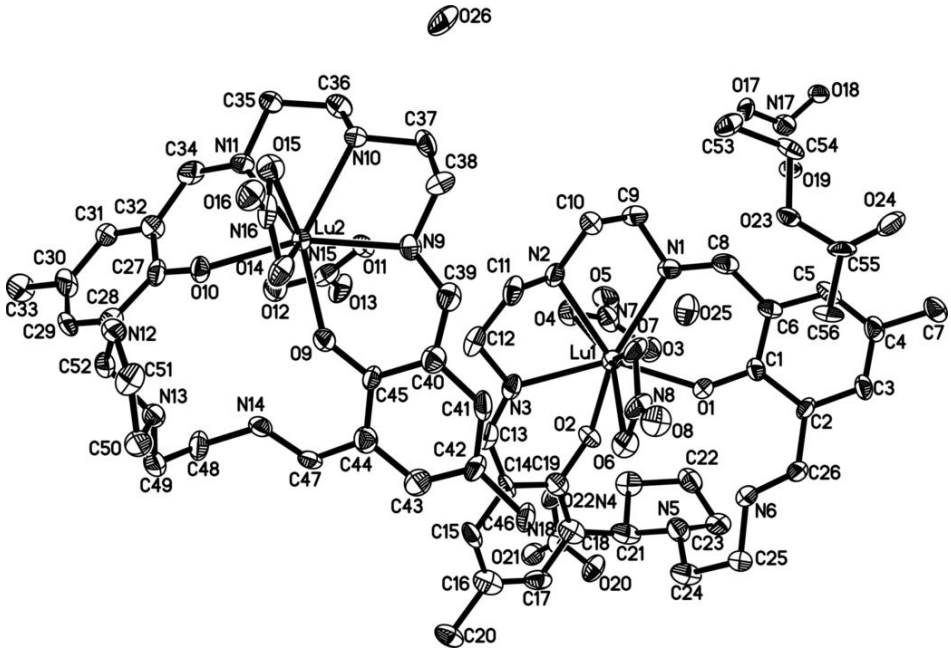
O26
C36
C35
C37
C34
N11
O15
N10
C38
O16
C31
C32
N16
Lu2
N9
C30
C27
N15
O14
O11
C39
C11
N2
O5
C10
C9
N1
C8
O17
N17
O18
C53
C54
O19
O24
O23
C55
C5
C33
C28
O10
O12
O13
C29
N12
O9
C12
O4
N7
O7
O25
C6
C56
C4
C7
Lu1
O3
C1
C52
C51
C45
C40
N3
N8
O1
C3
N13
N14
C41
O2
C13
O8
C2
C50
C48
C44
C42
O6
C22
C26
C49
C47
C14
C19
O22
N4
N5
N6
C43
C46
N18
C18
C21
C23
C25
C15
O21
O20
C24
C16
C17
C20

Fig. 2