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[μ-*N*,*N*′-Bis(3-ethoxy-2-oxidobenzylidene)propane-1,2-diamine](methanol)trinitratocopper(II)neodymium(III)

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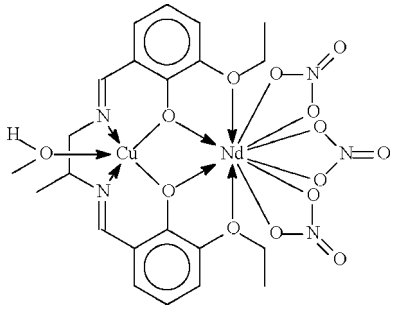
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.013 Å; disorder in main residue; R factor = 0.052; wR factor = 0.154; data-to-parameter ratio = 16.8.

The Cu atom in the title compound (systematic name: {6,6′-diethoxy-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1κ^4O^1,$O^{1'}$,O^6,$O^{6'}$:2κ^4O^1,N,N',$O^{1'}$}(methanol-2κO)trinitrato-1κ^6O,O'-copper(II)neodymium(III)), [CuNd($C_{21}H_{22}N_2O_4$)(NO_3)$_3$(CH_4O)], 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 ($C_{21}H_{24}N_2O_4$)(CH_4O)Cu unit uses the two ethoxy and two hydroxy O atoms to chelate the (NO_3)$_3$Nd unit. The Cu^{II} atom exists in a square-pyramidal geometry and the Nd^{III} atom in a bicapped square-antiprismatic geometry. Molecules are linked by O—H···O hydrogen bonds into a linear chain along the b axis. Some C and H atoms of the Schiff base are disordered equally over two positions.

Related literature

For the isostructural lutetium compound, see Sui *et al.* (2007).



Experimental

Crystal data

[CuNd($C_{21}H_{22}N_2O_4$)(NO_3)$_3$(CH_4O)]
M_r = 794.27
Monoclinic, $P2_1/c$
a = 9.2004 (4) Å
b = 20.5069 (8) Å
c = 15.6901 (6) Å
β = 93.111 (1)°
V = 2955.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.53 mm^{-1}
T = 295 (2) K
0.34 × 0.13 × 0.11 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.426, T_{max} = 0.768
21321 measured reflections
6644 independent reflections
5212 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.154
S = 1.14
6644 reflections
395 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected bond lengths (Å).

Nd1—O1	2.641 (5)	Nd1—O12	2.600 (6)
Nd1—O2	2.408 (5)	Nd1—O13	2.567 (6)
Nd1—O3	2.424 (5)	Cu1—O2	1.899 (5)
Nd1—O4	2.666 (5)	Cu1—O3	1.918 (5)
Nd1—O6	2.511 (7)	Cu1—O5	2.351 (7)
Nd1—O7	2.545 (7)	Cu1—N1	1.925 (7)
Nd1—O9	2.530 (7)	Cu1—N2	1.918 (7)
Nd1—O10	2.487 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*o*···O14^{i}	0.82	2.08	2.89 (1)	165

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: CI2405).

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Bruker (2004). *APEX2* (Version 1.22) and *SAINT* (Version 7.06A). Bruker AXS Inc., Madison, Winconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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Westrip, S. P. (2007). *publCIF*. In preparation.

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supplementary materials

Acta Cryst. (2007). E**63**, m2122 [**doi:10.1107/S1600536807033247**]

[μ-*N*,*N*'-Bis(3-ethoxy-2-oxidobenzylidene)propane-1,2-diamine](methanol)trinitratocopper(II)neodymium(III)

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

Comment

The isostructural lutetium compound is described in the preceding report (Sui *et al.*, 2007).

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. Neodymium nitrate hexahydrate (0.44 g, 1 mmol) was added and then 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 1.2 Å from O6.

Figures

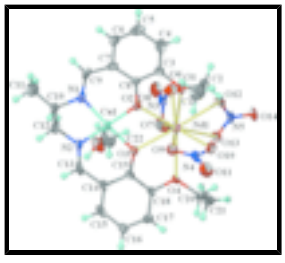


Fig. 1. Displacement ellipsoid plot of [$CuNd(C_{21}H_{22}N_2O_4)(CH_4O)(NO_3)_3$]; ellipsoids are drawn at the 30% probabilty level, and H atoms are shown as spheres of arbitrary radius. Only one disorder component is shown.

