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{6,6′-Diethoxy-2,2′-[ethane-1,2-diyl-bis(nitrilomethylidyne)]diphenolato}-trinitratosamarium(III)copper(II)

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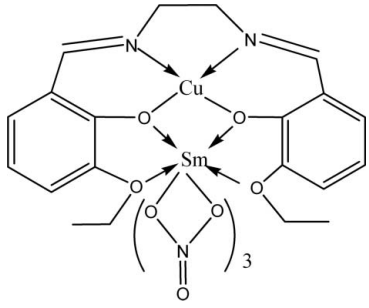
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.022; wR factor = 0.048; data-to-parameter ratio = 17.0.

A heteronuclear Cu^{II}–Sm^{III} complex (systematic name: {6,6′-diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}trinitrato-1$\kappa^6O,O'$-samarium(III)copper(II)), $[CuSm(C_{20}H_{22}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-ethoxysalicylidene)ethylene-1,2-diamine, has been synthesized and structurally characterized. The Cu and Sm atoms are doubly bridged by two phenolate O atoms provided by the Schiff base ligand. The coordination of the Cu atom is square planar, formed by two imine N and two phenolate O atoms. The Sm^{III} atom has a decacoordination environment, formed by the phenolate O atoms, two ethoxy O atoms and two O atoms each from the three nitrates. No classical intermolecular hydrogen bonds are found. Some weak C—H···O and O···Cu interactions [O···Cu = 3.167 (4) Å] generate a two-dimensional zigzag sheet.

Related literature

For related literature, see: Baggio *et al.* (2000); Brewer *et al.* (2001); Caravan *et al.* (1999); Edder *et al.* (2000); Mohanta *et al.* (2002); Wong *et al.* (2002).



Experimental

Crystal data

$[CuSm(C_{20}H_{22}N_2O_4)(NO_3)_3]$
M_r = 754.32
Orthorhombic, $P2_12_12_1$
a = 8.6208 (8) Å
b = 13.8333 (13) Å
c = 21.151 (2) Å
V = 2522.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.23 mm^{-1}
T = 293 (2) K
0.28 × 0.17 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.533, T_{max} = 0.622
19177 measured reflections
6184 independent reflections
5236 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.048
S = 1.00
6184 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}
Absolute structure: Flack (1983), 2621 Friedel pairs
Flack parameter: −0.013 (9)

Table 1
Selected geometric parameters (Å, °).

Sm1—O1	2.4189 (19)	Sm1—O9	2.569 (2)
Sm1—O2	2.3697 (19)	Sm1—O11	2.513 (2)
Sm1—O3	2.6602 (19)	Sm1—O12	2.460 (2)
Sm1—O4	2.6115 (19)	Cu1—O1	1.900 (2)
Sm1—O5	2.545 (2)	Cu1—O2	1.901 (2)
Sm1—O6	2.513 (2)	Cu1—N1	1.908 (3)
Sm1—O8	2.495 (2)	Cu1—N2	1.909 (2)
O1—Sm1—O3	59.96 (6)	O8—Sm1—O4	122.64 (7)
O1—Sm1—O4	121.46 (6)	O8—Sm1—O5	68.78 (8)
O1—Sm1—O5	69.87 (8)	O8—Sm1—O6	71.94 (8)
O1—Sm1—O6	113.86 (7)	O8—Sm1—O9	49.93 (8)
O1—Sm1—O8	113.06 (8)	O8—Sm1—O11	138.00 (8)
O1—Sm1—O9	161.23 (8)	O9—Sm1—O3	102.71 (8)
O1—Sm1—O11	72.27 (8)	O9—Sm1—O4	77.26 (8)
O1—Sm1—O12	114.83 (8)	O11—Sm1—O3	79.81 (7)
O2—Sm1—O1	64.75 (6)	O11—Sm1—O4	78.04 (7)
O2—Sm1—O3	124.60 (6)	O11—Sm1—O5	140.82 (8)
O2—Sm1—O4	61.50 (6)	O11—Sm1—O6	146.79 (8)
O2—Sm1—O5	74.31 (8)	O11—Sm1—O9	113.94 (8)
O2—Sm1—O6	73.79 (7)	O12—Sm1—O3	79.58 (7)
O2—Sm1—O8	140.44 (7)	O12—Sm1—O4	78.42 (7)
O2—Sm1—O9	132.55 (9)	O12—Sm1—O5	162.85 (8)
O2—Sm1—O11	80.88 (8)	O12—Sm1—O6	130.86 (8)
O2—Sm1—O12	122.83 (7)	O12—Sm1—O8	94.75 (8)
O4—Sm1—O3	155.54 (7)	O12—Sm1—O9	64.78 (9)
O5—Sm1—O3	89.80 (7)	O12—Sm1—O11	50.63 (8)
O5—Sm1—O4	114.03 (7)	O1—Cu1—O2	84.85 (8)
O5—Sm1—O9	105.17 (9)	O1—Cu1—N1	95.24 (10)
O6—Sm1—O3	132.51 (7)	O1—Cu1—N2	172.36 (10)
O6—Sm1—O4	71.18 (7)	O2—Cu1—N1	177.37 (10)
O6—Sm1—O5	50.15 (8)	O2—Cu1—N2	94.10 (9)
O6—Sm1—O9	71.36 (9)	N1—Cu1—N2	86.15 (11)
O8—Sm1—O3	69.74 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20A···O8	0.96	2.43	3.139 (4)	130
C9—H9A···O7^{i}	0.97	2.41	3.284 (4)	150
C7—H7···O7^{ii}	0.93	2.36	3.279 (4)	167

