Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Yan Sui,* Xiao-Niu Fang, Xiao-Chun Zhou, Qiu-Yan Luo and Ya-Ping Xu

JiangXi Province Key Laboratory of Coordination Chemistry, College of Chemistry and Chemical Engineering, JingGangShan University, 343009 Ji'an, JiangXi, People's Republic of China
Correspondence e-mail: ysui@163.com

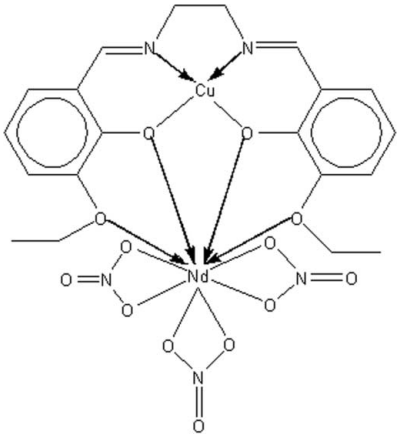
Received 28 June 2007; accepted 4 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.025; wR factor = 0.051; data-to-parameter ratio = 17.0.

In the title heteronuclear Cu^{II}–Nd^{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$\kappa^6O,O'$-neodymium(III)copper(II)), $[CuNd(C_{20}H_{22}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-ethoxysalicylidene)ethylenediamine, the Cu and Nd atoms are doubly bridged by two phenolate O atoms provided by the Schiff base ligand. The coordination of the Cu atom is square planar with the donor centers of two imine N atoms and two phenolate O atoms. The neodymium(III) center has a decacoordination environment of O atoms, involving the phenolate O atoms, two ethoxy O atoms and two O atoms each from the three nitrate ligands. Some weak C—H···O and O···Cu [O···Cu = 3.169 (3) Å] interactions generate a two-dimensional zigzag sheet.

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).



Experimental

Crystal data

$[CuNd(C_{20}H_{22}N_2O_4)(NO_3)_3]$
M_r = 748.21
Orthorhombic, $P2_12_12_1$
a = 8.6439 (16) Å
b = 13.861 (3) Å
c = 21.135 (4) Å
V = 2532.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.95 mm^{-1}
T = 293 (2) K
0.22 × 0.17 × 0.08 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.570, T_{max} = 0.794
19224 measured reflections
6179 independent reflections
4830 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.051
S = 1.01
6179 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}
Absolute structure: Flack (1983), 2611 Friedel pairs
Flack parameter: −0.008 (10)

Table 1
Selected bond lengths (Å).

Nd1—O1	2.437 (2)	Nd1—O11	2.521 (3)
Nd1—O3	2.671 (2)	Nd1—O12	2.578 (3)
Nd1—O4	2.631 (2)	O2—Cu1	1.904 (2)
Nd1—O5	2.536 (3)	O2—Nd1	2.396 (2)
Nd1—O6	2.569 (3)	Cu1—O1	1.900 (2)
Nd1—O8	2.493 (2)	Cu1—N1	1.906 (3)
Nd1—O9	2.543 (3)	Cu1—N2	1.911 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O7^{i}	0.93	2.36	3.277 (4)	168
C9—H9A···O7^{ii}	0.97	2.42	3.290 (5)	149
C20—H20A···O11	0.96	2.45	3.154 (5)	130

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$.

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 (No. 2007317), and the Natural Science Foundation of JiangXi Province (No. 0620029).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2252).

References

Baggio, R., Garland, M. T., Moreno, Y., Pena, O., Perec, M. & Spodine, E. (2000). *J. Chem. Soc. Dalton Trans.* pp. 2061–2066.

Bruker (2004). *APEX2* (Version 1.22) and *SADABS* (Version 1.22). Bruker AXS Inc., Madison, Wisconsin, USA.

Caravan, P., Ellison, J. J., McMurry, T. J. & Lauffer, R. B. (1999). *Chem. Rev.* **99**, 2293–2352.