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

Crystal data

$[CuNd(C_{21}H_{22}N_2O_4)(NO_3)_3(CH_4O)]$	F_{000} = 1584
M_r = 794.27	D_x = 1.785 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8519 reflections
a = 9.2004 (4) Å	θ = 2.2–27.4º
b = 20.5069 (8) Å	μ = 2.53 mm^{-1}
c = 15.6901 (6) Å	T = 295 (2) K
β = 93.111 (1)º	Block, red
V = 2955.9 (2) Å^3	0.34 × 0.13 × 0.11 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	6644 independent reflections
Radiation source: fine-focus sealed tube	5212 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.426, T_{max} = 0.768	k = −26→26
21321 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
$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters constrained
$wR(F^2)$ = 0.154	$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 17.0691P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.14	$(\Delta/\sigma)_{max}$ = 0.001
6644 reflections	$\Delta\rho_{max}$ = 1.04 e Å^{-3}
395 parameters	$\Delta\rho_{min}$ = −0.68 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)
Nd1	0.36649 (4)	0.341072 (17)	0.25006 (3)	0.04394 (13)	
Cu1	0.33005 (10)	0.50577 (4)	0.29959 (6)	0.0486 (2)	
O1	0.1453 (6)	0.3478 (2)	0.1359 (4)	0.0575 (14)	
O2	0.2273 (6)	0.4403 (2)	0.2355 (4)	0.0578 (14)	
O3	0.4766 (6)	0.4393 (2)	0.3103 (4)	0.0562 (14)	
O4	0.6487 (5)	0.3420 (2)	0.2987 (4)	0.0523 (12)	
O5	0.4301 (11)	0.5592 (4)	0.1838 (5)	0.118 (3)	
H5O	0.4926	0.5868	0.1952	0.141*	
O6	0.1577 (8)	0.3228 (5)	0.3439 (5)	0.096 (2)	
O7	0.3543 (9)	0.3409 (5)	0.4117 (5)	0.105 (3)	
O8	0.1590 (10)	0.3344 (3)	0.4808 (5)	0.095 (2)	
O9	0.4799 (8)	0.3825 (3)	0.1171 (4)	0.0774 (18)	
O10	0.4850 (8)	0.2788 (3)	0.1368 (4)	0.0755 (18)	
O11	0.6037 (12)	0.3199 (5)	0.0342 (6)	0.127 (3)	
O12	0.2348 (7)	0.2302 (3)	0.2231 (5)	0.0765 (19)	
O13	0.4328 (7)	0.2252 (3)	0.3004 (4)	0.0702 (17)	
O14	0.3190 (8)	0.1367 (3)	0.2636 (5)	0.090 (2)	
N1	0.1700 (8)	0.5660 (3)	0.3028 (5)	0.066 (2)	
N2	0.4296 (8)	0.5647 (3)	0.3777 (5)	0.0597 (17)	
N3	0.2211 (10)	0.3338 (3)	0.4139 (5)	0.0647 (19)	
N4	0.5249 (10)	0.3268 (4)	0.0932 (5)	0.076 (2)	
N5	0.3294 (8)	0.1962 (3)	0.2621 (5)	0.0582 (17)	
C1	0.1630 (14)	0.3442 (6)	−0.0207 (7)	0.101 (4)	
H1A	0.1443	0.3168	−0.0697	0.152*	
H1B	0.2632	0.3575	−0.0179	0.152*	
H1C	0.1017	0.3820	−0.0254	0.152*	
C2	0.1310 (11)	0.3065 (4)	0.0602 (6)	0.068 (2)	
H2A	0.0330	0.2891	0.0545	0.082*	
H2B	0.1979	0.2701	0.0669	0.082*	
C3	0.0446 (9)	0.3977 (4)	0.1433 (5)	0.0556 (19)	
C4	−0.0931 (11)	0.3986 (5)	0.1044 (7)	0.079 (3)	
H4	−0.1254	0.3647	0.0688	0.095*	
C5	−0.1829 (11)	0.4514 (6)	0.1196 (7)	0.084 (3)	
H5	−0.2765	0.4527	0.0941	0.101*	
C6	−0.1359 (10)	0.5010 (5)	0.1708 (7)	0.071 (3)	
H6	−0.1992	0.5352	0.1804	0.086*	
C7	0.0062 (8)	0.5027 (4)	0.2104 (6)	0.0553 (19)	
C8	0.0942 (8)	0.4479 (3)	0.1983 (5)	0.0496 (17)	
C9	0.0431 (11)	0.5567 (4)	0.2632 (6)	0.072 (3)	
H9	−0.0284	0.5880	0.2703	0.086*	
C10	0.2181 (17)	0.6309 (6)	0.3334 (14)	0.074 (5)	0.50
H10	0.2650	0.6545	0.2880	0.089*	0.50
C10'	0.195 (2)	0.6127 (7)	0.3723 (10)	0.074 (5)	0.50
H10'	0.1631	0.5889	0.4222	0.089*	0.50
C11	0.1042 (13)	0.6729 (5)	0.3711 (9)	0.108 (4)	

H11A	0.1491	0.7114	0.3954	0.162*	0.50
H11B	0.0581	0.6491	0.4149	0.162*	0.50
H11C	0.0325	0.6852	0.3273	0.162*	0.50
H11D	0.0031	0.6621	0.3614	0.162*	0.50
H11E	0.1181	0.6956	0.4245	0.162*	0.50
H11F	0.1342	0.7004	0.3257	0.162*	0.50
C12	0.328 (3)	0.6143 (14)	0.405 (2)	0.096 (7)	0.50
H12A	0.3810	0.6533	0.4219	0.116*	0.50
H12B	0.2775	0.5985	0.4532	0.116*	0.50
C12'	0.353 (2)	0.6253 (11)	0.395 (3)	0.096 (7)	0.50
H12C	0.3885	0.6605	0.3599	0.116*	0.50
H12D	0.3674	0.6374	0.4542	0.116*	0.50
C13	0.5624 (10)	0.5605 (4)	0.4056 (5)	0.062 (2)	
H13	0.6008	0.5944	0.4391	0.074*	
C14	0.6573 (10)	0.5057 (4)	0.3882 (5)	0.058 (2)	
C15	0.8015 (10)	0.5096 (4)	0.4202 (6)	0.066 (2)	
H15	0.8330	0.5468	0.4497	0.079*	
C16	0.8963 (10)	0.4605 (4)	0.4093 (6)	0.066 (2)	
H16	0.9930	0.4652	0.4289	0.079*	
C17	0.8515 (8)	0.4033 (4)	0.3693 (5)	0.0566 (19)	
H17	0.9168	0.3693	0.3627	0.068*	
C18	0.7074 (9)	0.3974 (4)	0.3391 (5)	0.0501 (18)	
C19	0.6091 (8)	0.4481 (3)	0.3459 (5)	0.0471 (16)	
C20	0.7444 (9)	0.2873 (4)	0.2865 (6)	0.063 (2)	
H20A	0.8360	0.3034	0.2671	0.075*	
H20B	0.7012	0.2593	0.2423	0.075*	
C21	0.7736 (12)	0.2480 (5)	0.3661 (7)	0.087 (3)	
H21A	0.7747	0.2025	0.3518	0.130*	
H21B	0.6986	0.2561	0.4049	0.130*	
H21C	0.8662	0.2602	0.3924	0.130*	
C22	0.3945 (19)	0.5487 (7)	0.1005 (8)	0.131 (6)	
H22A	0.4779	0.5565	0.0678	0.196*	
H22B	0.3173	0.5777	0.0819	0.196*	
H22C	0.3629	0.5044	0.0926	0.196*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.0452 (2)	0.03140 (19)	0.0547 (2)	0.00066 (16)	−0.00207 (16)	−0.00479 (16)
Cu1	0.0533 (5)	0.0312 (4)	0.0611 (6)	0.0019 (4)	0.0023 (4)	−0.0057 (4)
O1	0.059 (3)	0.046 (3)	0.066 (3)	0.000 (2)	−0.013 (3)	−0.008 (2)
O2	0.053 (3)	0.038 (3)	0.081 (4)	0.009 (2)	−0.013 (3)	−0.009 (3)
O3	0.050 (3)	0.039 (3)	0.078 (4)	0.007 (2)	−0.018 (3)	−0.015 (2)
O4	0.045 (3)	0.041 (3)	0.070 (3)	−0.002 (2)	−0.003 (2)	−0.011 (2)
O5	0.164 (9)	0.118 (7)	0.074 (5)	−0.075 (6)	0.033 (5)	−0.004 (5)
O6	0.067 (4)	0.156 (8)	0.066 (4)	0.019 (5)	0.007 (4)	0.006 (5)
O7	0.085 (6)	0.162 (9)	0.066 (4)	−0.037 (5)	−0.002 (4)	−0.010 (5)
O8	0.136 (7)	0.077 (5)	0.078 (5)	−0.009 (4)	0.045 (5)	0.002 (4)