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *APEX2*; program(s) used to refine structure: *APEX2*; molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2240).

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supplementary materials

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{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}trinitratosamarium(III)copper(II)

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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). Recently, some 3 d-4f heterometallic Schiff base complexes have been synthesized, such as Cu^{II}—Gd^{III}, Ni^{II}—Gd^{III} and Zn^{II}—Ho^{III} heterodinuclear complexes (Brewer *et al.*, 2001; Mohanta *et al.*, 2002; Wong *et al.*, 2002), which exhibits novel magnetic and luminescent properties, however, there are relatively few studies on Cu^{II}—Sm^{III} dinuclear complexes. As part of our investigations into the structure and applications of 3 d-4f hetorometallic Schiff base complexes, we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Cu^{II}—Sm^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-ethoxysalicylidene) ethylene-1,2-diamine(H_2L).

Complex (I) crystallizes in the space group $P2_12_12_1$, with copper and samarium doubly bridged by two phenolate O atoms provided by a salen-type Schiff base ligand. The inner salen-type cavity is occupied by copper(II), while samarium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand. The dihedral angles between the mean planes of Cu1/O1/O2 and Sm1/O1/O2 is 3.7 (2)° suggesting that the bridging moiety is almost planar; the deviation of atoms from the least squares Cu1/O1/O2/Sm1 plane being 0.0315 (2)Å for Cu, 0.0218 (2)Å for Sm, −0.0263 (4)Å for O1 and −0.0270 (3)Å for O2.

The samarium(III) center in (I) has a decacoordination environment of O atoms. In addition to the phenolate ligands, two ethoxy O atoms coordinate to this metal center, two O atoms from each of the three nitrates chelate to samarium to complete the decacoordination. The three kinds of Sm—O bond distances are significantly different, the shortest being the Sm—O(phenolate) and longest being the Sm—*O*(methoxy) separations.

The coordination of copper(II) is square planar. The donor centers are alternatively above and below the mean N_2O_2 plane with an average deviation from the plane of 0.0844 (2) Å, while Cu1 is just 0.0407 (2)Å below this square plane.

Adjacent molecules are held together by weak interactions (O10···Cu1=3.167 (4) Å, C7—H7···O7^{i} and C9—H9···O7^{ii}; symmetry codes:(i)-*x* + 1, *y* − 1/2, 1/2 − *z*; (ii)*x* − 1, Y, *Z*). these link the molecules into a two-dimensional zugzag sheet(Fig 2).

Experimental

H_2L was prepared by the 2:1 condensation of 3-ethoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of copper(II) acetate monohydrate (0.168 g, 1 mmol) with H_2L(0.356 g, 1 mmol) in methanol solution (50 ml) under reflux for 3 h and then for another 3 h after the addition of samarium(III) nitrate hexahydrate (0.444 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 $C_{20}H_{22}CuN_5O_{13}Sm$: C 31.85, H 2.94, Cu 8.42, N 9.28, Sm 19.93%; found: C 31.80, H 2.91, Cu 8.45, N 9.33, Sm 19.95%. IR(KBr, cm^{-1}): 1640(C=N), 1384,1491(nitrate).

Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.97 (methylene) and 0.96 Å (methyl), and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms.