Edder, C., Piguet, C., Bernardinelli, G., Mareda, J., Bochet, C. G., Bunzli, J.-C. G. & Hopfgartner, G. (2000). *Inorg. Chem.* **39**, 5059–5073.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Knoer, R., Lin, H.-H., Wei, H.-H. & Mohanta, S. (2005). *Inorg. Chem.* **44**, 3524–3536.

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

Sui, Y., Fang, X.-N., Xiao, Y.-A., Luo, Q.-Y. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m2230–m2232.

Westrip, S. P. (2007). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2007). E**63**, m2087-m2088 [**doi:10.1107/S1600536807032552**]

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

Y. Sui, X.-N. Fang, X.-C. Zhou, Q.-Y. Luo and Y.-P. Xu

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 hetorometallic 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 hetorometallic Schiff base complexes(Sui *et al.*, 2006), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Cu^{II}—Nd^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-ethoxysalicylidene) ethylenediamine(H_2L).

Complex (I) crystallizes in the space group $P2_12_12_1$, with copper and neodymium 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 neodymium(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 Nd1/O1/O2 is 3.63 (14)° suggesting that the bridging moiety is almost planar; the deviation of atoms from the least squares Cu1/O1/O2/Nd1 plane being −0.0308 (3)Å for Cu, −0.0211 (2)Å for Nd, 0.0256 (3)Å for O1 and 0.0262 (3)Å for O2.

The neodymium(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 neodymium to complete the decacoordination. The three kinds of Nd—O bond distances are significantly different, the shortest being the Nd—O(phenolate) and longest being the Nd—*O*(ethoxy) separations.

The coordination of copper(II) is approximately square planar. The donor centers are alternatively above and below the mean N_2O_2 plane with an average deviation from the plane of 0.0887 (2) Å, while Cu1 is 0.0395 (3)Å above this square plane.

Adjacent molecules are held together by weak interactions (O13···Cu1=3.169 (3) Å, C7—H7···$O7^{i}$=3.277 (4) and C9—H9A···$O7^{ii}$=3.290 (5); symmetry codes:(i)-*x* + 1, *y* − 1/2, 3/2 − *z*; (ii)1 + *x*, *y*, *z*). these link the molecules into a two-dimensional zigzag 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 (60 ml) under reflux for 3 h and then for another 3 h after the addition of neodymium(III) nitrate hexahydrate (0.438 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 $C_{20}H_{22}CuN_5NdO_{13}$: C 32.11, H 2.96, Cu 8.49, N 9.36,Nd 19.28%; found: C 32.00, H 2.86, Cu 8.53, N 9.47,Nd 19.30%. IR(KBr, cm^{-1}): 1642(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 (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

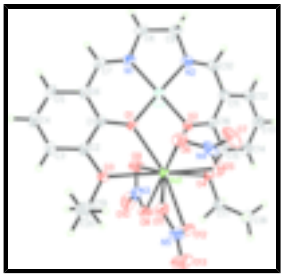


Fig.1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

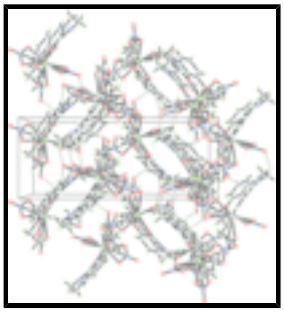


Fig.2. The packing diagram of (I), viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

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*'-\ neodymium(III)copper(II))

Crystal data

$[CuNd(C_{20}H_{22}N_2O_4)(NO_3)_3]$	F_{000} = 1480
M_r = 748.21	D_x = 1.962 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 19224 reflections
a = 8.6439 (16) Å	θ = 1.8–28.3º
b = 13.861 (3) Å	μ = 2.95 mm^{-1}
c = 21.135 (4) Å	*T* = 293 (2) K
V = 2532.4 (8) $Å^3$	Block, red
Z = 4	0.22 × 0.17 × 0.08 mm