O9	0.088 (5)	0.064 (4)	0.081 (4)	−0.002 (3)	0.017 (4)	0.012 (3)
O10	0.098 (5)	0.058 (4)	0.072 (4)	0.000 (3)	0.020 (4)	−0.008 (3)
O11	0.156 (9)	0.129 (7)	0.102 (6)	−0.027 (6)	0.074 (6)	−0.020 (5)
O12	0.064 (4)	0.049 (3)	0.114 (5)	−0.006 (3)	−0.019 (4)	0.006 (3)
O13	0.059 (4)	0.051 (3)	0.098 (5)	−0.008 (3)	−0.018 (3)	0.010 (3)
O14	0.103 (5)	0.031 (3)	0.137 (7)	−0.012 (3)	0.013 (5)	−0.002 (3)
N1	0.059 (5)	0.042 (4)	0.098 (6)	0.013 (3)	−0.001 (4)	−0.010 (4)
N2	0.071 (5)	0.042 (3)	0.067 (4)	0.001 (3)	0.002 (4)	−0.013 (3)
N3	0.090 (6)	0.042 (4)	0.063 (5)	0.000 (4)	0.017 (4)	−0.003 (3)
N4	0.083 (6)	0.082 (6)	0.063 (5)	−0.011 (5)	0.012 (4)	−0.008 (4)
N5	0.068 (5)	0.034 (3)	0.074 (5)	−0.007 (3)	0.017 (4)	−0.002 (3)
C1	0.111 (10)	0.126 (11)	0.066 (7)	−0.008 (8)	0.001 (6)	−0.001 (7)
C2	0.076 (6)	0.055 (5)	0.070 (6)	−0.001 (4)	−0.018 (5)	−0.014 (4)
C3	0.051 (5)	0.049 (4)	0.066 (5)	0.007 (3)	−0.002 (4)	0.005 (4)
C4	0.078 (7)	0.073 (6)	0.084 (7)	0.009 (5)	−0.021 (5)	0.000 (5)
C5	0.056 (6)	0.099 (8)	0.096 (8)	0.021 (6)	−0.012 (5)	0.010 (6)
C6	0.048 (5)	0.062 (5)	0.102 (7)	0.007 (4)	−0.006 (5)	0.008 (5)
C7	0.036 (4)	0.055 (5)	0.074 (5)	0.018 (3)	−0.006 (4)	0.009 (4)
C8	0.040 (4)	0.040 (4)	0.069 (5)	0.002 (3)	0.000 (3)	0.009 (3)
C9	0.078 (7)	0.051 (5)	0.089 (7)	0.027 (5)	0.023 (5)	0.004 (4)
C10	0.102 (11)	0.030 (7)	0.091 (14)	0.014 (7)	0.016 (10)	−0.004 (7)
C10'	0.102 (11)	0.030 (7)	0.091 (14)	0.014 (7)	0.016 (10)	−0.004 (7)
C11	0.100 (9)	0.075 (7)	0.151 (12)	0.020 (7)	0.013 (8)	−0.012 (7)
C12	0.072 (10)	0.065 (9)	0.149 (13)	0.015 (8)	−0.016 (9)	−0.058 (9)
C12'	0.072 (10)	0.065 (9)	0.149 (13)	0.015 (8)	−0.016 (9)	−0.058 (9)
C13	0.078 (6)	0.045 (4)	0.061 (5)	−0.007 (4)	−0.011 (4)	−0.016 (4)
C14	0.075 (6)	0.043 (4)	0.055 (4)	−0.005 (4)	−0.004 (4)	−0.002 (3)
C15	0.075 (6)	0.060 (5)	0.061 (5)	−0.024 (5)	−0.015 (4)	−0.006 (4)
C16	0.051 (5)	0.067 (6)	0.078 (6)	−0.008 (4)	−0.015 (4)	−0.006 (4)
C17	0.038 (4)	0.063 (5)	0.068 (5)	0.003 (3)	−0.005 (4)	−0.001 (4)
C18	0.058 (5)	0.045 (4)	0.047 (4)	−0.011 (3)	−0.002 (3)	−0.005 (3)
C19	0.046 (4)	0.042 (4)	0.053 (4)	−0.003 (3)	−0.004 (3)	−0.003 (3)
C20	0.050 (5)	0.055 (5)	0.082 (6)	0.011 (4)	−0.006 (4)	−0.012 (4)
C21	0.079 (7)	0.070 (6)	0.108 (8)	0.000 (5)	−0.013 (6)	0.012 (6)
C22	0.195 (17)	0.123 (11)	0.078 (8)	−0.026 (11)	0.042 (9)	0.018 (8)