Figures

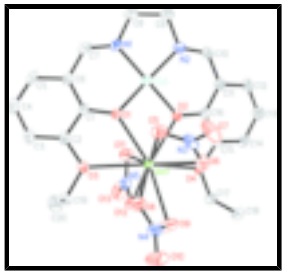

Fig.1. The molecular structure of (I), showing 30% probability displacement ellipsoids. All the H atoms on carbon have been omitted for clarity.

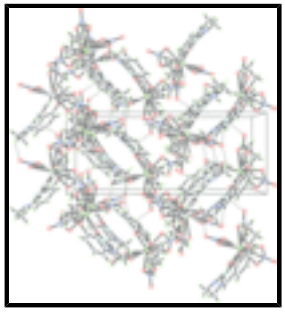

Fig.2. The packing diagram of (I), viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

Table 1. Selected geometric parameters (Å, °).

{6,6'-diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1κ^4*O*^{1},*O*$^{1'}$,*O*^{6},*O*$^{6'}$:2κ^4*O*^{1},*N*,*N*',*O*$^{1'}$}trinitrato-1κ^6*O*,*O*'- samarium(III)copper(II)

Crystal data

$[CuSm(C_{20}H_{22}N_2O_4)(NO_3)_3]$	$F_{000} = 1488$
$M_r = 754.32$	$D_x = 1.986$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 19177 reflections
$a = 8.6208$ (8) Å	θ = 1.8–28.4º
$b = 13.8333$ (13) Å	μ = 3.23 mm^{-1}
$c = 21.151$ (2) Å	$T = 293$ (2) K
$V = 2522.4$ (4) Å^3	Block, red
$Z = 4$	0.28 × 0.17 × 0.15 mm

Data collection

Bruker APEX II area-detector diffractometer	6184 independent reflections
Radiation source: fine-focus sealed tube	5236 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
Detector resolution: 0 pixels mm^{-1}	$\theta_{max} = 28.4^{o}$
$T = 293(2)$ K	$\theta_{min} = 1.8^{o}$
φ and ω scans	$h = -11 \rightarrow 10$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$k = -18 \rightarrow 18$
$T_{min} = 0.533$, $T_{max} = 0.622$	$l = -28 \rightarrow 27$
19177 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.019P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.048$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.00$	$\Delta\rho_{max} = 0.35$ e $Å^{-3}$
6184 reflections	$\Delta\rho_{min} = -0.65$ e $Å^{-3}$
363 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2621 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.013 (9)

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 $F^2 > 2$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}
Sm1	0.758979 (15)	1.000545 (10)	0.097186 (6)	0.03280 (4)
Cu1	0.43532 (4)	0.94387 (2)	0.183302 (17)	0.03690 (9)
N5	0.6347 (4)	0.9937 (2)	−0.03107 (12)	0.0513 (7)

