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[μ_2-*N*,*N*′-Bis(2-oxy-3-ethoxybenzylidene)propane-1,2-diamine](methanol)trinitratocopper(II)lutetium(III)

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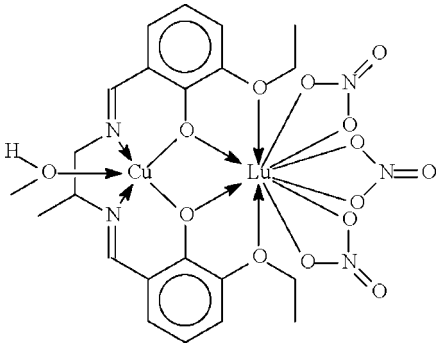
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.015 Å; disorder in main residue; R factor = 0.059; wR factor = 0.196; data-to-parameter ratio = 16.8.

The Cu atom in the title compound (systematic name: {6,6′-diethoxy-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-2$\kappa O$)trinitrato-1$\kappa^6O,O'$-copper(II)lutetium(III)), [CuLu($C_{21}H_{22}N_2O_4$)(CH_4O)(NO_3)$_3$] is *N*,*N*′,*O*,*O*′ chelated by the deprotonated Schiff base, the four chelating atoms forming a square plane above which lies the methanol molecule. The [Cu($C_{21}H_{24}N_2O_4$)(CH_4O)] unit uses the two ethoxy and two hydroxy O atoms to chelate the [Lu(NO_3)$_3$] unit. The Cu^{II} atom exists in a square-pyramidal geometry and the Lu^{III} atom in a bicapped square-antiprismatic geometry. Molecules are linked into a chain along the *b* axis by O—H···O hydrogen bonds. Two CH_2 groups of the C_2N_2Cu ring and the H atoms of the attached methyl group are disordered equally over two positions.

Related literature

See Elmali & Elerman (2004) for a related CuNd complex, Elmali & Elerman (2005) for a CuDy complex, and Koner *et al.* (2005) for a CuGd complex.



Experimental

Crystal data

[CuLu($C_{21}H_{22}N_2O_4$)(CH_4O)(NO_3)$_3$]
M_r = 825.00
Monoclinic, $P2_1/c$
a = 9.1795 (5) Å
b = 20.407 (1) Å
c = 15.7058 (9) Å
β = 93.126 (1)°
V = 2937.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.14 mm^{-1}
T = 295 (2) K
0.20 × 0.09 × 0.08 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.183, T_{max} = 0.733
21167 measured reflections
6636 independent reflections
3788 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.196
S = 1.07
6636 reflections
394 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −1.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Lu1—O1	2.616 (7)	Lu1—O12	2.574 (7)
Lu1—O2	2.368 (6)	Lu1—O13	2.514 (6)
Lu1—O3	2.397 (6)	Cu1—O2	1.874 (6)
Lu1—O4	2.634 (6)	Cu1—O3	1.909 (6)
Lu1—O6	2.482 (8)	Cu1—O5	2.335 (8)
Lu1—O7	2.493 (9)	Cu1—N1	1.922 (8)
Lu1—O9	2.485 (7)	Cu1—N2	1.900 (8)
Lu1—O10	2.447 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5O···O14^{i}	0.82	2.13	2.93 (1)	164

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2404).

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supplementary materials

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[μ_2-*N*,*N*'-Bis(2-oxy-3-ethoxybenzylidene)propane-1,2-diamine](methanol)trinitratocopper(II)lutetium(III)

Y. Sui, R.-H. Hu, J.-L. Peng and S. W. Ng

Comment

3-Alkoxysalicylaldehyde condenses with ethylenediamine and related diamines to form a class of Schiff bases that react with divalent transition-metal salts to afford another class of compounds that react with lanthanum(III) salts to yield bi-metallic compounds. Bis(2-oxy-3-methoxybenzylidene)ethylenediamine)(acetone)tris(nitrato)-copper- neodymium (Elmali *et al.*, 2004), bis(2-oxy-3-methoxybenzylidene)ethylenediamine)(acetone)tris(nitrato)-copper- dysprosium (Elmali *et al.*, 2005) and (1,2-cyclohexane)bis(3-ethoxysalicylideneaminato)aquatris(nitrato)\ coppergadolinium (Koner *et al.*, 2005) represent the copper compounds that are coordinated to lanthanum trinitrate. Their copper atoms are chelated by the deprotonated Schiff bases but the geometry is a square-pyramid owing to the coordinated solvent molecules. On the other hand, the lanthanum atom is chelated by three nitrate groups, so a ten-coordinate geometry results from the involvement of the four oxygen atoms of the copper-Schiff base portion of the bimetallic molecule. The title compound (Fig. 1) has a similar bonding mode; the lutetium atom shows bicapped square-antiprismatic coordination.

Experimental

The Schiff base used to make the title compound was synthesized by the condensation of 3-ethoxysalicylaldehyde and 1,2- diaminopropane in a 2:1 molar ratio. Copper diacetate monohydrate (0.17 g, 1 mmol) and the ligand (0.37 g, 1 mmol) were heated in methanol (50 ml) for 3 h. Lutetium nitrate hexahydrate (0.47 g, 1 mmol) was added and the mixture was heated for another 3 h. Cooling the solution gave a precipitate, which was collected and washed with diethyl ether. Crystals were obtained upon recrystallization from methanol.

Refinement

The part of the Schiff base that is made up of the C10 and C11 atoms (that belong to the cyclic system) is disordered over two positions; the occupancies of each set of atoms was arbitrarily fixed as 0.5. The displacement parameters of primed atoms were set to those of the unprimed ones. The C10—C11 and C11—C12 bond lengths were restrained to 1.50 (1) Å and the C10···C12 distance to 2.45 (1) Å. The displacement parameters of C10, C11 and C12 were restrained to approximate isotropic behaviour. The carbon- and oxygen-bound H atoms were positioned geometrically (C–H = 0.93–0.97 Å and O—H = 0.82 Å), and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2–1.5U_{eq}(C,*O*). The final difference Fourier map had a large peak at 0.5 Å from H12D and a deep hole at 0.5 Å from Lu1.