Geometric parameters (Å, °)

Nd1—O1	2.641 (5)	C4—C5	1.390 (14)
Nd1—O2	2.408 (5)	C4—H4	0.93
Nd1—O3	2.424 (5)	C5—C6	1.351 (14)
Nd1—O4	2.666 (5)	C5—H5	0.93
Nd1—O6	2.511 (7)	C6—C7	1.417 (11)
Nd1—O7	2.545 (7)	C6—H6	0.93
Nd1—O9	2.530 (7)	C7—C8	1.404 (10)
Nd1—O10	2.487 (6)	C7—C9	1.414 (13)
Nd1—O12	2.600 (6)	C9—H9	0.93
Nd1—O13	2.567 (6)	C10—C11	1.504 (10)
Cu1—O2	1.899 (5)	C10—C12	1.502 (10)

Cu1—O3	1.918 (5)	C10—H10	0.98
Cu1—O5	2.351 (7)	C10'—C11	1.492 (9)
Cu1—N1	1.925 (7)	C10'—C12'	1.499 (10)
Cu1—N2	1.918 (7)	C10'—H10'	0.98
O1—C3	1.389 (9)	C11—H11A	0.96
O1—C2	1.459 (9)	C11—H11B	0.96
O2—C8	1.336 (9)	C11—H11C	0.96
O3—C19	1.326 (9)	C11—H11D	0.96
O4—C18	1.397 (8)	C11—H11E	0.96
O4—C20	1.444 (9)	C11—H11F	0.96
O5—C22	1.347 (14)	C12—H12A	0.97
O5—H5O	0.8200	C12—H12B	0.97
O6—N3	1.236 (10)	C12'—H12C	0.97
O7—N3	1.236 (10)	C12'—H12D	0.97
O8—N3	1.221 (9)	C13—C14	1.458 (12)
O9—N4	1.279 (10)	C13—H13	0.93
O10—N4	1.264 (10)	C14—C15	1.396 (12)
O11—N4	1.215 (11)	C14—C19	1.414 (10)
O12—N5	1.249 (9)	C15—C16	1.349 (13)
O13—N5	1.248 (9)	C15—H15	0.93
O14—N5	1.225 (8)	C16—C17	1.382 (12)
N1—C9	1.306 (12)	C16—H16	0.93
N1—C10'	1.460 (9)	C17—C18	1.389 (11)
N1—C10	1.474 (9)	C17—H17	0.93
N2—C13	1.278 (11)	C18—C19	1.385 (11)
N2—C12'	1.461 (10)	C20—C21	1.498 (13)
N2—C12	1.461 (10)	C20—H20A	0.97
C1—C2	1.528 (14)	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—C4	1.377 (12)	C22—H22C	0.96
C3—C8	1.404 (11)		
O2—Nd1—O3	62.85 (17)	O1—C2—H2A	109.3
O2—Nd1—O10	128.1 (2)	C1—C2—H2A	109.3
O3—Nd1—O10	121.0 (2)	O1—C2—H2B	109.3
O2—Nd1—O6	76.2 (2)	C1—C2—H2B	109.3
O3—Nd1—O6	102.2 (3)	H2A—C2—H2B	107.9
O10—Nd1—O6	136.2 (3)	C4—C3—O1	125.1 (8)
O2—Nd1—O9	83.0 (2)	C4—C3—C8	121.5 (8)
O3—Nd1—O9	81.9 (2)	O1—C3—C8	113.3 (7)
O10—Nd1—O9	50.7 (2)	C3—C4—C5	118.4 (10)
O6—Nd1—O9	153.7 (2)	C3—C4—H4	120.8
O2—Nd1—O7	92.5 (3)	C5—C4—H4	120.8
O3—Nd1—O7	69.7 (2)	C6—C5—C4	120.9 (9)
O10—Nd1—O7	139.1 (3)	C6—C5—H5	119.6
O6—Nd1—O7	48.6 (2)	C4—C5—H5	119.6