Data collection

Bruker APEX II area-detector diffractometer	6179 independent reflections
Radiation source: fine-focus sealed tube	4830 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
Detector resolution: 0 pixels mm^{-1}	$\theta_{max} = 28.3°$
$T = 293(2)$ K	$\theta_{min} = 1.8°$
φ and ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$k = -18 \rightarrow 18$
$T_{min} = 0.570$, $T_{max} = 0.794$	$l = -28 \rightarrow 27$
19224 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.017P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.051$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
6179 reflections	$\Delta\rho_{min} = -0.85$ e Å^{-3}
363 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2611 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.008 (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}
C11	0.6447 (4)	1.1718 (2)	0.80399 (17)	0.0393 (9)
O2	0.4613 (2)	1.05648 (15)	0.84587 (10)	0.0361 (5)
C14	0.5175 (4)	1.3051 (2)	0.88820 (18)	0.0446 (9)

H14	0.4767	1.3496	0.9166	0.053*
Nd1	0.241515 (18)	0.999977 (13)	0.904190 (7)	0.03374 (5)
Cu1	0.56585 (5)	0.94407 (3)	0.81664 (2)	0.03818 (10)
O1	0.4129 (3)	0.87540 (14)	0.86294 (11)	0.0393 (6)
N3	0.3700 (4)	0.9940 (3)	1.03348 (15)	0.0519 (7)
N2	0.6995 (3)	1.0138 (2)	0.76099 (13)	0.0409 (7)
O9	0.4502 (3)	0.9690 (2)	0.98654 (12)	0.0620 (8)
N1	0.6781 (4)	0.8324 (2)	0.79083 (14)	0.0399 (8)
C1	0.4124 (4)	0.7805 (2)	0.87300 (16)	0.0325 (8)
O3	0.1882 (3)	0.81437 (15)	0.93014 (11)	0.0396 (6)
O10	0.4244 (4)	1.0009 (2)	1.08698 (13)	0.0815 (8)
C2	0.2910 (4)	0.7440 (2)	0.90989 (16)	0.0357 (8)
C7	0.6500 (4)	0.7459 (3)	0.80840 (18)	0.0413 (9)
H7	0.7161	0.6978	0.7939	0.050*
C5	0.5126 (4)	0.6185 (2)	0.86622 (18)	0.0494 (10)
H5	0.5875	0.5756	0.8519	0.059*
O8	0.2296 (3)	1.0111 (2)	1.02179 (11)	0.0565 (6)
C4	0.3961 (4)	0.5855 (2)	0.90305 (19)	0.0513 (10)
H4	0.3925	0.5205	0.9139	0.062*
C10	0.7205 (4)	1.1050 (3)	0.76113 (16)	0.0415 (8)
H10	0.7892	1.1305	0.7317	0.050*
C6	0.5231 (4)	0.7166 (2)	0.84912 (16)	0.0367 (8)
C19	0.0527 (4)	0.7830 (2)	0.96501 (17)	0.0446 (9)
H19A	0.0097	0.8375	0.9878	0.053*
H19B	0.0832	0.7348	0.9958	0.053*
O6	0.1803 (3)	0.9675 (2)	0.78716 (13)	0.0539 (8)
O5	0.1368 (3)	1.11173 (18)	0.81937 (13)	0.0523 (6)
N4	0.1369 (4)	1.0515 (3)	0.77486 (17)	0.0520 (8)
C3	0.2823 (4)	0.6474 (2)	0.92465 (17)	0.0448 (9)
H3	0.2008	0.6241	0.9489	0.054*
C8	0.8123 (4)	0.8556 (3)	0.75078 (18)	0.0478 (9)
H8A	0.8305	0.8042	0.7205	0.057*
H8B	0.9043	0.8632	0.7766	0.057*
C9	0.7763 (4)	0.9481 (3)	0.71683 (16)	0.0463 (9)
H9A	0.8710	0.9772	0.7013	0.056*
H9B	0.7093	0.9354	0.6810	0.056*
C20	−0.0682 (5)	0.7417 (3)	0.9226 (2)	0.0627 (12)
H20A	−0.1044	0.7907	0.8941	0.094*
H20B	−0.1531	0.7185	0.9476	0.094*
H20C	−0.0250	0.6892	0.8988	0.094*
O11	−0.0411 (3)	0.96243 (18)	0.88817 (13)	0.0575 (7)
O4	0.3447 (3)	1.17580 (15)	0.92475 (11)	0.0390 (6)
O13	−0.2383 (3)	1.0394 (3)	0.92662 (16)	0.0963 (11)
C16	0.5209 (4)	1.1451 (2)	0.84417 (15)	0.0334 (7)
O12	−0.0021 (3)	1.0835 (2)	0.94837 (15)	0.0706 (9)
O7	0.0968 (4)	1.0759 (2)	0.72145 (14)	0.0835 (11)
C13	0.6365 (5)	1.3318 (3)	0.84766 (19)	0.0536 (10)
H13	0.6748	1.3945	0.8492	0.064*
N5	−0.0977 (4)	1.0284 (2)	0.92122 (16)	0.0559 (9)