Figures

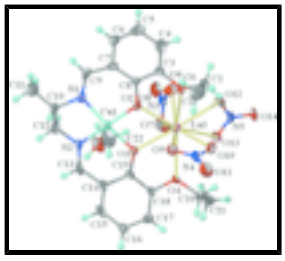


Fig. 1. Displacement ellipsoid plot of [CuLu($C_{21}H_{22}N_2O_4$)(CH_4O)(NO_3)$_3$]; ellipsoids are drawn at the 30% probabilty level, and H atoms are shown as spheres of arbitrary radius. Only one disorder component is shown.

[μ$_2$-*N*,*N*'-Bis(2-oxy-3-ethoxybenzylidene)ethylene-1,2-diamine] (methanol)tris(nitrato)copper(II)lutetium(III)

Crystal data

[CuLu($C_{21}H_{22}N_2O_4$)(CH_4O)(NO_3)$_3$]	F_{000} = 1628
M_r = 825.00	D_x = 1.865 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4544 reflections
a = 9.1795 (5) Å	θ = 2.4–22.2º
b = 20.407 (1) Å	μ = 4.14 mm^{-1}
c = 15.7058 (9) Å	T = 295 (2) K
β = 93.126 (1)º	Block, red
V = 2937.7 (3) Å^3	0.20 × 0.09 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	6636 independent reflections
Radiation source: fine-focus sealed tube	3788 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.183, T_{max} = 0.733	k = −26→26
21167 measured reflections	l = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.196	$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
6636 reflections	$\Delta\rho_{max}$ = 1.20 e Å^{-3}
394 parameters	$\Delta\rho_{min}$ = −1.29 e Å^{-3}
10 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Lu1	0.36449 (5)	0.34232 (2)	0.25150 (3)	0.05488 (19)	
Cu1	0.32833 (12)	0.50585 (5)	0.30039 (7)	0.0460 (3)	
O1	0.1485 (8)	0.3477 (3)	0.1360 (4)	0.0525 (16)	
O2	0.2284 (7)	0.4406 (3)	0.2367 (4)	0.0550 (16)	
O3	0.4753 (7)	0.4397 (3)	0.3108 (4)	0.0519 (16)	
O4	0.6441 (7)	0.3413 (3)	0.2989 (4)	0.0489 (15)	
O5	0.4254 (11)	0.5592 (4)	0.1848 (5)	0.101 (3)	
H5O	0.4865	0.5875	0.1969	0.122*	
O6	0.1569 (10)	0.3251 (5)	0.3439 (6)	0.097 (3)	
O7	0.3518 (12)	0.3407 (5)	0.4097 (5)	0.099 (3)	
O8	0.1587 (12)	0.3342 (4)	0.4790 (6)	0.093 (3)	
O9	0.4776 (8)	0.3859 (4)	0.1229 (5)	0.067 (2)	
O10	0.4809 (9)	0.2812 (4)	0.1396 (5)	0.071 (2)	
O11	0.5937 (12)	0.3224 (5)	0.0349 (6)	0.104 (3)	
O12	0.2362 (8)	0.2317 (3)	0.2230 (6)	0.075 (2)	
O13	0.4277 (8)	0.2285 (3)	0.3023 (5)	0.067 (2)	
O14	0.3179 (10)	0.1381 (3)	0.2648 (6)	0.086 (3)	
N1	0.1675 (10)	0.5659 (3)	0.3038 (6)	0.064 (2)	
N2	0.4260 (9)	0.5652 (3)	0.3773 (5)	0.053 (2)	
N3	0.2196 (11)	0.3338 (4)	0.4138 (6)	0.056 (2)	
N4	0.5218 (12)	0.3308 (5)	0.0953 (7)	0.070 (3)	
N5	0.3281 (10)	0.1984 (4)	0.2624 (5)	0.055 (2)	
C1	0.1685 (19)	0.3436 (7)	−0.0203 (8)	0.107 (5)	
H1A	0.1514	0.3160	−0.0693	0.160*	
H1B	0.2687	0.3574	−0.0167	0.160*	
H1C	0.1062	0.3813	−0.0253	0.160*	
C2	0.1348 (14)	0.3045 (5)	0.0622 (6)	0.069 (3)	
H2A	0.0367	0.2868	0.0565	0.082*	
H2B	0.2025	0.2681	0.0698	0.082*	
C3	0.0473 (10)	0.3983 (4)	0.1446 (6)	0.050 (2)	
C4	−0.0902 (14)	0.3990 (6)	0.1026 (7)	0.081 (4)	
H4	−0.1196	0.3659	0.0647	0.097*	
C5	−0.1824 (13)	0.4515 (7)	0.1197 (8)	0.086 (4)	
H5	−0.2774	0.4521	0.0959	0.103*	
C6	−0.1351 (12)	0.5010 (5)	0.1702 (8)	0.070 (3)	
H6	−0.1970	0.5363	0.1781	0.084*	
C7	0.0070 (10)	0.5015 (5)	0.2122 (7)	0.056 (2)	
C8	0.0955 (9)	0.4482 (4)	0.1980 (6)	0.048 (2)	