O1	0.5890 (3)	0.87546 (13)	0.13701 (10)	0.0395 (5)
N1	0.3237 (3)	0.83138 (18)	0.20885 (12)	0.0377 (6)
O3	0.8146 (2)	0.81613 (14)	0.06966 (10)	0.0396 (5)
O11	0.5526 (3)	0.97137 (18)	0.01551 (11)	0.0590 (7)
O13	0.5818 (4)	0.9988 (2)	−0.08480 (11)	0.0792 (8)
C1	0.5900 (4)	0.78076 (19)	0.12685 (13)	0.0312 (7)
C2	0.7140 (4)	0.74466 (19)	0.09014 (13)	0.0346 (7)
C5	0.4912 (4)	0.6173 (2)	0.13322 (15)	0.0469 (8)
H5	0.4163	0.5739	0.1472	0.056*
C7	0.3536 (4)	0.7445 (2)	0.19117 (15)	0.0406 (8)
H7	0.2884	0.6958	0.2058	0.049*
O12	0.7763 (3)	1.00950 (19)	−0.01877 (10)	0.0540 (6)
C4	0.6083 (4)	0.5856 (2)	0.09699 (16)	0.0524 (9)
H4	0.6123	0.5206	0.0859	0.063*
C6	0.4800 (4)	0.7162 (2)	0.15052 (13)	0.0354 (7)
O2	0.5405 (2)	1.05638 (13)	0.15454 (9)	0.0351 (4)
N2	0.3009 (3)	1.01365 (18)	0.23861 (11)	0.0393 (6)
O4	0.6581 (2)	1.17546 (13)	0.07559 (9)	0.0373 (5)
O6	0.8625 (3)	1.11130 (16)	0.18137 (11)	0.0500 (6)
O5	0.8189 (3)	0.96652 (18)	0.21287 (11)	0.0532 (7)
O8	1.0395 (3)	0.96285 (16)	0.11271 (12)	0.0546 (6)
N3	0.8613 (3)	1.0503 (3)	0.22574 (14)	0.0490 (7)
C19	0.9510 (4)	0.7847 (2)	0.03452 (14)	0.0437 (8)
H19A	0.9935	0.8392	0.0115	0.052*
H19B	0.9204	0.7361	0.0039	0.052*
C3	0.7241 (4)	0.6480 (2)	0.07552 (14)	0.0434 (8)
H3	0.8068	0.6246	0.0518	0.052*
O9	1.0010 (3)	1.0865 (2)	0.05411 (13)	0.0689 (8)
C16	0.4796 (4)	1.14461 (18)	0.15585 (13)	0.0328 (6)
C8	0.1878 (4)	0.8545 (2)	0.24860 (15)	0.0474 (8)
H8A	0.1691	0.8030	0.2787	0.057*
H8B	0.0960	0.8621	0.2225	0.057*
C15	0.5414 (4)	1.21220 (19)	0.11348 (13)	0.0338 (7)
C10	0.2786 (4)	1.1052 (2)	0.23833 (14)	0.0389 (7)
H10	0.2083	1.1307	0.2672	0.047*
O10	1.2361 (3)	1.0403 (3)	0.07445 (15)	0.0932 (9)
C17	0.7306 (4)	1.2406 (2)	0.02956 (13)	0.0444 (8)
H17A	0.6507	1.2790	0.0093	0.053*
H17B	0.7813	1.2024	−0.0029	0.053*
O7	0.9014 (4)	1.0745 (2)	0.27940 (12)	0.0809 (10)
N4	1.0959 (4)	1.0303 (2)	0.07988 (14)	0.0534 (8)
C11	0.3562 (4)	1.1717 (2)	0.19575 (15)	0.0378 (8)
C9	0.2234 (4)	0.9478 (2)	0.28284 (14)	0.0448 (7)
H9A	0.1282	0.9768	0.2982	0.054*
H9B	0.2902	0.9351	0.3188	0.054*
C14	0.4830 (4)	1.3055 (2)	0.11118 (16)	0.0420 (8)
H14	0.5238	1.3500	0.0828	0.050*
C12	0.3022 (4)	1.2679 (2)	0.19381 (17)	0.0471 (9)
H12	0.2247	1.2879	0.2214	0.057*