C15	0.4601 (4)	1.2122 (2)	0.88621 (16)	0.0352 (8)
C12	0.6984 (4)	1.2675 (3)	0.80550 (19)	0.0492 (11)
H12	0.7759	1.2872	0.7778	0.059*
C17	0.2725 (4)	1.2405 (2)	0.97093 (16)	0.0447 (9)
H17A	0.3520	1.2793	0.9910	0.054*
H17B	0.2223	1.2024	1.0035	0.054*
C18	0.1549 (5)	1.3063 (3)	0.9406 (2)	0.0595 (12)
H18A	0.2071	1.3539	0.9155	0.089*
H18B	0.0952	1.3377	0.9729	0.089*
H18C	0.0873	1.2690	0.9140	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.036 (2)	0.0354 (18)	0.047 (2)	−0.0048 (15)	0.0028 (17)	−0.0019 (18)
O2	0.0360 (12)	0.0246 (10)	0.0477 (13)	−0.0027 (10)	0.0114 (11)	−0.0024 (11)
C14	0.048 (2)	0.0276 (18)	0.058 (2)	−0.0006 (14)	−0.0061 (19)	−0.0105 (17)
Nd1	0.03385 (8)	0.02793 (7)	0.03943 (8)	0.00136 (11)	0.00417 (8)	−0.00230 (9)
Cu1	0.0381 (2)	0.02996 (18)	0.0464 (2)	0.00145 (18)	0.0109 (2)	−0.0040 (2)
O1	0.0419 (14)	0.0237 (10)	0.0523 (15)	0.0026 (10)	0.0147 (12)	0.0001 (10)
N3	0.067 (2)	0.0368 (15)	0.0518 (19)	0.001 (2)	−0.0018 (16)	0.007 (2)
N2	0.0382 (14)	0.0444 (18)	0.0401 (15)	−0.0006 (13)	0.0055 (11)	−0.0015 (15)
O9	0.0502 (15)	0.084 (2)	0.0516 (15)	0.0084 (14)	0.0009 (14)	0.0027 (14)
N1	0.0384 (17)	0.0395 (17)	0.0417 (18)	0.0031 (13)	0.0055 (14)	−0.0102 (15)
C1	0.037 (2)	0.0277 (16)	0.0329 (18)	0.0005 (14)	−0.0024 (16)	−0.0024 (15)
O3	0.0354 (13)	0.0328 (12)	0.0506 (15)	−0.0020 (10)	0.0100 (11)	0.0016 (11)
O10	0.114 (2)	0.0766 (19)	0.0540 (17)	0.012 (2)	−0.0269 (17)	−0.002 (2)
C2	0.0441 (19)	0.0260 (15)	0.0369 (18)	−0.0003 (13)	−0.0045 (16)	−0.0048 (15)
C7	0.038 (2)	0.0379 (19)	0.048 (2)	0.0122 (15)	−0.0037 (18)	−0.0101 (18)
C5	0.056 (2)	0.0292 (18)	0.063 (3)	0.0116 (16)	−0.003 (2)	−0.0040 (18)
O8	0.0605 (17)	0.0622 (17)	0.0469 (13)	0.0087 (17)	0.0071 (12)	−0.0003 (13)
C4	0.066 (3)	0.0263 (17)	0.061 (2)	0.0002 (16)	−0.012 (2)	−0.0049 (18)
C10	0.039 (2)	0.047 (2)	0.0385 (19)	−0.0080 (17)	0.0035 (16)	0.0003 (17)
C6	0.041 (2)	0.0271 (16)	0.0415 (19)	0.0031 (14)	−0.0063 (17)	−0.0028 (16)
C19	0.0379 (19)	0.0436 (19)	0.052 (2)	−0.0067 (16)	0.0101 (19)	0.0034 (18)
O6	0.0582 (18)	0.0578 (17)	0.0457 (16)	−0.0026 (13)	0.0010 (13)	−0.0126 (13)
O5	0.0603 (17)	0.0462 (14)	0.0503 (16)	−0.0021 (12)	−0.0057 (14)	0.0040 (15)
N4	0.0408 (18)	0.069 (2)	0.046 (2)	−0.0183 (19)	−0.0010 (16)	0.012 (2)
C3	0.053 (2)	0.0341 (17)	0.048 (2)	−0.0029 (16)	−0.0019 (18)	0.0059 (16)
C8	0.038 (2)	0.057 (2)	0.049 (2)	0.0061 (17)	0.0084 (18)	−0.0130 (19)
C9	0.046 (2)	0.0496 (19)	0.0436 (19)	−0.0016 (18)	0.0120 (17)	−0.0123 (18)
C20	0.057 (3)	0.052 (2)	0.079 (3)	−0.013 (2)	−0.003 (2)	0.009 (2)
O11	0.0442 (15)	0.0472 (15)	0.081 (2)	0.0035 (12)	0.0041 (14)	−0.0056 (14)
O4	0.0468 (14)	0.0273 (11)	0.0431 (14)	0.0019 (10)	0.0070 (11)	−0.0051 (11)
O13	0.0380 (16)	0.139 (3)	0.113 (3)	0.022 (2)	0.0050 (18)	−0.003 (2)
C16	0.0365 (19)	0.0275 (16)	0.0362 (17)	0.0000 (13)	−0.0041 (15)	0.0000 (15)
O12	0.0493 (18)	0.086 (2)	0.077 (2)	0.0160 (15)	0.0005 (16)	−0.0320 (19)
O7	0.087 (2)	0.115 (3)	0.0478 (16)	−0.047 (2)	−0.0185 (17)	0.0250 (19)

