(μ-6-Oxido-4-oxo-1,2-dihydro-pyrimidine-5-carboxylato-κ^4O^5,O^6:-O^2,N^3)bis[aquabis(4-oxido-2-oxo-1,2-dihydropyrimidin-3-ium-5-carboxylato-κ^2O^4,O^5)(1,10-phenanthroline-κ^2N,N')neodymium(III)] hexahydrate

Hui-Hui Xing,[a] Zi-Lu Chen[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Gulin 541004, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603, Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

The water-coordinated neodymium(III) atom in the centrosymmetric title compound, [Nd$_2$(C$_5$H$_2$N$_2$O$_4$)(C$_5$H$_3$N$_2$O$_4$)$_4$(C$_{12}$H$_8$N$_2$)$_2$(H$_2$O)$_2$]·6H$_2$O is chelated by a 1,10-phenanthroline heterocycle and two 2,4-dihydroxypyrimidine-5-carboxylate dianions. Two tris-chelated water-coordinated units are bridged by a 2,4-dihydroxypyrimidine-5-carboxylate dianion, which is disordered about a center of inversion. The metal center has a monocapped square-antiprismatic coordination.

Related literature

The title neodymium compound is isostructural with the praseodymium analog (Sun & Jin, 2004). For a related structure, see: Xing *et al.* (2008).
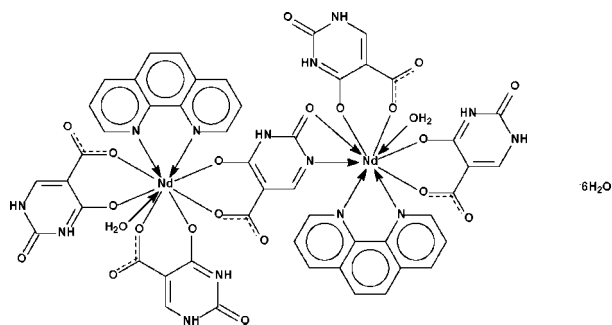
Experimental

Crystal data

[Nd$_2$(C$_5$H$_2$N$_2$O$_4$)(C$_5$H$_3$N$_2$O$_4$)$_4$-(C$_{12}$H$_8$N$_2$)$_2$(H$_2$O)$_2$]·6H$_2$O
M_r = 1567.48
Triclinic, $P\bar{1}$
a = 10.1980 (7) Å
b = 12.8896 (9) Å
c = 13.3383 (9) Å
α = 118.711 (1)°

β = 90.010 (1)°
γ = 108.612 (1)°
V = 1432.25 (17) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.90 mm^{-1}
T = 295 (2) K
0.10 × 0.04 × 0.02 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.724, T_{max} = 0.963

12405 measured reflections
6377 independent reflections
5349 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.136
S = 1.04
6377 reflections
454 parameters

84 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O2	2.526 (4)	Nd1—O10	2.526 (4)
Nd1—O3	2.502 (9)	Nd1—O1W	2.475 (4)
Nd1—O5	2.392 (4)	Nd1—N7	2.638 (5)
Nd1—O6	2.575 (4)	Nd1—N8	2.725 (5)
Nd1—O9	2.341 (4)		
O2—Nd1—O3	67.5 (2)	O5—Nd1—O1W	78.2 (2)
O2—Nd1—O5	71.6 (1)	O5—Nd1—N7	83.8 (2)
O2—Nd1—O6	123.5 (1)	O5—Nd1—N8	138.8 (2)
O2—Nd1—O9	127.7 (1)	O6—Nd1—O9	72.6 (1)
O2—Nd1—O10	71.8 (1)	O6—Nd1—O10	67.7 (1)
O2—Nd1—O1W	136.6 (2)	O6—Nd1—O1W	69.0 (1)
O2—Nd1—N7	70.6 (2)	O6—Nd1—N7	138.2 (2)
O2—Nd1—N8	111.7 (2)	O6—Nd1—N8	124.8 (2)
O3—Nd1—O5	138.7 (2)	O9—Nd1—O10	71.5 (1)
O3—Nd1—O6	133.6 (3)	O9—Nd1—O1W	95.5 (2)
O3—Nd1—O9	68.6 (3)	O9—Nd1—N7	133.8 (2)
O3—Nd1—O10	76.5 (3)	O9—Nd1—N8	72.8 (2)
O3—Nd1—O1W	138.2 (3)	O10—Nd1—O1W	136.7 (2)
O3—Nd1—N7	87.9 (3)	O10—Nd1—N7	142.5 (2)
O3—Nd1—N8	65.6 (3)	O10—Nd1—N8	135.1 (2)
O5—Nd1—O6	67.9 (1)	O1W—Nd1—N7	75.78 (16)
O5—Nd1—O9	139.7 (2)	O1W—Nd1—N8	72.93 (16)
O5—Nd1—O10	85.9 (1)	N7—Nd1—N8	61.14 (16)