C9	0.0390 (13)	0.5572 (5)	0.2657 (7)	0.063 (3)	
H9	−0.0338	0.5879	0.2735	0.076*	
C10	0.2161 (17)	0.6300 (6)	0.3366 (12)	0.053 (4)	0.50
H10	0.2633	0.6537	0.2913	0.063*	0.50
C10'	0.187 (2)	0.6104 (6)	0.3762 (10)	0.053 (4)	0.50
H10'	0.1607	0.5865	0.4273	0.063*	0.50
C11	0.1109 (15)	0.6748 (6)	0.3762 (10)	0.108 (5)	
H11A	0.1626	0.7116	0.4011	0.163*	0.50
H11B	0.0622	0.6517	0.4197	0.163*	0.50
H11C	0.0402	0.6899	0.3334	0.163*	0.50
H11D	0.0074	0.6677	0.3727	0.163*	0.50
H11E	0.1379	0.6985	0.4275	0.163*	0.50
H11F	0.1381	0.6996	0.3277	0.163*	0.50
C12	0.328 (3)	0.6153 (14)	0.4072 (18)	0.096 (8)	0.50
H12A	0.3824	0.6547	0.4226	0.115*	0.50
H12B	0.2805	0.5998	0.4570	0.115*	0.50
C12'	0.347 (2)	0.6264 (10)	0.386 (3)	0.096 (8)	0.50
H12C	0.3728	0.6575	0.3429	0.115*	0.50
H12D	0.3696	0.6456	0.4419	0.115*	0.50
C13	0.5558 (15)	0.5608 (5)	0.4052 (7)	0.069 (3)	
H13	0.5925	0.5951	0.4390	0.083*	
C14	0.6568 (12)	0.5056 (4)	0.3894 (6)	0.053 (2)	
C15	0.7976 (13)	0.5104 (5)	0.4195 (6)	0.068 (3)	
H15	0.8283	0.5477	0.4494	0.081*	
C16	0.8962 (11)	0.4607 (5)	0.4065 (6)	0.057 (2)	
H16	0.9939	0.4659	0.4242	0.068*	
C17	0.8500 (11)	0.4039 (5)	0.3676 (6)	0.058 (3)	
H17	0.9161	0.3701	0.3597	0.070*	
C18	0.7030 (10)	0.3963 (4)	0.3395 (6)	0.046 (2)	
C19	0.6058 (10)	0.4479 (4)	0.3458 (5)	0.046 (2)	
C20	0.7437 (10)	0.2855 (5)	0.2863 (7)	0.062 (3)	
H20A	0.8354	0.3019	0.2670	0.075*	
H20B	0.7011	0.2570	0.2422	0.075*	
C21	0.7735 (12)	0.2457 (6)	0.3676 (8)	0.077 (3)	
H21A	0.7709	0.1998	0.3541	0.115*	
H21B	0.7004	0.2553	0.4072	0.115*	
H21C	0.8680	0.2569	0.3926	0.115*	
C22	0.3956 (19)	0.5501 (8)	0.1039 (9)	0.114 (5)	
H22A	0.4755	0.5654	0.0723	0.171*	
H22B	0.3088	0.5739	0.0865	0.171*	
H22C	0.3805	0.5042	0.0931	0.171*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Lu1	0.0553 (3)	0.0411 (3)	0.0676 (3)	0.00042 (19)	−0.0023 (2)	−0.0050 (2)
Cu1	0.0493 (7)	0.0293 (5)	0.0591 (7)	0.0017 (5)	0.0012 (5)	−0.0057 (5)
O1	0.057 (4)	0.041 (4)	0.058 (4)	0.000 (3)	−0.010 (3)	−0.003 (3)

O2	0.054 (4)	0.036 (3)	0.074 (4)	0.012 (3)	−0.006 (3)	−0.009 (3)
O3	0.047 (4)	0.036 (3)	0.070 (4)	0.008 (3)	−0.018 (3)	−0.012 (3)
O4	0.047 (4)	0.034 (3)	0.065 (4)	−0.006 (3)	0.001 (3)	−0.011 (3)
O5	0.135 (9)	0.086 (6)	0.084 (6)	−0.053 (6)	0.017 (6)	0.002 (5)
O6	0.074 (6)	0.145 (9)	0.072 (6)	0.021 (6)	0.019 (5)	0.023 (5)
O7	0.101 (8)	0.132 (9)	0.062 (5)	−0.032 (6)	−0.010 (5)	−0.003 (5)
O8	0.138 (9)	0.076 (6)	0.070 (6)	−0.008 (5)	0.040 (6)	0.007 (4)
O9	0.066 (5)	0.063 (5)	0.074 (5)	−0.008 (4)	0.009 (4)	0.015 (4)
O10	0.083 (6)	0.060 (5)	0.071 (5)	0.005 (4)	0.012 (4)	−0.019 (4)
O11	0.119 (8)	0.114 (7)	0.085 (6)	−0.026 (6)	0.061 (6)	−0.014 (5)
O12	0.058 (5)	0.046 (4)	0.119 (6)	−0.013 (4)	−0.023 (4)	0.011 (4)
O13	0.057 (5)	0.045 (4)	0.096 (5)	−0.009 (3)	−0.018 (4)	0.011 (4)
O14	0.101 (6)	0.031 (4)	0.127 (7)	−0.013 (4)	0.006 (5)	−0.014 (4)
N1	0.064 (6)	0.035 (4)	0.092 (6)	0.016 (4)	−0.007 (5)	−0.004 (4)
N2	0.061 (6)	0.031 (4)	0.067 (5)	0.003 (4)	−0.006 (4)	−0.008 (4)
N3	0.069 (7)	0.041 (5)	0.060 (6)	−0.002 (4)	0.015 (5)	−0.010 (4)
N4	0.072 (7)	0.066 (7)	0.071 (6)	−0.020 (5)	−0.005 (5)	−0.001 (5)
N5	0.070 (6)	0.029 (4)	0.068 (5)	0.000 (4)	0.023 (5)	−0.003 (4)
C1	0.124 (14)	0.143 (14)	0.054 (7)	0.011 (10)	0.007 (8)	0.003 (8)
C2	0.086 (8)	0.054 (6)	0.064 (7)	−0.005 (6)	−0.016 (6)	−0.006 (5)
C3	0.046 (6)	0.044 (5)	0.058 (6)	0.002 (4)	−0.005 (4)	0.009 (4)
C4	0.101 (10)	0.066 (8)	0.071 (8)	0.012 (7)	−0.027 (7)	0.000 (6)
C5	0.054 (7)	0.112 (11)	0.091 (9)	0.020 (7)	−0.007 (6)	0.025 (8)
C6	0.057 (7)	0.053 (6)	0.101 (9)	0.012 (5)	0.012 (6)	0.007 (6)
C7	0.038 (5)	0.057 (6)	0.073 (6)	0.008 (4)	−0.007 (5)	0.020 (5)
C8	0.029 (5)	0.040 (5)	0.076 (6)	0.004 (4)	0.000 (4)	0.014 (5)
C9	0.073 (8)	0.043 (6)	0.075 (7)	0.025 (5)	0.012 (6)	−0.001 (5)
C10	0.077 (11)	0.028 (8)	0.051 (11)	0.013 (7)	−0.009 (9)	0.005 (6)
C10'	0.077 (11)	0.028 (8)	0.051 (11)	0.013 (7)	−0.009 (9)	0.005 (6)
C11	0.090 (11)	0.083 (9)	0.152 (14)	0.015 (8)	0.003 (10)	−0.003 (9)
C12	0.107 (13)	0.053 (10)	0.124 (18)	0.022 (9)	−0.024 (11)	−0.044 (11)
C12'	0.107 (13)	0.053 (10)	0.124 (18)	0.022 (9)	−0.024 (11)	−0.044 (11)
C13	0.108 (10)	0.037 (5)	0.063 (6)	−0.012 (6)	0.010 (7)	−0.020 (5)
C14	0.069 (7)	0.041 (5)	0.049 (5)	−0.010 (5)	−0.005 (5)	−0.006 (4)
C15	0.087 (9)	0.060 (7)	0.054 (6)	−0.032 (6)	−0.018 (6)	−0.005 (5)
C16	0.051 (6)	0.051 (6)	0.065 (6)	−0.004 (5)	−0.020 (5)	−0.002 (5)
C17	0.049 (6)	0.061 (6)	0.065 (6)	0.010 (5)	0.004 (5)	0.004 (5)
C18	0.045 (6)	0.042 (5)	0.049 (5)	−0.008 (4)	−0.003 (4)	−0.001 (4)
C19	0.041 (5)	0.049 (5)	0.048 (5)	−0.009 (4)	0.002 (4)	−0.005 (4)
C20	0.037 (6)	0.062 (6)	0.087 (7)	0.013 (5)	−0.010 (5)	−0.024 (6)
C21	0.059 (7)	0.064 (7)	0.106 (9)	0.000 (6)	−0.017 (7)	0.010 (7)
C22	0.159 (16)	0.104 (11)	0.080 (10)	−0.022 (10)	0.010 (10)	0.006 (9)