C13	0.055 (2)	0.0370 (19)	0.069 (3)	−0.0125 (18)	−0.001 (2)	−0.001 (2)
N5	0.0396 (19)	0.072 (3)	0.057 (2)	0.0079 (16)	0.0062 (16)	0.0123 (17)
C15	0.036 (2)	0.0303 (17)	0.0387 (19)	0.0008 (14)	−0.0041 (16)	0.0029 (15)
C12	0.044 (2)	0.0382 (19)	0.065 (3)	−0.0093 (16)	0.007 (2)	0.0051 (19)
C17	0.060 (2)	0.0344 (17)	0.0399 (19)	0.0043 (17)	0.0102 (19)	−0.0106 (15)
C18	0.063 (3)	0.044 (2)	0.071 (3)	0.0109 (19)	0.019 (2)	0.004 (2)

Geometric parameters (Å, °)

C11—C12	1.407 (5)	C5—C4	1.353 (5)
C11—C16	1.415 (5)	C5—C6	1.409 (4)
C11—C10	1.451 (5)	C5—H5	0.9300
O2—C16	1.333 (3)	C4—C3	1.383 (5)
C14—C15	1.380 (4)	C4—H4	0.9300
C14—C13	1.389 (5)	C10—H10	0.9300
C14—H14	0.9300	C19—C20	1.492 (5)
Nd1—O1	2.437 (2)	C19—H19A	0.9700
Nd1—O3	2.671 (2)	C19—H19B	0.9700
Nd1—O4	2.631 (2)	O6—N4	1.250 (4)
Nd1—O5	2.536 (3)	O5—N4	1.258 (4)
Nd1—O6	2.569 (3)	N4—O7	1.229 (4)
Nd1—O8	2.493 (2)	C3—H3	0.9300
Nd1—O9	2.543 (3)	C8—C9	1.502 (5)
Nd1—O11	2.521 (3)	C8—H8A	0.9700
Nd1—O12	2.578 (3)	C8—H8B	0.9700
O2—Cu1	1.904 (2)	C9—H9A	0.9700
O2—Nd1	2.396 (2)	C9—H9B	0.9700
Cu1—O1	1.900 (2)	C20—H20A	0.9600
Cu1—N1	1.906 (3)	C20—H20B	0.9600
Cu1—N2	1.911 (3)	C20—H20C	0.9600
O1—C1	1.333 (3)	O11—N5	1.250 (4)
N3—O10	1.228 (4)	O4—C15	1.383 (4)
N3—O9	1.259 (4)	O4—C17	1.465 (4)
N3—O8	1.261 (4)	O13—N5	1.230 (4)
N2—C10	1.278 (4)	C16—C15	1.390 (4)
N2—C9	1.463 (4)	O12—N5	1.263 (4)
N1—C7	1.280 (4)	C13—C12	1.369 (5)
N1—C8	1.472 (4)	C13—H13	0.9300
C1—C6	1.398 (4)	C12—H12	0.9300
C1—C2	1.402 (5)	C17—C18	1.509 (5)
O3—C2	1.387 (4)	C17—H17A	0.9700
O3—C19	1.450 (4)	C17—H17B	0.9700
C2—C3	1.376 (4)	C18—H18A	0.9600
C7—C6	1.452 (5)	C18—H18B	0.9600
C7—H7	0.9300	C18—H18C	0.9600
C12—C11—C16	118.8 (3)	O3—C2—C1	113.4 (3)
C12—C11—C10	117.8 (3)	N1—C7—C6	125.3 (3)
C16—C11—C10	123.3 (3)	N1—C7—H7	117.4
C16—O2—Cu1	124.18 (19)	C6—C7—H7	117.4