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from the Pr analog (Sun & Jin, 2004); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2552).

metal-organic compounds

References

Barbour, L. J. (2001). *J. Supramol. Chem.*, **1**, 189–191.
Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Winconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sun, C.-Y. & Jin, L. P. (2004). *Polyhedron*, **23**, 2085–2093.
Westrip, S. P. (2008). *publCIF*. In preparation.
Xing, H.-H., Chen, Z.-L. & Ng, S. W. (2008). *Acta Cryst.* E**64**, m418.

supporting information

(*µ*-6-Oxido-4-oxo-1,2-dihydropyrimidine-5-carboxylato-*κ*⁴*O*⁵,*O*⁶:*O*²,*N*³)bis-[aquabis(4-oxido-2-oxo-1,2-dihydropyrimidin-3-ium-5-carboxylato-*κ*²*O*⁴,*O*⁵)(1,10-phenanthroline-*κ*²*N*,*N*′)neodymium(III)] hexahydrate

Hui-Hui Xing, Zi-Lu Chen and Seik Weng Ng

S1. Comment

The 1,10-phenanthroline-chelated rare-earth compound, $Pr_2(C_{12}H_8N_2)_2(C_5H_2N_2O_4)(C_5H_3N_2O_4)_4(H_2O)_2$– $\cdot$3H$_2$O, represents the first example of dinculear lanthanum derivatives of 2,4-dihydroxpyrimidine-5-carboxylic acid (Sun & Jin, 2004). The present neodymium compound is isostructural with the praseodymium analog.

S2. Experimental

2,4-Dihydroxypyrimidine-5-carboxylic acid (0.044 g, 0.25 mmol), neodymium trichloride hexahydrate (0.090 g, 0.25 mmol), 1,10-phenanthroline (0.050 g, 0.25 mmol), sodium hydroxide (0.010 g, 0.25 mmol) and water (15 ml) was sealed in a 25-ml, Teflon-lined, stainless-steel Parr bomb. The bomb was heated to 383 K for 120 h. It was then cooled over 48 h to give lilac crystals in 70% yield. CH&N elemental analysis. Found (Calculated) for $C_{49}H_{46}N_{14}O_{28}Nd_2$: C 37.37, H 3.07, N 12.62% (37.54, 2.96, 12.51%).

S3. Refinement

The bridging dianion is disordered about a center of inversion; all atoms were assigned only half site-occupancy except for O2, which had full site occupancy. The pyrimidine ring was refined as a rigid hexagon of 1.39 Å sides.