C20	1.0732 (5)	0.7438 (3)	0.07655 (17)	0.0574 (9)
H20A	1.1080	0.7926	0.1055	0.086*
H20B	1.1591	0.7221	0.0514	0.086*
H20C	1.0314	0.6902	0.0998	0.086*
C13	0.3639 (4)	1.3319 (2)	0.15125 (16)	0.0520 (9)
H13	0.3247	1.3945	0.1493	0.062*
C18	0.8475 (4)	1.3070 (2)	0.05914 (18)	0.0570 (10)
H18A	0.7953	1.3525	0.0861	0.085*
H18B	0.9023	1.3413	0.0266	0.085*
H18C	0.9197	1.2699	0.0837	0.085*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.03259 (8)	0.02752 (6)	0.03830 (7)	−0.00114 (9)	0.00422 (6)	0.00242 (7)
Cu1	0.0367 (2)	0.02826 (16)	0.04569 (19)	−0.00167 (15)	0.01072 (18)	0.00384 (17)
N5	0.068 (2)	0.0352 (14)	0.0505 (16)	0.0006 (17)	−0.0011 (14)	−0.0049 (16)
O1	0.0424 (14)	0.0231 (9)	0.0531 (13)	−0.0029 (9)	0.0163 (10)	0.0000 (9)
N1	0.0363 (16)	0.0367 (13)	0.0402 (14)	−0.0025 (11)	0.0021 (12)	0.0097 (12)
O3	0.0372 (13)	0.0316 (11)	0.0500 (12)	0.0013 (9)	0.0097 (10)	−0.0024 (9)
O11	0.0513 (15)	0.0772 (19)	0.0486 (13)	−0.0061 (13)	0.0037 (12)	−0.0006 (12)
O13	0.114 (2)	0.0737 (16)	0.0498 (14)	−0.015 (2)	−0.0223 (14)	0.0004 (16)
C1	0.0333 (18)	0.0248 (13)	0.0355 (14)	−0.0010 (12)	−0.0027 (14)	0.0015 (12)
C2	0.0403 (18)	0.0270 (13)	0.0364 (15)	0.0011 (12)	−0.0034 (13)	0.0012 (11)
C5	0.058 (2)	0.0247 (14)	0.058 (2)	−0.0105 (14)	−0.0036 (17)	0.0042 (14)
C7	0.0361 (19)	0.0393 (16)	0.0465 (19)	−0.0103 (14)	−0.0042 (16)	0.0121 (15)
O12	0.0528 (15)	0.0618 (15)	0.0474 (11)	−0.0086 (15)	0.0062 (10)	−0.0008 (11)
C4	0.069 (3)	0.0239 (15)	0.064 (2)	0.0013 (14)	−0.009 (2)	−0.0038 (15)
C6	0.0396 (19)	0.0280 (14)	0.0385 (15)	−0.0044 (12)	−0.0048 (14)	0.0058 (13)
O2	0.0336 (12)	0.0252 (9)	0.0465 (11)	0.0024 (9)	0.0098 (9)	0.0029 (9)
N2	0.0368 (13)	0.0419 (15)	0.0392 (13)	0.0022 (11)	0.0071 (10)	0.0057 (12)
O4	0.0419 (13)	0.0281 (10)	0.0420 (11)	−0.0008 (9)	0.0055 (10)	0.0070 (9)
O6	0.0565 (16)	0.0441 (12)	0.0495 (13)	0.0017 (11)	−0.0047 (12)	−0.0042 (12)
O5	0.0574 (17)	0.0570 (15)	0.0453 (13)	0.0029 (12)	0.0021 (12)	0.0139 (11)
O8	0.0418 (14)	0.0462 (12)	0.0758 (16)	−0.0018 (11)	0.0056 (13)	0.0054 (12)
N3	0.0388 (17)	0.0639 (19)	0.0442 (17)	0.0188 (16)	−0.0005 (13)	−0.0085 (17)
C19	0.0402 (19)	0.0439 (17)	0.0470 (18)	0.0045 (15)	0.0123 (16)	−0.0056 (14)
C3	0.054 (2)	0.0312 (14)	0.0452 (16)	0.0062 (15)	−0.0021 (16)	−0.0058 (13)
O9	0.0485 (17)	0.086 (2)	0.0719 (17)	−0.0149 (14)	0.0014 (14)	0.0335 (16)
C16	0.0353 (18)	0.0260 (13)	0.0370 (14)	−0.0005 (11)	−0.0053 (13)	−0.0009 (12)
C8	0.042 (2)	0.054 (2)	0.0462 (19)	−0.0054 (15)	0.0103 (16)	0.0144 (16)
C15	0.0345 (18)	0.0275 (13)	0.0394 (16)	−0.0012 (12)	−0.0053 (14)	−0.0015 (12)
C10	0.0344 (18)	0.0436 (16)	0.0386 (15)	0.0075 (14)	0.0046 (14)	−0.0011 (14)
O10	0.0393 (17)	0.135 (3)	0.106 (2)	−0.0233 (18)	0.0062 (16)	0.003 (2)
C17	0.057 (2)	0.0361 (15)	0.0403 (16)	−0.0041 (16)	0.0092 (17)	0.0076 (12)
O7	0.083 (2)	0.113 (2)	0.0464 (14)	0.0462 (19)	−0.0178 (14)	−0.0234 (15)
N4	0.0389 (18)	0.065 (2)	0.0563 (17)	−0.0093 (14)	0.0061 (14)	−0.0100 (14)
C11	0.0376 (19)	0.0331 (14)	0.0428 (19)	0.0037 (13)	0.0008 (15)	0.0004 (14)

C9	0.040 (2)	0.0484 (17)	0.0458 (16)	0.0021 (15)	0.0091 (15)	0.0137 (15)
C14	0.0426 (19)	0.0270 (14)	0.057 (2)	0.0006 (12)	−0.0032 (16)	0.0086 (14)
C12	0.042 (2)	0.0357 (16)	0.064 (2)	0.0088 (14)	0.0041 (17)	−0.0084 (16)
C20	0.052 (2)	0.052 (2)	0.069 (2)	0.0130 (18)	−0.005 (2)	−0.0070 (18)
C13	0.058 (2)	0.0279 (15)	0.070 (2)	0.0138 (15)	0.0001 (19)	0.0014 (16)
C18	0.059 (2)	0.0439 (19)	0.068 (2)	−0.0123 (17)	0.0199 (19)	−0.0001 (18)

Geometric parameters (Å, °)