C16—O2—Nd1	128.46 (19)	C4—C5—C6	121.5 (3)
Cu1—O2—Nd1	106.00 (9)	C4—C5—H5	119.3
C15—C14—C13	119.8 (3)	C6—C5—H5	119.3
C15—C14—H14	120.1	N3—O8—Nd1	98.3 (2)
C13—C14—H14	120.1	C5—C4—C3	120.6 (3)
O2—Nd1—O1	64.25 (7)	C5—C4—H4	119.7
O2—Nd1—O8	121.70 (8)	C3—C4—H4	119.7
O1—Nd1—O8	115.21 (8)	N2—C10—C11	124.6 (3)
O2—Nd1—O11	140.06 (8)	N2—C10—H10	117.7
O1—Nd1—O11	113.26 (8)	C11—C10—H10	117.7
O8—Nd1—O11	96.12 (9)	C1—C6—C5	118.3 (3)
O2—Nd1—O5	73.72 (8)	C1—C6—C7	123.7 (3)
O1—Nd1—O5	113.39 (8)	C5—C6—C7	118.0 (3)
O8—Nd1—O5	130.71 (9)	O3—C19—C20	112.1 (3)
O11—Nd1—O5	71.65 (8)	O3—C19—H19A	109.2
O2—Nd1—O9	81.07 (9)	C20—C19—H19A	109.2
O1—Nd1—O9	72.18 (9)	O3—C19—H19B	109.2
O8—Nd1—O9	50.01 (8)	C20—C19—H19B	109.2
O11—Nd1—O9	138.13 (9)	H19A—C19—H19B	107.9
O5—Nd1—O9	147.13 (9)	N4—O6—Nd1	95.7 (2)
O2—Nd1—O6	74.05 (8)	N4—O5—Nd1	97.1 (2)
O1—Nd1—O6	69.91 (9)	O7—N4—O6	122.2 (4)
O8—Nd1—O6	164.25 (9)	O7—N4—O5	120.3 (4)
O11—Nd1—O6	68.60 (9)	O6—N4—O5	117.6 (3)
O5—Nd1—O6	49.68 (8)	C2—C3—C4	119.4 (3)
O9—Nd1—O6	140.84 (9)	C2—C3—H3	120.3
O2—Nd1—O12	133.41 (9)	C4—C3—H3	120.3
O1—Nd1—O12	160.81 (9)	N1—C8—C9	107.3 (3)
O8—Nd1—O12	64.99 (9)	N1—C8—H8A	110.3
O11—Nd1—O12	49.43 (9)	C9—C8—H8A	110.3
O5—Nd1—O12	71.96 (10)	N1—C8—H8B	110.3
O9—Nd1—O12	114.04 (9)	C9—C8—H8B	110.3
O6—Nd1—O12	105.02 (10)	H8A—C8—H8B	108.5
O2—Nd1—O4	60.89 (7)	N2—C9—C8	108.7 (3)
O1—Nd1—O4	120.62 (7)	N2—C9—H9A	110.0
O8—Nd1—O4	77.98 (8)	C8—C9—H9A	110.0
O11—Nd1—O4	122.82 (8)	N2—C9—H9B	110.0
O5—Nd1—O4	70.86 (8)	C8—C9—H9B	110.0
O9—Nd1—O4	78.62 (8)	H9A—C9—H9B	108.3
O6—Nd1—O4	113.02 (8)	C19—C20—H20A	109.5
O12—Nd1—O4	78.54 (9)	C19—C20—H20B	109.5