O9—Nd1—O7	149.8 (2)	C5—C6—C7	122.5 (9)
O2—Nd1—O13	158.0 (2)	C5—C6—H6	118.7
O3—Nd1—O13	124.21 (18)	C7—C6—H6	118.7
O10—Nd1—O13	68.8 (2)	C8—C7—C6	116.5 (8)
O6—Nd1—O13	81.8 (3)	C8—C7—C9	125.8 (7)
O9—Nd1—O13	117.6 (2)	C6—C7—C9	117.6 (8)
O7—Nd1—O13	73.4 (3)	O2—C8—C3	116.2 (7)
O2—Nd1—O12	118.85 (19)	O2—C8—C7	123.8 (7)
O3—Nd1—O12	166.3 (2)	C3—C8—C7	120.0 (7)
O10—Nd1—O12	69.7 (2)	N1—C9—C7	124.9 (7)
O6—Nd1—O12	66.4 (3)	N1—C9—H9	117.5
O9—Nd1—O12	111.7 (2)	C7—C9—H9	117.5
O7—Nd1—O12	96.6 (3)	N1—C10—C11	116.3 (11)
O13—Nd1—O12	48.82 (19)	N1—C10—C12	102.5 (16)
O2—Nd1—O1	60.35 (17)	C11—C10—C12	106.9 (12)
O3—Nd1—O1	120.77 (16)	N1—C10—H10	110.3
O10—Nd1—O1	83.9 (2)	C11—C10—H10	110.3
O6—Nd1—O1	79.6 (2)	C12—C10—H10	110.3
O9—Nd1—O1	76.1 (2)	N1—C10'—C11	117.9 (11)
O7—Nd1—O1	127.0 (2)	N1—C10'—C12'	113.6 (16)
O13—Nd1—O1	114.73 (17)	C11—C10'—C12'	113.2 (12)
O12—Nd1—O1	66.42 (18)	N1—C10'—H10'	103.2
O2—Nd1—O4	121.74 (16)	C11—C10'—H10'	103.2
O3—Nd1—O4	60.19 (16)	C12'—C10'—H10'	103.2
O10—Nd1—O4	75.5 (2)	C10—C11—H11A	109.5
O6—Nd1—O4	126.6 (2)	C10—C11—H11B	109.5
O9—Nd1—O4	78.2 (2)	H11A—C11—H11B	109.5
O7—Nd1—O4	79.0 (2)	C10—C11—H11C	109.5
O13—Nd1—O4	72.95 (17)	H11A—C11—H11C	109.5
O12—Nd1—O4	119.37 (17)	H11B—C11—H11C	109.5
O1—Nd1—O4	153.69 (19)	C10'—C11—H11D	110.3
O2—Cu1—O3	82.6 (2)	C10'—C11—H11E	110.0
O2—Cu1—N2	172.2 (3)	H11D—C11—H11E	109.5
O3—Cu1—N2	94.7 (3)	C10'—C11—H11F	108.1
O2—Cu1—N1	96.2 (3)	H11D—C11—H11F	109.5
O3—Cu1—N1	171.4 (3)	H11E—C11—H11F	109.5
N2—Cu1—N1	85.3 (3)	N2—C12—C10	111.0 (15)
O2—Cu1—O5	97.2 (3)	N2—C12—H12A	109.4
O3—Cu1—O5	95.5 (3)	C10—C12—H12A	109.4
N2—Cu1—O5	90.4 (3)	N2—C12—H12B	109.4
N1—Cu1—O5	93.1 (4)	C10—C12—H12B	109.4
C3—O1—C2	117.7 (6)	H12A—C12—H12B	108.0
C3—O1—Nd1	118.3 (4)	N2—C12'—C10'	106.3 (14)
C2—O1—Nd1	123.7 (5)	N2—C12'—H12C	110.5
C8—O2—Cu1	124.5 (5)	C10'—C12'—H12C	110.5
C8—O2—Nd1	127.6 (4)	N2—C12'—H12D	110.5
Cu1—O2—Nd1	107.5 (2)	C10'—C12'—H12D	110.5
C19—O3—Cu1	124.5 (4)	H12C—C12'—H12D	108.7
C19—O3—Nd1	129.2 (4)	N2—C13—C14	124.0 (7)

Cu1—O3—Nd1	106.2 (2)	N2—C13—H13	118.0
C18—O4—C20	117.9 (6)	C14—C13—H13	118.0
C18—O4—Nd1	118.8 (4)	C15—C14—C19	119.0 (8)
C20—O4—Nd1	123.2 (4)	C15—C14—C13	117.1 (7)
C22—O5—Cu1	126.2 (8)	C19—C14—C13	123.8 (8)
C22—O5—H5O	116.9	C16—C15—C14	121.3 (8)
Cu1—O5—H5O	116.9	C16—C15—H15	119.3
N3—O6—Nd1	98.9 (6)	C14—C15—H15	119.3
N3—O7—Nd1	97.2 (5)	C15—C16—C17	120.8 (8)
N4—O9—Nd1	95.5 (5)	C15—C16—H16	119.6
N4—O10—Nd1	98.0 (5)	C17—C16—H16	119.6
N5—O12—Nd1	95.8 (4)	C16—C17—C18	119.0 (8)
N5—O13—Nd1	97.5 (4)	C16—C17—H17	120.5
C9—N1—C10'	123.5 (10)	C18—C17—H17	120.5
C9—N1—C10	122.1 (10)	C19—C18—C17	121.6 (7)
C9—N1—Cu1	124.0 (6)	C19—C18—O4	114.1 (6)
C10'—N1—Cu1	110.5 (7)	C17—C18—O4	124.3 (7)
C10—N1—Cu1	111.8 (7)	O3—C19—C18	117.1 (6)
C13—N2—C12'	117.2 (11)	O3—C19—C14	124.7 (7)
C13—N2—C12	124.4 (12)	C18—C19—C14	118.3 (7)
C13—N2—Cu1	126.2 (5)	O4—C20—C21	113.0 (8)
C12'—N2—Cu1	115.7 (11)	O4—C20—H20A	109.0
C12—N2—Cu1	109.3 (11)	C21—C20—H20A	109.0
O8—N3—O7	122.2 (9)	O4—C20—H20B	109.0
O8—N3—O6	123.0 (9)	C21—C20—H20B	109.0
O7—N3—O6	114.7 (8)	H20A—C20—H20B	107.8
O11—N4—O10	121.7 (9)	C20—C21—H21A	109.5
O11—N4—O9	123.0 (9)	C20—C21—H21B	109.5
O10—N4—O9	115.3 (8)	H21A—C21—H21B	109.5
O14—N5—O13	121.6 (8)	C20—C21—H21C	109.5
O14—N5—O12	120.8 (8)	H21A—C21—H21C	109.5
O13—N5—O12	117.6 (6)	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	111.7 (8)		
O2—Nd1—O1—C3	−16.6 (5)	O6—Nd1—O12—N5	−103.0 (5)
O3—Nd1—O1—C3	−34.8 (6)	O9—Nd1—O12—N5	105.4 (5)
O10—Nd1—O1—C3	−157.5 (6)	O7—Nd1—O12—N5	−64.0 (5)
O6—Nd1—O1—C3	63.3 (6)	O13—Nd1—O12—N5	−2.9 (5)
O9—Nd1—O1—C3	−106.5 (6)	O1—Nd1—O12—N5	168.4 (6)
O7—Nd1—O1—C3	51.9 (6)	O4—Nd1—O12—N5	17.1 (6)
O13—Nd1—O1—C3	139.3 (5)	O2—Nd1—O13—N5	65.8 (8)
O12—Nd1—O1—C3	132.0 (6)	O3—Nd1—O13—N5	168.0 (4)
O4—Nd1—O1—C3	−119.0 (6)	O10—Nd1—O13—N5	−78.2 (5)
O2—Nd1—O1—C2	156.5 (7)	O6—Nd1—O13—N5	68.7 (5)