Sm1—O1	2.4189 (19)	O4—C17	1.467 (3)
Sm1—O2	2.3697 (19)	O6—N3	1.262 (4)
Sm1—O3	2.6602 (19)	O5—N3	1.245 (4)
Sm1—O4	2.6115 (19)	O8—N4	1.261 (4)
Sm1—O5	2.545 (2)	N3—O7	1.233 (3)
Sm1—O6	2.513 (2)	C19—C20	1.490 (5)
Sm1—O8	2.495 (2)	C19—H19A	0.9700
Sm1—O9	2.569 (2)	C19—H19B	0.9700
Sm1—O11	2.513 (2)	C3—H3	0.9300
Sm1—O12	2.460 (2)	O9—N4	1.254 (4)
Cu1—O1	1.900 (2)	C16—C15	1.400 (4)
Cu1—O2	1.901 (2)	C16—C11	1.409 (4)
Cu1—N1	1.908 (3)	C8—C9	1.511 (5)
Cu1—N2	1.909 (2)	C8—H8A	0.9700
N5—O13	1.227 (3)	C8—H8B	0.9700
N5—O11	1.252 (3)	C15—C14	1.386 (4)
N5—O12	1.267 (3)	C10—C11	1.450 (4)
O1—C1	1.328 (3)	C10—H10	0.9300
N1—C7	1.285 (4)	O10—N4	1.222 (4)
N1—C8	1.478 (4)	C17—C18	1.500 (5)
O3—C2	1.385 (3)	C17—H17A	0.9700
O3—C19	1.458 (4)	C17—H17B	0.9700
C1—C6	1.395 (4)	C11—C12	1.411 (4)
C1—C2	1.412 (4)	C9—H9A	0.9700
C2—C3	1.376 (4)	C9—H9B	0.9700
C5—C4	1.341 (5)	C14—C13	1.381 (5)
C5—C6	1.420 (4)	C14—H14	0.9300
C5—H5	0.9300	C12—C13	1.370 (5)
C7—C6	1.442 (4)	C12—H12	0.9300
C7—H7	0.9300	C20—H20A	0.9600
C4—C3	1.396 (5)	C20—H20B	0.9600
C4—H4	0.9300	C20—H20C	0.9600
O2—C16	1.329 (3)	C13—H13	0.9300
N2—C10	1.282 (4)	C18—H18A	0.9600
N2—C9	1.467 (4)	C18—H18B	0.9600
O4—C15	1.383 (4)	C18—H18C	0.9600
O1—Sm1—O3	59.96 (6)	C1—C6—C7	123.6 (3)
O1—Sm1—O4	121.46 (6)	C5—C6—C7	117.8 (3)
O1—Sm1—O5	69.87 (8)	C16—O2—Cu1	123.83 (18)
O1—Sm1—O6	113.86 (7)	C16—O2—Sm1	128.61 (17)