Geometric parameters (Å, °)

Lu1—O1	2.616 (7)	C4—C5	1.402 (16)
Lu1—O2	2.368 (6)	C4—H4	0.93
Lu1—O3	2.397 (6)	C5—C6	1.342 (17)
Lu1—O4	2.634 (6)	C5—H5	0.93

Lu1—O6	2.482 (8)	C6—C7	1.429 (15)
Lu1—O7	2.493 (9)	C6—H6	0.93
Lu1—O9	2.485 (7)	C7—C8	1.385 (13)
Lu1—O10	2.447 (7)	C7—C9	1.433 (14)
Lu1—O12	2.574 (7)	C9—H9	0.93
Lu1—O13	2.514 (6)	C10—C11	1.490 (10)
Cu1—O2	1.874 (6)	C10—C12	1.500 (10)
Cu1—O3	1.909 (6)	C10—H10	0.98
Cu1—O5	2.335 (8)	C10'—C11	1.487 (9)
Cu1—N1	1.922 (8)	C10'—C12'	1.502 (10)
Cu1—N2	1.900 (8)	C10'—H10'	0.98
O1—C3	1.400 (11)	C11—H11A	0.96
O1—C2	1.458 (11)	C11—H11B	0.96
O2—C8	1.342 (11)	C11—H11C	0.96
O3—C19	1.301 (10)	C11—H11D	0.96
O4—C18	1.387 (10)	C11—H11E	0.96
O4—C20	1.481 (10)	C11—H11F	0.96
O5—C22	1.299 (14)	C12—H12A	0.97
O5—H5O	0.82	C12—H12B	0.97
O6—N3	1.225 (12)	C12'—H12C	0.97
O7—N3	1.227 (13)	C12'—H12D	0.97
O8—N3	1.193 (11)	C13—C14	1.488 (14)
O9—N4	1.278 (11)	C13—H13	0.93
O10—N4	1.296 (11)	C14—C15	1.355 (15)
O11—N4	1.196 (12)	C14—C19	1.429 (12)
O12—N5	1.224 (10)	C15—C16	1.383 (15)
O13—N5	1.242 (10)	C15—H15	0.93
O14—N5	1.235 (10)	C16—C17	1.367 (14)
N1—C9	1.305 (13)	C16—H16	0.93
N1—C10'	1.458 (9)	C17—C18	1.405 (13)
N1—C10	1.466 (9)	C17—H17	0.93
N2—C13	1.250 (13)	C18—C19	1.387 (12)
N2—C12'	1.459 (10)	C20—C21	1.524 (14)
N2—C12	1.458 (10)	C20—H20A	0.97
C1—C2	1.567 (15)	C20—H20B	0.97
C1—H1A	0.96	C21—H21A	0.96
C1—H1B	0.96	C21—H21B	0.96
C1—H1C	0.96	C21—H21C	0.96
C2—H2A	0.97	C22—H22A	0.96
C2—H2B	0.97	C22—H22B	0.96
C3—C8	1.376 (13)	C22—H22C	0.96
C3—C4	1.392 (14)		
O2—Lu1—O3	63.0 (2)	O1—C2—H2A	109.7
O2—Lu1—O10	127.6 (2)	C1—C2—H2A	109.7
O3—Lu1—O10	120.6 (3)	O1—C2—H2B	109.7
O2—Lu1—O9	81.9 (2)	C1—C2—H2B	109.7
O3—Lu1—O9	80.3 (2)	H2A—C2—H2B	108.2
O10—Lu1—O9	51.7 (3)	C8—C3—C4	122.3 (9)
O2—Lu1—O6	76.1 (3)	C8—C3—O1	114.3 (8)