O2—Nd1—O3	123.87 (7)	H20A—C20—H20B	109.5
O1—Nd1—O3	59.71 (7)	C19—C20—H20C	109.5
O8—Nd1—O3	81.25 (8)	H20A—C20—H20C	109.5
O11—Nd1—O3	70.21 (8)	H20B—C20—H20C	109.5
O5—Nd1—O3	132.22 (8)	N5—O11—Nd1	98.8 (2)
O9—Nd1—O3	79.59 (8)	C15—O4—C17	118.4 (2)
O6—Nd1—O3	89.63 (8)	C15—O4—Nd1	119.02 (18)
O12—Nd1—O3	102.54 (9)	C17—O4—Nd1	122.19 (19)

O4—Nd1—O3	156.47 (8)	O2—C16—C15	117.0 (3)
O1—Cu1—O2	84.99 (9)	O2—C16—C11	123.3 (3)
O1—Cu1—N1	95.44 (11)	C15—C16—C11	119.7 (3)
O2—Cu1—N1	177.03 (12)	N5—O12—Nd1	95.7 (2)
O1—Cu1—N2	172.22 (12)	C12—C13—C14	121.1 (3)
O2—Cu1—N2	94.18 (11)	C12—C13—H13	119.4
N1—Cu1—N2	85.79 (13)	C14—C13—H13	119.4
C1—O1—Cu1	125.4 (2)	O13—N5—O11	122.0 (4)
C1—O1—Nd1	129.8 (2)	O13—N5—O12	121.9 (4)
Cu1—O1—Nd1	104.61 (8)	O11—N5—O12	116.1 (3)
O10—N3—O9	122.4 (3)	C14—C15—O4	125.6 (3)
O10—N3—O8	122.3 (3)	C14—C15—C16	120.5 (3)
O9—N3—O8	115.3 (3)	O4—C15—C16	113.9 (3)
C10—N2—C9	123.6 (3)	C13—C12—C11	120.0 (4)
C10—N2—Cu1	125.8 (3)	C13—C12—H12	120.0
C9—N2—Cu1	110.6 (2)	C11—C12—H12	120.0
N3—O9—Nd1	95.9 (2)	O4—C17—C18	111.9 (3)
C7—N1—C8	121.4 (3)	O4—C17—H17A	109.2
C7—N1—Cu1	125.6 (3)	C18—C17—H17A	109.2
C8—N1—Cu1	112.9 (2)	O4—C17—H17B	109.2
O1—C1—C6	124.4 (3)	C18—C17—H17B	109.2
O1—C1—C2	116.6 (3)	H17A—C17—H17B	107.9
C6—C1—C2	119.0 (3)	C17—C18—H18A	109.5
C2—O3—C19	117.6 (2)	C17—C18—H18B	109.5
C2—O3—Nd1	120.25 (18)	H18A—C18—H18B	109.5
C19—O3—Nd1	122.16 (18)	C17—C18—H18C	109.5
C3—C2—O3	125.4 (3)	H18A—C18—H18C	109.5
C3—C2—C1	121.2 (3)	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O7^{i}	0.93	2.36	3.277 (4)	168
C9—H9A···O7^{ii}	0.97	2.42	3.290 (5)	149
C20—H20A···O11	0.96	2.45	3.154 (5)	130