O1—Sm1—O8	113.06 (8)	Cu1—O2—Sm1	106.02 (8)
O1—Sm1—O9	161.23 (8)	C10—N2—C9	123.3 (3)
O1—Sm1—O11	72.27 (8)	C10—N2—Cu1	126.0 (2)
O1—Sm1—O12	114.83 (8)	C9—N2—Cu1	110.7 (2)
O2—Sm1—O1	64.75 (6)	C15—O4—C17	118.0 (2)
O2—Sm1—O3	124.60 (6)	C15—O4—Sm1	118.78 (15)
O2—Sm1—O4	61.50 (6)	C17—O4—Sm1	122.91 (17)
O2—Sm1—O5	74.31 (8)	N3—O6—Sm1	96.66 (18)
O2—Sm1—O6	73.79 (7)	N3—O5—Sm1	95.60 (18)
O2—Sm1—O8	140.44 (7)	N4—O8—Sm1	98.4 (2)
O2—Sm1—O9	132.55 (9)	O7—N3—O5	122.5 (3)
O2—Sm1—O11	80.88 (8)	O7—N3—O6	120.0 (3)
O2—Sm1—O12	122.83 (7)	O5—N3—O6	117.5 (3)
O4—Sm1—O3	155.54 (7)	O3—C19—C20	112.3 (3)
O5—Sm1—O3	89.80 (7)	O3—C19—H19A	109.1
O5—Sm1—O4	114.03 (7)	C20—C19—H19A	109.1
O5—Sm1—O9	105.17 (9)	O3—C19—H19B	109.1
O6—Sm1—O3	132.51 (7)	C20—C19—H19B	109.1
O6—Sm1—O4	71.18 (7)	H19A—C19—H19B	107.9
O6—Sm1—O5	50.15 (8)	C2—C3—C4	118.8 (3)
O6—Sm1—O9	71.36 (9)	C2—C3—H3	120.6
O8—Sm1—O3	69.74 (7)	C4—C3—H3	120.6
O8—Sm1—O4	122.64 (7)	N4—O9—Sm1	95.08 (19)
O8—Sm1—O5	68.78 (8)	O2—C16—C15	116.7 (3)
O8—Sm1—O6	71.94 (8)	O2—C16—C11	123.7 (3)
O8—Sm1—O9	49.93 (8)	C15—C16—C11	119.5 (2)
O8—Sm1—O11	138.00 (8)	N1—C8—C9	107.2 (3)
O9—Sm1—O3	102.71 (8)	N1—C8—H8A	110.3
O9—Sm1—O4	77.26 (8)	C9—C8—H8A	110.3
O11—Sm1—O3	79.81 (7)	N1—C8—H8B	110.3
O11—Sm1—O4	78.04 (7)	C9—C8—H8B	110.3
O11—Sm1—O5	140.82 (8)	H8A—C8—H8B	108.5
O11—Sm1—O6	146.79 (8)	O4—C15—C14	125.9 (3)
O11—Sm1—O9	113.94 (8)	O4—C15—C16	113.7 (2)
O12—Sm1—O3	79.58 (7)	C14—C15—C16	120.4 (3)
O12—Sm1—O4	78.42 (7)	N2—C10—C11	124.1 (3)
O12—Sm1—O5	162.85 (8)	N2—C10—H10	118.0
O12—Sm1—O6	130.86 (8)	C11—C10—H10	118.0
O12—Sm1—O8	94.75 (8)	O4—C17—C18	112.7 (3)
O12—Sm1—O9	64.78 (9)	O4—C17—H17A	109.1
O12—Sm1—O11	50.63 (8)	C18—C17—H17A	109.1
O1—Cu1—O2	84.85 (8)	O4—C17—H17B	109.1
O1—Cu1—N1	95.24 (10)	C18—C17—H17B	109.1
O1—Cu1—N2	172.36 (10)	H17A—C17—H17B	107.8
O2—Cu1—N1	177.37 (10)	O10—N4—O9	122.3 (3)
O2—Cu1—N2	94.10 (9)	O10—N4—O8	121.1 (4)
N1—Cu1—N2	86.15 (11)	O9—N4—O8	116.5 (3)
O13—N5—O11	122.2 (3)	C16—C11—C12	118.9 (3)
O13—N5—O12	122.6 (3)	C16—C11—C10	123.5 (3)

O11—N5—O12	115.2 (3)	C12—C11—C10	117.6 (3)
C1—O1—Cu1	125.42 (19)	N2—C9—C8	108.5 (2)
C1—O1—Sm1	130.21 (18)	N2—C9—H9A	110.0
Cu1—O1—Sm1	104.22 (8)	C8—C9—H9A	110.0
C7—N1—C8	121.8 (3)	N2—C9—H9B	110.0
C7—N1—Cu1	125.4 (2)	C8—C9—H9B	110.0
C8—N1—Cu1	112.6 (2)	H9A—C9—H9B	108.4
C2—O3—C19	116.9 (2)	C13—C14—C15	119.7 (3)
C2—O3—Sm1	120.22 (16)	C13—C14—H14	120.1
C19—O3—Sm1	122.91 (16)	C15—C14—H14	120.1
N5—O11—Sm1	95.79 (19)	C13—C12—C11	120.0 (3)
O1—C1—C6	124.7 (3)	C13—C12—H12	120.0
O1—C1—C2	116.3 (3)	C11—C12—H12	120.0
C6—C1—C2	119.0 (2)	C19—C20—H20A	109.5
C3—C2—O3	125.7 (3)	C19—C20—H20B	109.5
C3—C2—C1	121.0 (3)	H20A—C20—H20B	109.5
O3—C2—C1	113.2 (2)	C19—C20—H20C	109.5
C4—C5—C6	120.9 (3)	H20A—C20—H20C	109.5
C4—C5—H5	119.6	H20B—C20—H20C	109.5
C6—C5—H5	119.6	C12—C13—C14	121.4 (3)
N1—C7—C6	125.4 (3)	C12—C13—H13	119.3
N1—C7—H7	117.3	C14—C13—H13	119.3
C6—C7—H7	117.3	C17—C18—H18A	109.5
N5—O12—Sm1	97.91 (17)	C17—C18—H18B	109.5
C5—C4—C3	121.5 (3)	H18A—C18—H18B	109.5
C5—C4—H4	119.3	C17—C18—H18C	109.5
C3—C4—H4	119.3	H18A—C18—H18C	109.5
C1—C6—C5	118.6 (3)	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20A···O8	0.96	2.43	3.139 (4)	130
C9—H9A···O7^{i}	0.97	2.41	3.284 (4)	150
C7—H7···O7^{ii}	0.93	2.36	3.279 (4)	167