O3—Lu1—O6	102.3 (3)	C4—C3—O1	123.4 (9)
O10—Lu1—O6	136.6 (3)	C3—C4—C5	117.2 (11)
O9—Lu1—O6	153.3 (3)	C3—C4—H4	121.4
O2—Lu1—O7	93.2 (3)	C5—C4—H4	121.4
O3—Lu1—O7	70.5 (3)	C6—C5—C4	120.7 (11)
O10—Lu1—O7	139.0 (3)	C6—C5—H5	119.7
O9—Lu1—O7	149.2 (3)	C4—C5—H5	119.7
O6—Lu1—O7	48.4 (3)	C5—C6—C7	122.4 (10)
O2—Lu1—O13	157.8 (2)	C5—C6—H6	118.8
O3—Lu1—O13	123.9 (2)	C7—C6—H6	118.8
O10—Lu1—O13	69.8 (3)	C8—C7—C9	127.9 (9)
O9—Lu1—O13	119.3 (3)	C8—C7—C6	116.6 (10)
O6—Lu1—O13	81.7 (3)	C9—C7—C6	115.4 (9)
O7—Lu1—O13	72.2 (3)	O2—C8—C3	116.5 (8)
O2—Lu1—O12	119.5 (2)	O2—C8—C7	122.9 (9)
O3—Lu1—O12	167.1 (2)	C3—C8—C7	120.6 (9)
O10—Lu1—O12	69.0 (3)	N1—C9—C7	121.9 (8)
O9—Lu1—O12	112.3 (3)	N1—C9—H9	119.0
O6—Lu1—O12	67.6 (3)	C7—C9—H9	119.0
O7—Lu1—O12	96.7 (3)	N1—C10—C11	120.1 (12)
O13—Lu1—O12	48.7 (2)	N1—C10—C12	105.3 (17)
O2—Lu1—O1	61.3 (2)	C11—C10—C12	104.3 (11)
O3—Lu1—O1	121.59 (19)	N1—C10—H10	108.9
O10—Lu1—O1	82.4 (2)	C11—C10—H10	108.9
O9—Lu1—O1	75.8 (2)	C12—C10—H10	108.9
O6—Lu1—O1	80.5 (3)	N1—C10'—C11	120.9 (11)
O7—Lu1—O1	128.1 (3)	N1—C10'—C12'	107.1 (18)
O13—Lu1—O1	114.3 (2)	C11—C10'—C12'	105.2 (12)
O12—Lu1—O1	66.0 (2)	N1—C10'—H10'	107.6
O2—Lu1—O4	122.4 (2)	C11—C10'—H10'	107.6
O3—Lu1—O4	60.70 (18)	C12'—C10'—H10'	107.6
O10—Lu1—O4	75.1 (2)	C10—C11—H11A	109.5
O9—Lu1—O4	77.8 (2)	C10—C11—H11B	109.5
O6—Lu1—O4	126.9 (3)	H11A—C11—H11B	109.5
O7—Lu1—O4	79.4 (3)	C10—C11—H11C	109.5
O13—Lu1—O4	72.4 (2)	H11A—C11—H11C	109.5
O12—Lu1—O4	118.2 (2)	H11B—C11—H11C	109.5
O1—Lu1—O4	152.5 (2)	C10'—C11—H11D	109.3
O2—Cu1—O3	82.3 (3)	C10'—C11—H11E	110.2
O2—Cu1—N2	172.7 (3)	H11D—C11—H11E	109.5
O3—Cu1—N2	95.1 (3)	C10'—C11—H11F	108.9
O2—Cu1—N1	96.5 (3)	H11D—C11—H11F	109.5
O3—Cu1—N1	171.4 (3)	H11E—C11—H11F	109.5
N2—Cu1—N1	85.0 (3)	N2—C12—C10	108.2 (14)
O2—Cu1—O5	96.4 (3)	N2—C12—H12A	110.1
O3—Cu1—O5	95.7 (3)	C10—C12—H12A	110.1
N2—Cu1—O5	90.6 (3)	N2—C12—H12B	110.1
N1—Cu1—O5	92.9 (4)	C10—C12—H12B	110.1
C3—O1—C2	119.6 (8)	H12A—C12—H12B	108.4

C3—O1—Lu1	116.5 (5)	N2—C12'—C10'	107.1 (15)
C2—O1—Lu1	123.7 (6)	N2—C12'—H12C	110.3
C8—O2—Cu1	124.5 (5)	C10'—C12'—H12C	110.3
C8—O2—Lu1	127.1 (5)	N2—C12'—H12D	110.3
Cu1—O2—Lu1	108.0 (3)	C10'—C12'—H12D	110.3
C19—O3—Cu1	125.1 (6)	H12C—C12'—H12D	108.5
C19—O3—Lu1	129.2 (5)	N2—C13—C14	125.8 (9)
Cu1—O3—Lu1	105.7 (3)	N2—C13—H13	117.1
C18—O4—C20	117.2 (7)	C14—C13—H13	117.1
C18—O4—Lu1	118.2 (5)	C15—C14—C19	120.5 (9)
C20—O4—Lu1	124.6 (5)	C15—C14—C13	118.6 (9)
C22—O5—Cu1	128.7 (9)	C19—C14—C13	120.9 (9)
C22—O5—H5O	115.7	C16—C15—C14	121.0 (9)
Cu1—O5—H5O	115.7	C16—C15—H15	119.5
N3—O6—Lu1	99.5 (7)	C14—C15—H15	119.5
N3—O7—Lu1	98.9 (7)	C17—C16—C15	119.9 (9)
N4—O9—Lu1	96.7 (6)	C17—C16—H16	120.0
N4—O10—Lu1	97.9 (6)	C15—C16—H16	120.0
N5—O12—Lu1	95.8 (5)	C16—C17—C18	120.2 (9)
N5—O13—Lu1	98.4 (5)	C16—C17—H17	119.9
C9—N1—C10'	120.7 (11)	C18—C17—H17	119.9
C9—N1—C10	122.2 (10)	C19—C18—O4	114.3 (8)
C9—N1—Cu1	125.2 (6)	C19—C18—C17	120.4 (8)
C10'—N1—Cu1	111.0 (8)	O4—C18—C17	125.2 (8)
C10—N1—Cu1	111.0 (8)	O3—C19—C18	117.0 (8)
C13—N2—C12'	119.9 (13)	O3—C19—C14	125.3 (8)
C13—N2—C12	122.0 (13)	C18—C19—C14	117.7 (8)
C13—N2—Cu1	125.9 (6)	O4—C20—C21	112.5 (9)
C12'—N2—Cu1	112.7 (12)	O4—C20—H20A	109.1
C12—N2—Cu1	111.9 (12)	C21—C20—H20A	109.1
O8—N3—O7	123.8 (11)	O4—C20—H20B	109.1
O8—N3—O6	123.5 (11)	C21—C20—H20B	109.1
O7—N3—O6	112.7 (9)	H20A—C20—H20B	107.8
O11—N4—O9	126.5 (10)	C20—C21—H21A	109.5
O11—N4—O10	120.1 (10)	C20—C21—H21B	109.5
O9—N4—O10	113.4 (9)	H21A—C21—H21B	109.5
O13—N5—O12	116.7 (8)	C20—C21—H21C	109.5
O13—N5—O14	122.1 (9)	H21A—C21—H21C	109.5
O12—N5—O14	121.1 (9)	H21B—C21—H21C	109.5
C2—C1—H1A	109.5	O5—C22—H22A	109.5
C2—C1—H1B	109.5	O5—C22—H22B	109.5
H1A—C1—H1B	109.5	H22A—C22—H22B	109.5
C2—C1—H1C	109.5	O5—C22—H22C	109.5
H1A—C1—H1C	109.5	H22A—C22—H22C	109.5
H1B—C1—H1C	109.5	H22B—C22—H22C	109.5
O1—C2—C1	109.7 (9)		
O2—Lu1—O1—C3	−17.2 (6)	O6—Lu1—O12—N5	−102.2 (6)
O3—Lu1—O1—C3	−36.6 (7)	O7—Lu1—O12—N5	−62.6 (6)
O10—Lu1—O1—C3	−158.0 (6)	O13—Lu1—O12—N5	−3.4 (5)