  Carbon-bound H atoms were generated geometrically, and were included in the refinements in the riding model approximation, as well the nitrogen-bound ones. For the water molecules, only those on the coordinated water were were placed in chemically sensible positions on the basis of hydrogen bonding interactions. TWo of the lattice water molecules are each disordered over two positions. The displacement parameters of the two components were restrained to be equal. The H atoms bound to the lattice water molecules could not be located. The final difference Fourier map had a large peak near Nd1.
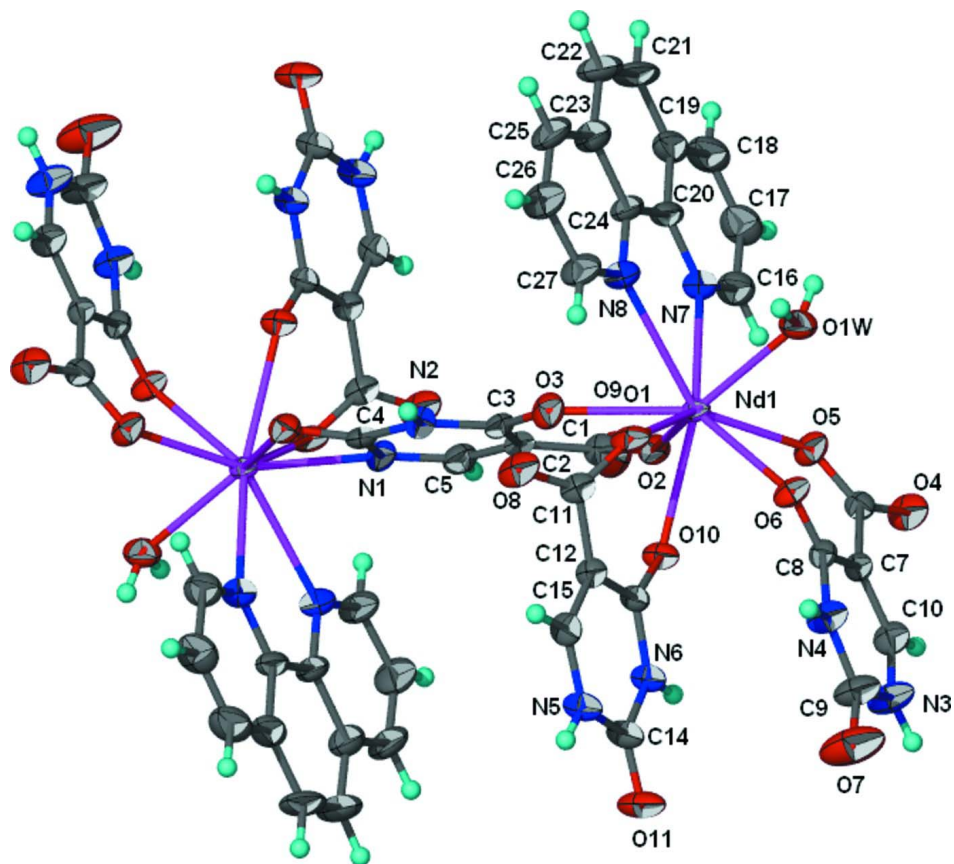
Figure 1

Displacement ellipsoid plot of $Nd_2(C_{12}H_8N_2)_2(C_5H_2N_2O_4)(C_5H_3N_2O_4)_4(H_2O)_2 \cdot 6H_2O$ drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - x, 1 - y, 1 - z). Lattice water molecules have been omitted for clarity. Only one disorder component is shown.
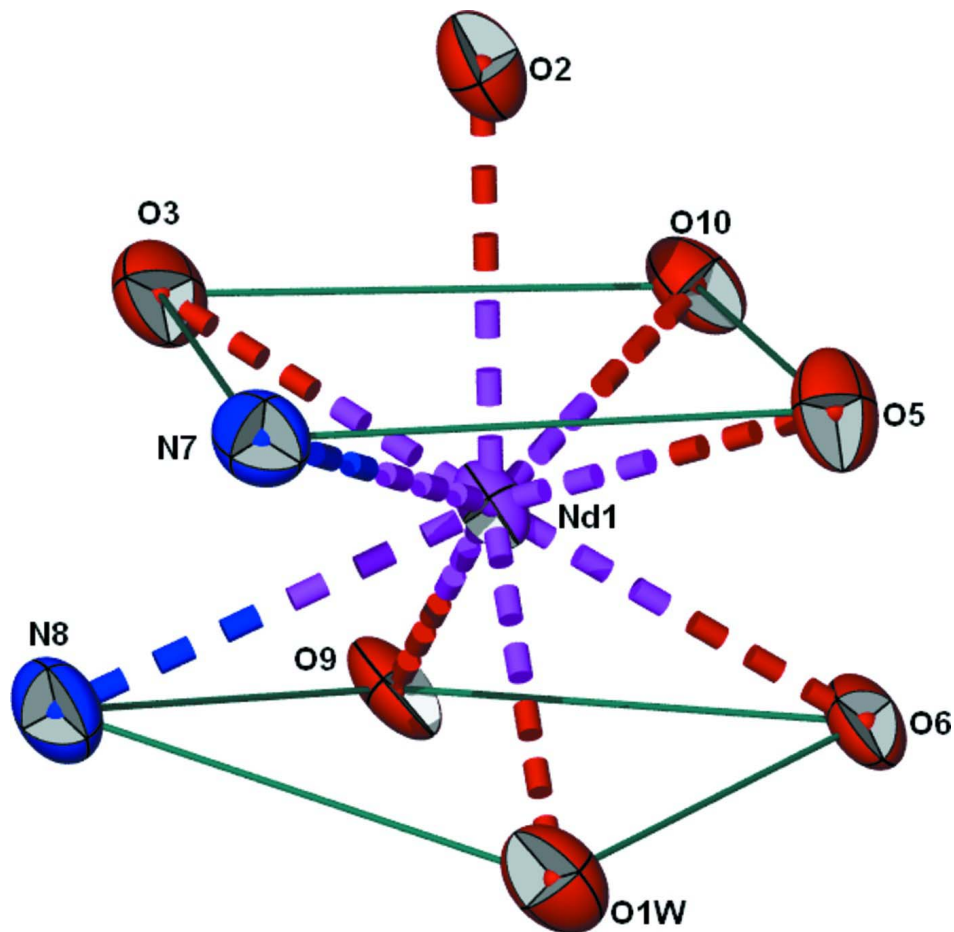
Figure 2