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

Fig. 1

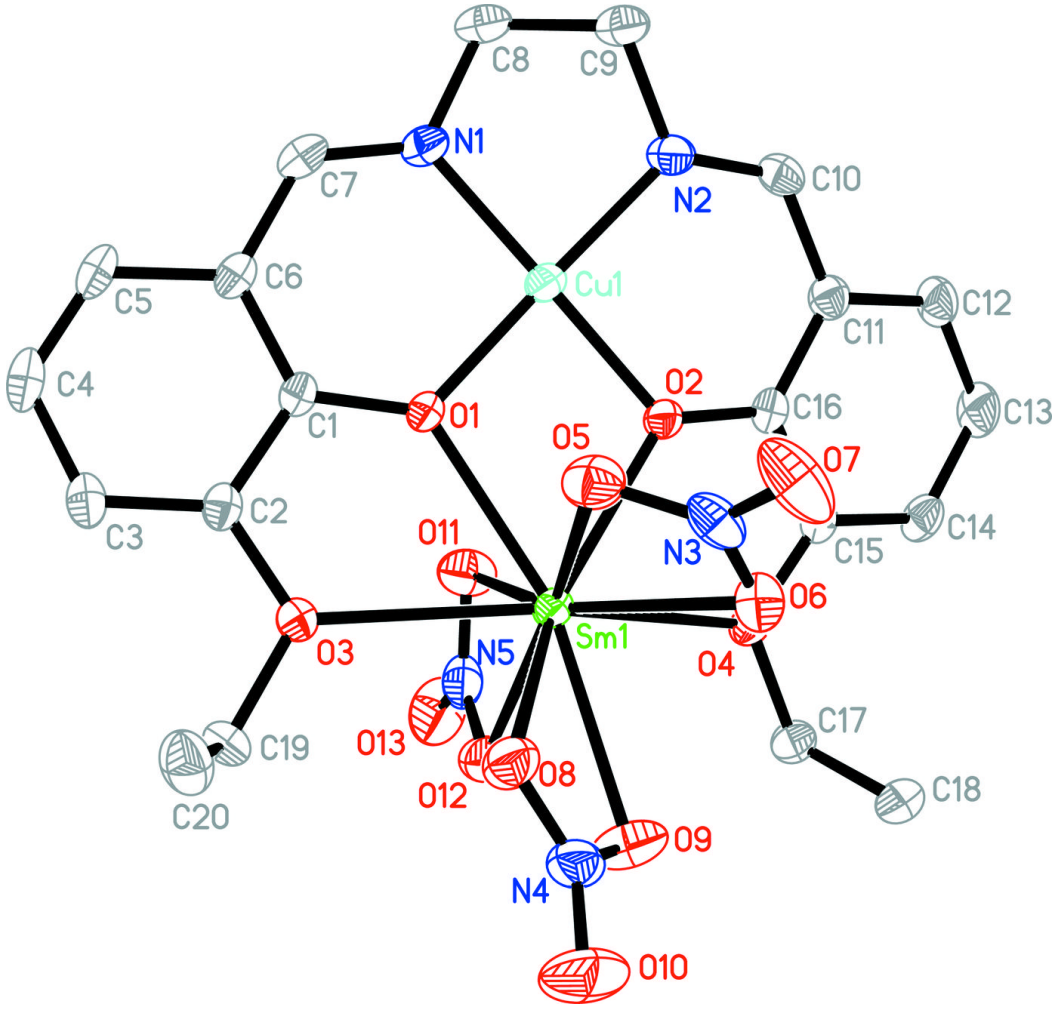
C8
C9
N1
C7
N2
C10
C6
C5
Cu1
C11
C12
C4
C1
O1
O2
C16
C13
O5
O7
C3
C2
O11
N3
C15
C14
O6
O3
N5
Sm1
O4
C17
C19
O13
O8
C18
C20
O12
O9
N4
O10

Fig. 2