O9—Lu1—O1—C3	−105.6 (6)	O1—Lu1—O12—N5	168.5 (7)
O6—Lu1—O1—C3	62.1 (6)	O4—Lu1—O12—N5	18.9 (7)
O7—Lu1—O1—C3	52.4 (7)	O2—Lu1—O13—N5	68.7 (9)
O13—Lu1—O1—C3	138.3 (6)	O3—Lu1—O13—N5	170.1 (5)
O12—Lu1—O1—C3	131.7 (6)	O10—Lu1—O13—N5	−76.0 (6)
O4—Lu1—O1—C3	−122.9 (6)	O9—Lu1—O13—N5	−91.6 (6)
O2—Lu1—O1—C2	158.6 (7)	O6—Lu1—O13—N5	70.8 (6)
O3—Lu1—O1—C2	139.3 (6)	O7—Lu1—O13—N5	119.7 (6)
O10—Lu1—O1—C2	17.9 (7)	O12—Lu1—O13—N5	3.4 (5)
O9—Lu1—O1—C2	70.3 (7)	O1—Lu1—O13—N5	−4.7 (6)
O6—Lu1—O1—C2	−122.1 (7)	O4—Lu1—O13—N5	−156.1 (6)
O7—Lu1—O1—C2	−131.7 (7)	O2—Cu1—N1—C9	−3.2 (9)
O13—Lu1—O1—C2	−45.8 (7)	N2—Cu1—N1—C9	−176.1 (9)
O12—Lu1—O1—C2	−52.5 (7)	O5—Cu1—N1—C9	93.6 (9)
O4—Lu1—O1—C2	52.9 (8)	O2—Cu1—N1—C10'	156.9 (11)
O3—Cu1—O2—C8	−178.4 (7)	N2—Cu1—N1—C10'	−15.9 (11)
N1—Cu1—O2—C8	10.2 (7)	O5—Cu1—N1—C10'	−106.3 (11)
O5—Cu1—O2—C8	−83.5 (7)	O2—Cu1—N1—C10	−169.1 (10)
O3—Cu1—O2—Lu1	8.3 (3)	N2—Cu1—N1—C10	18.0 (10)
N1—Cu1—O2—Lu1	−163.1 (3)	O5—Cu1—N1—C10	−72.3 (10)
O5—Cu1—O2—Lu1	103.2 (3)	O3—Cu1—N2—C13	12.6 (9)
O3—Lu1—O2—C8	179.5 (8)	N1—Cu1—N2—C13	−176.0 (9)
O10—Lu1—O2—C8	70.3 (8)	O5—Cu1—N2—C13	−83.1 (9)
O9—Lu1—O2—C8	96.3 (7)	O3—Cu1—N2—C12'	178.6 (18)
O6—Lu1—O2—C8	−68.6 (7)	N1—Cu1—N2—C12'	−10.0 (18)
O7—Lu1—O2—C8	−114.3 (7)	O5—Cu1—N2—C12'	82.9 (18)
O13—Lu1—O2—C8	−66.5 (10)	O3—Cu1—N2—C12	−162.6 (17)
O12—Lu1—O2—C8	−14.8 (8)	N1—Cu1—N2—C12	8.8 (17)
O1—Lu1—O2—C8	18.0 (7)	O5—Cu1—N2—C12	101.7 (17)
O4—Lu1—O2—C8	166.2 (7)	Lu1—O7—N3—O8	−175.4 (8)
O3—Lu1—O2—Cu1	−7.3 (3)	Lu1—O7—N3—O6	6.0 (10)
O10—Lu1—O2—Cu1	−116.5 (3)	Lu1—O6—N3—O8	175.4 (8)
O9—Lu1—O2—Cu1	−90.6 (3)	Lu1—O6—N3—O7	−6.0 (10)
O6—Lu1—O2—Cu1	104.5 (4)	Lu1—O9—N4—O11	−175.5 (11)
O7—Lu1—O2—Cu1	58.8 (4)	Lu1—O9—N4—O10	4.7 (9)
O13—Lu1—O2—Cu1	106.6 (6)	Lu1—O10—N4—O11	175.4 (10)
O12—Lu1—O2—Cu1	158.3 (3)	Lu1—O10—N4—O9	−4.8 (9)
O1—Lu1—O2—Cu1	−168.9 (4)	Lu1—O13—N5—O12	−6.0 (9)
O4—Lu1—O2—Cu1	−20.7 (4)	Lu1—O13—N5—O14	176.9 (7)
O2—Cu1—O3—C19	173.7 (8)	Lu1—O12—N5—O13	5.8 (9)
N2—Cu1—O3—C19	−13.2 (8)	Lu1—O12—N5—O14	−177.0 (7)
O5—Cu1—O3—C19	77.9 (7)	C3—O1—C2—C1	68.5 (12)
O2—Cu1—O3—Lu1	−8.1 (3)	Lu1—O1—C2—C1	−107.2 (9)
N2—Cu1—O3—Lu1	165.1 (3)	C2—O1—C3—C8	−159.1 (8)
O5—Cu1—O3—Lu1	−103.9 (3)	Lu1—O1—C3—C8	16.9 (10)
O2—Lu1—O3—C19	−174.7 (8)	C2—O1—C3—C4	20.3 (14)
O10—Lu1—O3—C19	−55.2 (8)	Lu1—O1—C3—C4	−163.7 (8)
O9—Lu1—O3—C19	−89.0 (8)	C8—C3—C4—C5	−3.0 (16)
O6—Lu1—O3—C19	118.0 (7)	O1—C3—C4—C5	177.7 (10)