Geometry of Nd.

(μ-6-Oxido-4-oxo-1,2-dihydropyrimidine-5-carboxylato- $\kappa^4O^5,O^6:O^2,N^3$)bis[aquabis(4-oxido- 2-oxo-1,2-dihydropyrimidin-3-ium-5-carboxylato- κ^2O^4,O^5)(1,10-phenanthroline- κ^2N,N')neodymium(III)] hexahydrate

Crystal data

[Nd$_2$(C$_5$H$_2$N$_2$O$_4$) (C$_5$H$_3$N$_2$O$_4$)$_4$(C$_{12}$H$_8$N$_2$)$_2$(H$_2$O)$_2$]·6H$_2$O	$V = 1432.25$ (17) Å^3
$M_r = 1567.48$	$Z = 1$
Triclinic, $P\bar{1}$	$F(000) = 782$
Hall symbol: -P 1	$D_x = 1.817$ Mg m^{-3}
$a = 10.1980$ (7) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 12.8896$ (9) Å	Cell parameters from 2901 reflections
$c = 13.3383$ (9) Å	$\theta = 2.3$–22.7°
$\alpha = 118.711$ (1)°	$\mu = 1.90$ mm^{-1}
$\beta = 90.010$ (1)°	$T = 295$ K
$\gamma = 108.612$ (1)°	Prism, lilac
	$0.10 \times 0.04 \times 0.02$ mm

Data collection

Bruker APEXII diffractometer	Graphite monochromator
Radiation source: fine-focus sealed tube	φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
$T_{min} = 0.724$, $T_{max} = 0.963$
12405 measured reflections
6377 independent reflections
5349 reflections with $I > 2\sigma(I)$