O3—Nd1—O1—C2	138.3 (6)	O9—Nd1—O13—N5	−92.6 (5)
O10—Nd1—O1—C2	15.6 (6)	O7—Nd1—O13—N5	117.8 (5)
O6—Nd1—O1—C2	−123.6 (6)	O12—Nd1—O13—N5	2.9 (5)
O9—Nd1—O1—C2	66.6 (6)	O1—Nd1—O13—N5	−5.9 (6)
O7—Nd1—O1—C2	−135.0 (6)	O4—Nd1—O13—N5	−158.9 (5)
O13—Nd1—O1—C2	−47.7 (6)	O2—Cu1—N1—C9	−4.2 (8)
O12—Nd1—O1—C2	−54.9 (6)	N2—Cu1—N1—C9	−176.5 (8)
O4—Nd1—O1—C2	54.1 (7)	O5—Cu1—N1—C9	93.3 (8)
O3—Cu1—O2—C8	−179.4 (7)	O2—Cu1—N1—C10'	160.1 (11)
N1—Cu1—O2—C8	9.1 (7)	N2—Cu1—N1—C10'	−12.2 (11)
O5—Cu1—O2—C8	−84.8 (7)	O5—Cu1—N1—C10'	−102.4 (11)
O3—Cu1—O2—Nd1	7.6 (3)	O2—Cu1—N1—C10	−167.9 (10)
N1—Cu1—O2—Nd1	−163.9 (3)	N2—Cu1—N1—C10	19.8 (11)
O5—Cu1—O2—Nd1	102.3 (3)	O5—Cu1—N1—C10	−70.3 (11)
O3—Nd1—O2—C8	−179.4 (7)	O3—Cu1—N2—C13	13.7 (8)
O10—Nd1—O2—C8	71.1 (7)	N1—Cu1—N2—C13	−174.8 (8)
O6—Nd1—O2—C8	−67.6 (6)	O5—Cu1—N2—C13	−81.8 (8)
O9—Nd1—O2—C8	96.1 (6)	O3—Cu1—N2—C12	−163.5 (17)
O7—Nd1—O2—C8	−113.8 (6)	N1—Cu1—N2—C12	7.9 (17)
O13—Nd1—O2—C8	−64.7 (9)	O5—Cu1—N2—C12	101.0 (17)
O12—Nd1—O2—C8	−14.8 (7)	Nd1—O7—N3—O8	−175.8 (7)
O1—Nd1—O2—C8	18.1 (6)	Nd1—O7—N3—O6	7.7 (9)
O4—Nd1—O2—C8	167.5 (6)	Nd1—O6—N3—O8	175.7 (7)
O3—Nd1—O2—Cu1	−6.7 (2)	Nd1—O6—N3—O7	−7.8 (9)
O10—Nd1—O2—Cu1	−116.2 (3)	Nd1—O10—N4—O11	171.8 (9)
O6—Nd1—O2—Cu1	105.1 (3)	Nd1—O10—N4—O9	−6.4 (9)
O9—Nd1—O2—Cu1	−91.2 (3)	Nd1—O9—N4—O11	−171.9 (10)
O7—Nd1—O2—Cu1	58.9 (3)	Nd1—O9—N4—O10	6.2 (9)
O13—Nd1—O2—Cu1	108.0 (5)	Nd1—O13—N5—O14	176.1 (7)
O12—Nd1—O2—Cu1	157.9 (3)	Nd1—O13—N5—O12	−5.2 (8)
O1—Nd1—O2—Cu1	−169.2 (4)	Nd1—O12—N5—O14	−176.2 (7)
O4—Nd1—O2—Cu1	−19.8 (4)	Nd1—O12—N5—O13	5.1 (8)
O2—Cu1—O3—C19	173.7 (7)	C3—O1—C2—C1	67.5 (11)
N2—Cu1—O3—C19	−13.7 (7)	Nd1—O1—C2—C1	−105.7 (8)
O5—Cu1—O3—C19	77.2 (6)	C2—O1—C3—C4	24.3 (13)
O2—Cu1—O3—Nd1	−7.5 (3)	Nd1—O1—C3—C4	−162.2 (8)
N2—Cu1—O3—Nd1	165.1 (3)	C2—O1—C3—C8	−158.0 (7)
O5—Cu1—O3—Nd1	−104.1 (3)	Nd1—O1—C3—C8	15.5 (9)
O2—Nd1—O3—C19	−174.7 (7)	O1—C3—C4—C5	178.5 (9)
O10—Nd1—O3—C19	−54.6 (7)	C8—C3—C4—C5	1.0 (15)
O6—Nd1—O3—C19	117.9 (7)	C3—C4—C5—C6	0.5 (17)
O9—Nd1—O3—C19	−88.4 (7)	C4—C5—C6—C7	1.1 (17)
O7—Nd1—O3—C19	81.3 (7)	C5—C6—C7—C8	−4.0 (15)
O13—Nd1—O3—C19	29.6 (7)	C5—C6—C7—C9	−179.5 (10)
O12—Nd1—O3—C19	84.6 (10)	Cu1—O2—C8—C3	170.9 (6)
O1—Nd1—O3—C19	−156.9 (6)	Nd1—O2—C8—C3	−17.5 (10)
O4—Nd1—O3—C19	−7.5 (6)	Cu1—O2—C8—C7	−8.0 (11)
O2—Nd1—O3—Cu1	6.6 (2)	Nd1—O2—C8—C7	163.6 (6)
O10—Nd1—O3—Cu1	126.7 (3)	C4—C3—C8—O2	177.0 (8)