O7—Lu1—O3—C19	80.9 (8)	C3—C4—C5—C6	4.4 (18)
O13—Lu1—O3—C19	29.9 (8)	C4—C5—C6—C7	−3.3 (19)
O12—Lu1—O3—C19	80.8 (13)	C5—C6—C7—C8	0.5 (17)
O1—Lu1—O3—C19	−155.7 (7)	C5—C6—C7—C9	−178.3 (11)
O4—Lu1—O3—C19	−7.7 (7)	Cu1—O2—C8—C3	171.5 (6)
O2—Lu1—O3—Cu1	7.1 (3)	Lu1—O2—C8—C3	−16.4 (11)
O10—Lu1—O3—Cu1	126.7 (3)	Cu1—O2—C8—C7	−10.8 (12)
O9—Lu1—O3—Cu1	92.8 (3)	Lu1—O2—C8—C7	161.2 (7)
O6—Lu1—O3—Cu1	−60.1 (3)	C4—C3—C8—O2	178.0 (9)
O7—Lu1—O3—Cu1	−97.2 (4)	O1—C3—C8—O2	−2.6 (12)
O13—Lu1—O3—Cu1	−148.3 (3)	C4—C3—C8—C7	0.4 (15)
O12—Lu1—O3—Cu1	−97.3 (10)	O1—C3—C8—C7	179.7 (8)
O1—Lu1—O3—Cu1	26.1 (4)	C9—C7—C8—O2	2.1 (16)
O4—Lu1—O3—Cu1	174.2 (4)	C6—C7—C8—O2	−176.6 (9)
O2—Lu1—O4—C18	18.9 (7)	C9—C7—C8—C3	179.6 (10)
O3—Lu1—O4—C18	5.3 (6)	C6—C7—C8—C3	1.0 (14)
O10—Lu1—O4—C18	144.2 (6)	C10'—N1—C9—C7	−161.7 (12)
O9—Lu1—O4—C18	90.9 (6)	C10—N1—C9—C7	161.1 (12)
O6—Lu1—O4—C18	−78.0 (7)	Cu1—N1—C9—C7	−3.3 (15)
O7—Lu1—O4—C18	−68.2 (6)	C8—C7—C9—N1	5.5 (17)
O13—Lu1—O4—C18	−142.7 (6)	C6—C7—C9—N1	−175.8 (10)
O12—Lu1—O4—C18	−160.1 (6)	C9—N1—C10—C11	37 (2)
O1—Lu1—O4—C18	108.1 (6)	C10'—N1—C10—C11	−60.1 (15)
O2—Lu1—O4—C20	−161.9 (7)	Cu1—N1—C10—C11	−156.2 (13)
O3—Lu1—O4—C20	−175.6 (7)	C9—N1—C10—C12	154.4 (17)
O10—Lu1—O4—C20	−36.6 (7)	C10'—N1—C10—C12	57 (3)
O9—Lu1—O4—C20	−89.9 (7)	Cu1—N1—C10—C12	−39.2 (18)
O6—Lu1—O4—C20	101.1 (7)	C9—N1—C10'—C11	−41 (2)
O7—Lu1—O4—C20	111.0 (7)	C10—N1—C10'—C11	61.2 (14)
O13—Lu1—O4—C20	36.5 (7)	Cu1—N1—C10'—C11	157.5 (16)
O12—Lu1—O4—C20	19.1 (8)	C9—N1—C10'—C12'	−161.7 (16)
O1—Lu1—O4—C20	−72.7 (8)	C10—N1—C10'—C12'	−59 (3)
O2—Cu1—O5—C22	9.4 (14)	Cu1—N1—C10'—C12'	37.2 (18)
O3—Cu1—O5—C22	92.3 (13)	N1—C10'—C11—C10	−61.2 (14)
N2—Cu1—O5—C22	−172.5 (13)	C12'—C10'—C11—C10	60 (3)
N1—Cu1—O5—C22	−87.5 (13)	N1—C10—C11—C10'	59.8 (14)
O2—Lu1—O6—N3	−103.6 (7)	C12—C10—C11—C10'	−58 (3)
O3—Lu1—O6—N3	−45.8 (7)	C13—N2—C12—C10	151.7 (17)
O10—Lu1—O6—N3	125.7 (7)	C12'—N2—C12—C10	63 (6)
O9—Lu1—O6—N3	−138.7 (6)	Cu1—N2—C12—C10	−33 (3)
O7—Lu1—O6—N3	3.7 (6)	N1—C10—C12—N2	46 (3)
O13—Lu1—O6—N3	77.2 (7)	C11—C10—C12—N2	173 (2)
O12—Lu1—O6—N3	125.9 (7)	C13—N2—C12'—C10'	−160.6 (17)
O1—Lu1—O6—N3	−166.2 (7)	C12—N2—C12'—C10'	−59 (5)
O4—Lu1—O6—N3	16.7 (8)	Cu1—N2—C12'—C10'	32 (3)
O2—Lu1—O7—N3	64.6 (6)	N1—C10'—C12'—N2	−44 (3)
O3—Lu1—O7—N3	124.4 (7)	C11—C10'—C12'—N2	−174 (2)
O10—Lu1—O7—N3	−121.1 (7)	C12'—N2—C13—C14	−170 (2)
O9—Lu1—O7—N3	144.0 (6)	C12—N2—C13—C14	170 (2)