$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -13 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.136$
$S = 1.04$
6377 reflections
454 parameters
84 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.4633P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.90$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Nd1	0.26520 (3)	0.27712 (3)	0.14686 (3)	0.02555 (12)	
O4	0.2306 (5)	−0.1369 (4)	−0.0511 (5)	0.0486 (12)	
O5	0.2203 (5)	0.0542 (4)	0.0456 (4)	0.0400 (11)	
O6	0.3131 (5)	0.1959 (4)	−0.0621 (4)	0.0349 (10)	
O7	0.6565 (7)	0.1207 (7)	−0.2689 (7)	0.090 (2)	
O8	0.5206 (5)	0.6553 (4)	0.2061 (5)	0.0490 (13)	
O9	0.3726 (4)	0.4550 (4)	0.1277 (4)	0.0370 (10)	
O10	0.5209 (4)	0.3057 (4)	0.1378 (4)	0.0334 (9)	
O11	0.9276 (5)	0.3690 (5)	0.0047 (5)	0.0535 (14)	
O1W	0.0466 (5)	0.1916 (4)	0.0068 (4)	0.0442 (11)	
H1W1	−0.0305	0.1557	0.0212	0.066*	
H1W2	0.0389	0.2526	0.0013	0.066*	
O2W	−0.0203 (12)	0.1690 (10)	−0.2139 (10)	0.156 (4)	
O3W	0.212 (2)	0.192 (2)	−0.3809 (18)	0.149 (5)	0.50
O4W	0.483 (2)	0.789 (2)	0.4468 (18)	0.155 (5)	0.50
O3′	0.144 (2)	−0.0260 (19)	−0.5588 (18)	0.149 (5)	0.50
O4′	0.418 (2)	0.918 (2)	0.4944 (18)	0.155 (5)	0.50
N3	0.5421 (7)	−0.0189 (6)	−0.2106 (6)	0.0512 (16)	
H3N	0.5912	−0.0654	−0.2433	0.061*	
N4	0.4768 (6)	0.1499 (5)	−0.1699 (5)	0.0415 (13)	
H4N	0.4830	0.2124	−0.1797	0.050*	
N5	0.8306 (5)	0.5190 (5)	0.0582 (5)	0.0373 (13)	
H5N	0.8986	0.5647	0.0416	0.045*	
N6	0.7237 (5)	0.3425 (5)	0.0743 (5)	0.0325 (11)	
H6N	0.7251	0.2736	0.0689	0.039*	
N7	0.0616 (5)	0.2175 (5)	0.2535 (5)	0.0359 (12)	
N8	0.1220 (6)	0.4365 (5)	0.2479 (5)	0.0404 (13)	
C6	0.2655 (6)	−0.0264 (6)	−0.0300 (5)	0.0302 (13)	

C7	0.3654 (6)	0.0150 (5)	−0.0962 (5)	0.0282 (12)	
C8	0.3800 (6)	0.1251 (5)	−0.1048 (5)	0.0291 (12)	
C9	0.5642 (8)	0.0857 (8)	−0.2206 (7)	0.053 (2)	
C10	0.4462 (7)	−0.0521 (6)	−0.1512 (6)	0.0386 (15)	
H10	0.4356	−0.1249	−0.1482	0.046*	