O6—Nd1—O3—Cu1	−60.8 (3)	O1—C3—C8—O2	−0.8 (10)
O9—Nd1—O3—Cu1	92.9 (3)	C4—C3—C8—C7	−4.1 (13)
O7—Nd1—O3—Cu1	−97.4 (3)	O1—C3—C8—C7	178.2 (7)
O13—Nd1—O3—Cu1	−149.1 (2)	C6—C7—C8—O2	−175.8 (8)
O12—Nd1—O3—Cu1	−94.1 (8)	C9—C7—C8—O2	−0.7 (14)
O1—Nd1—O3—Cu1	24.4 (4)	C6—C7—C8—C3	5.3 (12)
O4—Nd1—O3—Cu1	173.8 (3)	C9—C7—C8—C3	−179.5 (9)
O2—Nd1—O4—C18	18.1 (6)	C10'—N1—C9—C7	−164.5 (12)
O3—Nd1—O4—C18	4.7 (5)	C10—N1—C9—C7	159.9 (12)
O10—Nd1—O4—C18	144.3 (5)	Cu1—N1—C9—C7	−2.2 (14)
O6—Nd1—O4—C18	−78.3 (6)	C8—C7—C9—N1	6.2 (16)
O9—Nd1—O4—C18	92.2 (5)	C6—C7—C9—N1	−178.7 (9)
O7—Nd1—O4—C18	−68.0 (5)	C9—N1—C10—C11	39 (2)
O13—Nd1—O4—C18	−143.9 (5)	C10'—N1—C10—C11	−63.2 (14)
O12—Nd1—O4—C18	−159.5 (5)	Cu1—N1—C10—C11	−156.7 (13)
O1—Nd1—O4—C18	104.6 (6)	C9—N1—C10—C12	155.4 (16)
O2—Nd1—O4—C20	−162.8 (6)	C10'—N1—C10—C12	53 (2)
O3—Nd1—O4—C20	−176.2 (6)	Cu1—N1—C10—C12	−40.5 (16)
O10—Nd1—O4—C20	−36.6 (6)	C9—N1—C10'—C11	−31 (2)
O6—Nd1—O4—C20	100.8 (6)	C10—N1—C10'—C11	65.9 (14)
O9—Nd1—O4—C20	−88.7 (6)	Cu1—N1—C10'—C11	164.2 (14)
O7—Nd1—O4—C20	111.1 (6)	C9—N1—C10'—C12'	−167.3 (19)
O13—Nd1—O4—C20	35.2 (6)	C10—N1—C10'—C12'	−70 (3)
O12—Nd1—O4—C20	19.6 (7)	Cu1—N1—C10'—C12'	28 (2)
O1—Nd1—O4—C20	−76.3 (7)	N1—C10'—C11—C10	−65.8 (15)
O2—Cu1—O5—C22	10.2 (12)	C12'—C10'—C11—C10	70 (3)
O3—Cu1—O5—C22	93.4 (12)	N1—C10—C11—C10'	62.9 (14)
N2—Cu1—O5—C22	−171.8 (12)	C12—C10—C11—C10'	−51 (3)
N1—Cu1—O5—C22	−86.4 (12)	C13—N2—C12—C10	148.7 (17)
O2—Nd1—O6—N3	−101.4 (6)	C12'—N2—C12—C10	85 (9)
O3—Nd1—O6—N3	−43.7 (6)	Cu1—N2—C12—C10	−34 (3)
O10—Nd1—O6—N3	127.1 (6)	N1—C10—C12—N2	48 (3)
O9—Nd1—O6—N3	−140.3 (5)	C11—C10—C12—N2	170 (2)
O7—Nd1—O6—N3	4.6 (5)	C13—N2—C12'—C10'	−168.5 (18)
O13—Nd1—O6—N3	79.7 (6)	C12—N2—C12'—C10'	−45 (7)
O12—Nd1—O6—N3	128.1 (6)	Cu1—N2—C12'—C10'	22 (3)
O1—Nd1—O6—N3	−163.2 (6)	N1—C10'—C12'—N2	−32 (3)
O4—Nd1—O6—N3	18.1 (7)	C11—C10'—C12'—N2	−169.8 (19)
O2—Nd1—O7—N3	64.6 (6)	C12'—N2—C13—C14	−175 (2)
O3—Nd1—O7—N3	124.3 (7)	C12—N2—C13—C14	171 (2)
O10—Nd1—O7—N3	−121.4 (6)	Cu1—N2—C13—C14	−6.1 (13)
O6—Nd1—O7—N3	−4.6 (5)	N2—C13—C14—C15	177.3 (9)
O9—Nd1—O7—N3	145.0 (5)	N2—C13—C14—C19	−6.6 (14)
O13—Nd1—O7—N3	−98.3 (6)	C19—C14—C15—C16	2.0 (13)
O12—Nd1—O7—N3	−54.9 (6)	C13—C14—C15—C16	178.2 (9)
O1—Nd1—O7—N3	10.5 (7)	C14—C15—C16—C17	−3.0 (15)
O4—Nd1—O7—N3	−173.6 (6)	C15—C16—C17—C18	1.0 (14)
O2—Nd1—O9—N4	−158.2 (6)	C16—C17—C18—C19	2.0 (13)
O3—Nd1—O9—N4	138.3 (6)	C16—C17—C18—O4	−179.1 (8)