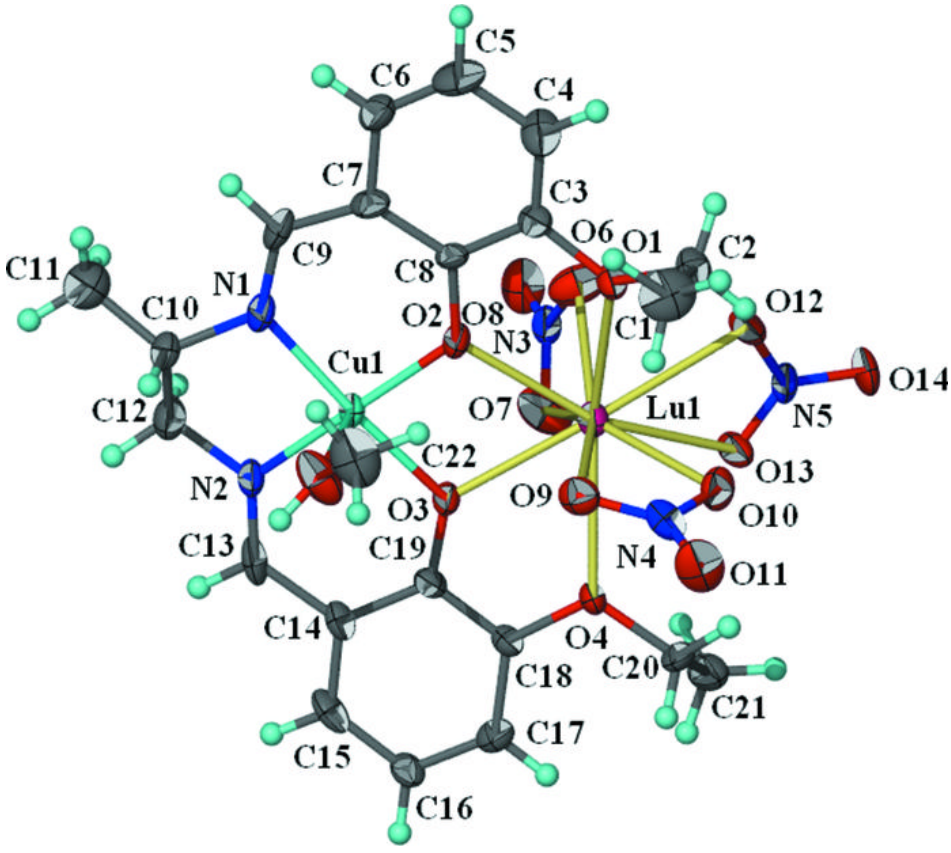
O6—Lu1—O7—N3	−3.6 (6)	Cu1—N2—C13—C14	−5.1 (16)
O13—Lu1—O7—N3	−98.3 (7)	N2—C13—C14—C15	175.5 (10)
O12—Lu1—O7—N3	−55.6 (7)	N2—C13—C14—C19	−6.5 (16)
O1—Lu1—O7—N3	9.1 (8)	C19—C14—C15—C16	2.1 (16)
O4—Lu1—O7—N3	−173.1 (7)	C13—C14—C15—C16	−179.9 (9)
O2—Lu1—O9—N4	−156.7 (6)	C14—C15—C16—C17	−4.3 (16)
O3—Lu1—O9—N4	139.4 (6)	C15—C16—C17—C18	1.1 (15)
O10—Lu1—O9—N4	−2.9 (6)	C20—O4—C18—C19	177.2 (8)
O6—Lu1—O9—N4	−122.4 (8)	Lu1—O4—C18—C19	−3.6 (10)
O7—Lu1—O9—N4	120.7 (8)	C20—O4—C18—C17	1.7 (13)
O13—Lu1—O9—N4	15.9 (7)	Lu1—O4—C18—C17	−179.1 (7)
O12—Lu1—O9—N4	−38.1 (6)	C16—C17—C18—C19	4.3 (15)
O1—Lu1—O9—N4	−94.3 (6)	C16—C17—C18—O4	179.6 (9)
O4—Lu1—O9—N4	77.5 (6)	Cu1—O3—C19—C18	−173.2 (6)
O2—Lu1—O10—N4	36.4 (7)	Lu1—O3—C19—C18	9.0 (12)
O3—Lu1—O10—N4	−41.5 (7)	Cu1—O3—C19—C14	6.3 (13)
O9—Lu1—O10—N4	2.9 (6)	Lu1—O3—C19—C14	−171.5 (6)
O6—Lu1—O10—N4	148.2 (6)	O4—C18—C19—O3	−2.5 (12)
O7—Lu1—O10—N4	−136.5 (6)	C17—C18—C19—O3	173.2 (8)
O13—Lu1—O10—N4	−159.7 (7)	O4—C18—C19—C14	178.0 (8)
O12—Lu1—O10—N4	148.0 (7)	C17—C18—C19—C14	−6.3 (13)
O1—Lu1—O10—N4	80.8 (6)	C15—C14—C19—O3	−176.4 (9)
O4—Lu1—O10—N4	−83.2 (6)	C13—C14—C19—O3	5.7 (15)
O2—Lu1—O12—N5	−160.1 (5)	C15—C14—C19—C18	3.2 (14)
O3—Lu1—O12—N5	−62.5 (13)	C13—C14—C19—C18	−174.8 (9)
O10—Lu1—O12—N5	77.7 (6)	C18—O4—C20—C21	77.7 (10)
O9—Lu1—O12—N5	106.7 (6)	Lu1—O4—C20—C21	−101.5 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5O···O14^{i}	0.82	2.13	2.93 (1)	164

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

Fig. 1


C5
C6
C4
C7
C3
O6
O1
C2
C11
C9
C8
O12
N1
C10
O2
O8
C1
N3
Cu1
O14
C12
O7
Lu1
N5
C22
O13
N2
O9
O3
O10
C13
C19
N4
O11
C14
O4
C20
C18
C21
C17
C15
C16