C11	0.4953 (7)	0.5402 (6)	0.1568 (5)	0.0319 (13)	
C12	0.6137 (6)	0.4941 (5)	0.1250 (5)	0.0300 (13)	
C13	0.6123 (6)	0.3775 (5)	0.1135 (5)	0.0279 (12)	
C14	0.8335 (6)	0.4081 (6)	0.0429 (6)	0.0379 (15)	
C15	0.7258 (6)	0.5607 (6)	0.0983 (5)	0.0338 (14)	
H15	0.7303	0.6383	0.1081	0.041*	
C16	0.0321 (8)	0.1146 (7)	0.2595 (6)	0.0479 (17)	
H16	0.0852	0.0640	0.2260	0.057*	
C17	−0.0746 (8)	0.0765 (8)	0.3131 (7)	0.058 (2)	
H17	−0.0915	0.0024	0.3154	0.069*	
C18	−0.1540 (8)	0.1494 (9)	0.3626 (7)	0.061 (2)	
H18	−0.2255	0.1251	0.3989	0.073*	
C19	−0.1288 (7)	0.2575 (8)	0.3586 (6)	0.0489 (18)	
C20	−0.0184 (6)	0.2911 (7)	0.3026 (5)	0.0382 (15)	
C21	−0.2097 (8)	0.3371 (10)	0.4055 (7)	0.067 (3)	
H21	−0.2834	0.3149	0.4410	0.080*	
C22	−0.1824 (8)	0.4419 (9)	0.3998 (7)	0.062 (2)	
H22	−0.2382	0.4906	0.4299	0.074*	
C23	−0.0688 (8)	0.4805 (8)	0.3481 (6)	0.0499 (18)	
C24	0.0120 (7)	0.4047 (6)	0.2980 (5)	0.0376 (15)	
C25	−0.0328 (9)	0.5927 (8)	0.3471 (7)	0.059 (2)	
H25	−0.0849	0.6447	0.3789	0.071*	
C26	0.0792 (9)	0.6270 (8)	0.2994 (7)	0.059 (2)	
H26	0.1058	0.7036	0.3005	0.071*	
C27	0.1537 (8)	0.5466 (7)	0.2491 (7)	0.0483 (18)	
H27	0.2284	0.5700	0.2149	0.058*	
O1	0.3919 (11)	0.1911 (9)	0.4221 (9)	0.059 (3)	0.50
O2	0.3542 (4)	0.2234 (4)	0.2860 (4)	0.0383 (10)	
O3	0.3932 (12)	0.4700 (9)	0.3390 (8)	0.042 (3)	0.50
C1	0.3988 (6)	0.2642 (7)	0.3854 (7)	0.034 (3)	0.50
C2	0.4626 (9)	0.4027 (5)	0.4640 (6)	0.021 (3)	0.50
C3	0.4558 (9)	0.4923 (6)	0.4366 (5)	0.032 (3)	0.50
N2	0.5211 (9)	0.6211 (6)	0.5170 (6)	0.028 (3)	0.50
H2N	0.5169	0.6766	0.5001	0.034*	0.50
C4	0.5931 (8)	0.6601 (5)	0.6250 (6)	0.033 (3)	0.50
N1	0.5999 (9)	0.5705 (8)	0.6524 (5)	0.033 (3)	0.50
C5	0.5346 (9)	0.4417 (7)	0.5719 (7)	0.040 (3)	0.50
H5	0.5391	0.3817	0.5903	0.048*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.02497 (18)	0.02326 (18)	0.03442 (19)	0.01369 (13)	0.01123 (12)	0.01601 (14)