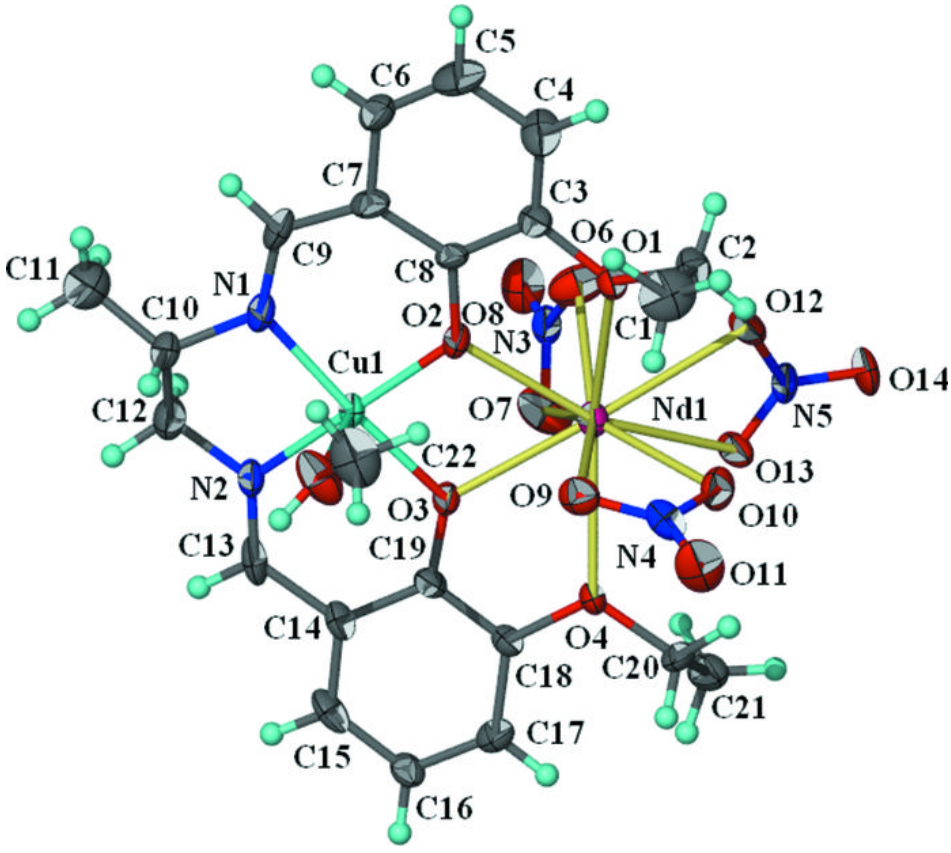
O10—Nd1—O9—N4	−3.7 (5)	C20—O4—C18—C19	178.2 (7)
O6—Nd1—O9—N4	−120.3 (7)	Nd1—O4—C18—C19	−2.7 (8)
O7—Nd1—O9—N4	118.8 (7)	C20—O4—C18—C17	−0.8 (11)
O13—Nd1—O9—N4	13.8 (6)	Nd1—O4—C18—C17	178.3 (6)
O12—Nd1—O9—N4	−39.9 (6)	Cu1—O3—C19—C18	−172.3 (5)
O1—Nd1—O9—N4	−97.1 (6)	Nd1—O3—C19—C18	9.2 (10)
O4—Nd1—O9—N4	77.2 (5)	Cu1—O3—C19—C14	6.4 (11)
O2—Nd1—O10—N4	36.6 (7)	Nd1—O3—C19—C14	−172.1 (6)
O3—Nd1—O10—N4	−41.6 (6)	C17—C18—C19—O3	175.8 (7)
O6—Nd1—O10—N4	148.9 (5)	O4—C18—C19—O3	−3.3 (10)
O9—Nd1—O10—N4	3.7 (5)	C17—C18—C19—C14	−2.9 (12)
O7—Nd1—O10—N4	−135.9 (6)	O4—C18—C19—C14	178.0 (7)
O13—Nd1—O10—N4	−159.7 (6)	C15—C14—C19—O3	−177.6 (8)
O12—Nd1—O10—N4	147.9 (6)	C13—C14—C19—O3	6.4 (13)
O1—Nd1—O10—N4	80.8 (6)	C15—C14—C19—C18	1.0 (12)
O4—Nd1—O10—N4	−82.7 (6)	C13—C14—C19—C18	−175.0 (8)
O2—Nd1—O12—N5	−160.6 (5)	C18—O4—C20—C21	78.0 (9)
O3—Nd1—O12—N5	−67.2 (10)	Nd1—O4—C20—C21	−101.1 (7)
O10—Nd1—O12—N5	76.2 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5O···O14^{i}	0.82	2.08	2.89 (1)	165

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

Fig. 1


C5
C6
C4
C7
C3
O6
O1
C2
C11
C9
C8
N1
C10
O2
O8
C1
O12
N3
Cu1
O14
C12
O7
Nd1
N5
C22
O13
N2
O9
O3
O10
C13
C19
N4
O11
C14
O4
C20
C18
C21
C17
C15
C16