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) *x*+1, *y*, *z*.

Fig. 1

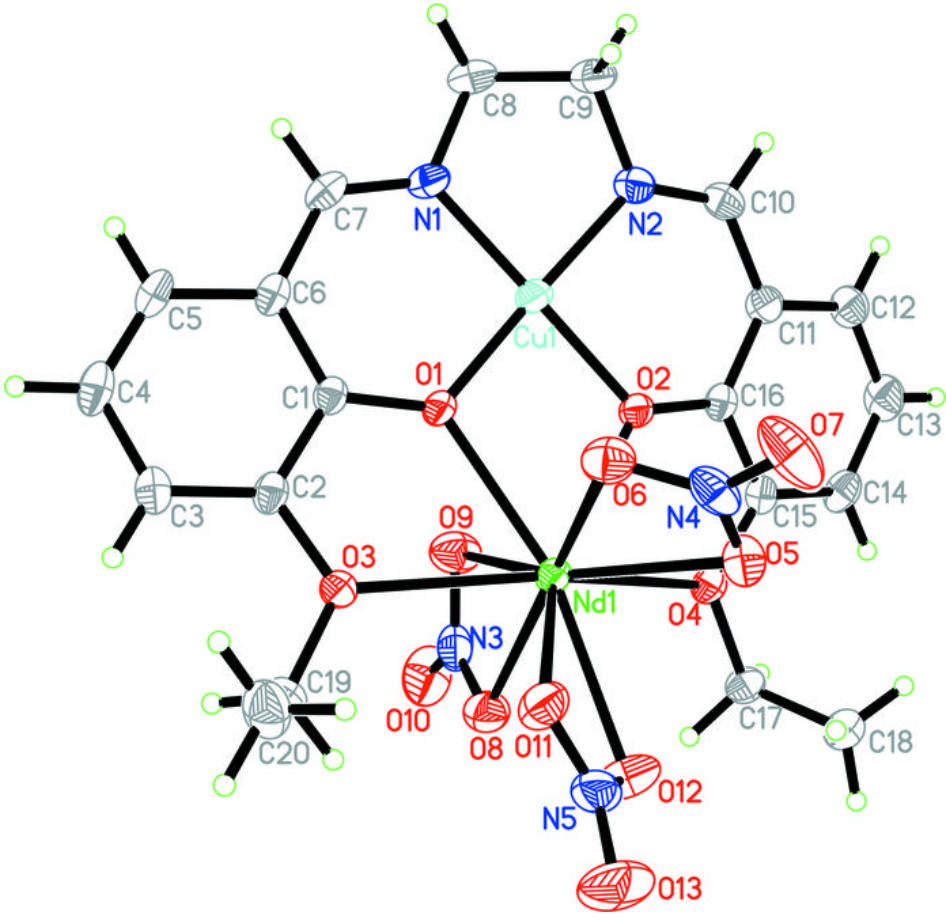

C8
C9
C7
N1
N2
C10
C6
C5
Cu1
C11
C12
C4
C1
O1
O2
C16
C13
O7
C2
C3
O6
N4
C15
C14
O9
O3
O5
Nd1
O4
N3
C19
O10
O8
O11
C17
C18
C20
O12
N5
O13

Fig. 2