O4	0.057 (3)	0.030 (2)	0.071 (3)	0.022 (2)	0.022 (3)	0.030 (3)
O5	0.051 (3)	0.025 (2)	0.047 (3)	0.015 (2)	0.021 (2)	0.019 (2)
O6	0.048 (3)	0.033 (2)	0.041 (2)	0.027 (2)	0.019 (2)	0.023 (2)
O7	0.103 (5)	0.095 (5)	0.133 (6)	0.066 (4)	0.085 (5)	0.084 (5)
O8	0.059 (3)	0.028 (2)	0.074 (3)	0.024 (2)	0.031 (3)	0.031 (2)
O9	0.038 (2)	0.035 (2)	0.057 (3)	0.026 (2)	0.021 (2)	0.030 (2)
O10	0.030 (2)	0.032 (2)	0.052 (3)	0.0154 (18)	0.0149 (19)	0.029 (2)
O11	0.038 (3)	0.046 (3)	0.100 (4)	0.025 (2)	0.036 (3)	0.048 (3)
O1W	0.035 (2)	0.046 (3)	0.058 (3)	0.021 (2)	0.011 (2)	0.026 (2)
O2W	0.174 (8)	0.147 (7)	0.156 (7)	0.074 (6)	0.026 (6)	0.075 (6)
O3W	0.195 (10)	0.126 (8)	0.143 (8)	0.064 (7)	0.005 (7)	0.077 (7)
O4W	0.177 (10)	0.163 (9)	0.127 (8)	0.035 (7)	0.036 (7)	0.092 (7)
O3′	0.195 (10)	0.126 (8)	0.143 (8)	0.064 (7)	0.005 (7)	0.077 (7)
O4′	0.177 (10)	0.163 (9)	0.127 (8)	0.035 (7)	0.036 (7)	0.092 (7)
N3	0.063 (4)	0.052 (4)	0.070 (4)	0.042 (3)	0.036 (3)	0.041 (3)
N4	0.051 (3)	0.037 (3)	0.057 (4)	0.025 (3)	0.027 (3)	0.034 (3)
N5	0.029 (3)	0.035 (3)	0.064 (4)	0.012 (2)	0.016 (3)	0.036 (3)
N6	0.028 (3)	0.027 (3)	0.053 (3)	0.011 (2)	0.012 (2)	0.027 (3)
N7	0.033 (3)	0.040 (3)	0.040 (3)	0.016 (2)	0.010 (2)	0.023 (3)
N8	0.038 (3)	0.044 (3)	0.045 (3)	0.025 (3)	0.015 (3)	0.021 (3)
C6	0.029 (3)	0.028 (3)	0.037 (3)	0.012 (2)	0.005 (2)	0.018 (3)
C7	0.030 (3)	0.024 (3)	0.031 (3)	0.013 (2)	0.003 (2)	0.013 (3)
C8	0.031 (3)	0.023 (3)	0.032 (3)	0.011 (2)	0.007 (2)	0.013 (3)
C9	0.057 (5)	0.060 (5)	0.067 (5)	0.037 (4)	0.037 (4)	0.040 (4)
C10	0.046 (4)	0.035 (3)	0.046 (4)	0.021 (3)	0.012 (3)	0.024 (3)
C11	0.041 (4)	0.033 (3)	0.038 (3)	0.020 (3)	0.016 (3)	0.026 (3)
C12	0.033 (3)	0.027 (3)	0.036 (3)	0.012 (3)	0.009 (3)	0.019 (3)
C13	0.023 (3)	0.027 (3)	0.035 (3)	0.009 (2)	0.005 (2)	0.017 (3)
C14	0.027 (3)	0.034 (3)	0.061 (4)	0.012 (3)	0.011 (3)	0.030 (3)
C15	0.037 (3)	0.023 (3)	0.045 (4)	0.010 (3)	0.006 (3)	0.020 (3)
C16	0.043 (4)	0.049 (4)	0.053 (4)	0.017 (3)	0.014 (3)	0.027 (4)
C17	0.050 (5)	0.060 (5)	0.063 (5)	0.010 (4)	0.014 (4)	0.038 (4)
C18	0.043 (4)	0.077 (6)	0.057 (5)	0.013 (4)	0.018 (4)	0.036 (5)
C19	0.036 (4)	0.064 (5)	0.035 (4)	0.014 (4)	0.011 (3)	0.019 (4)
C20	0.028 (3)	0.054 (4)	0.030 (3)	0.020 (3)	0.010 (3)	0.016 (3)
C21	0.041 (4)	0.104 (8)	0.054 (5)	0.037 (5)	0.031 (4)	0.032 (5)
C22	0.048 (5)	0.086 (7)	0.061 (5)	0.044 (5)	0.026 (4)	0.031 (5)
C23	0.047 (4)	0.058 (5)	0.041 (4)	0.031 (4)	0.009 (3)	0.015 (4)
C24	0.035 (3)	0.047 (4)	0.032 (3)	0.027 (3)	0.010 (3)	0.014 (3)
C25	0.063 (5)	0.063 (5)	0.051 (5)	0.047 (4)	0.016 (4)	0.014 (4)
C26	0.065 (5)	0.050 (5)	0.070 (5)	0.039 (4)	0.014 (4)	0.025 (4)
C27	0.053 (4)	0.040 (4)	0.064 (5)	0.030 (4)	0.022 (4)	0.027 (4)
O1	0.076 (6)	0.042 (5)	0.057 (6)	0.020 (5)	0.013 (5)	0.025 (4)
O2	0.036 (2)	0.028 (2)	0.048 (3)	0.0158 (19)	0.010 (2)	0.015 (2)
O3	0.050 (6)	0.027 (5)	0.046 (5)	0.017 (4)	0.006 (4)	0.015 (4)
C1	0.040 (6)	0.024 (5)	0.046 (6)	0.014 (5)	0.011 (5)	0.022 (5)
C2	0.028 (5)	0.023 (5)	0.029 (6)	0.017 (4)	0.009 (4)	0.022 (5)
C3	0.030 (6)	0.033 (6)	0.029 (6)	0.014 (5)	0.014 (4)	0.011 (5)

N2	0.040 (5)	0.027 (5)	0.030 (5)	0.021 (4)	0.002 (4)	0.018 (4)
C4	0.024 (5)	0.038 (6)	0.035 (6)	0.017 (5)	0.012 (4)	0.014 (5)
N1	0.039 (6)	0.029 (6)	0.034 (6)	0.021 (5)	0.004 (4)	0.013 (5)
C5	0.041 (6)	0.043 (7)	0.037 (6)	0.019 (5)	0.016 (5)	0.018 (5)

Geometric parameters (Å, º)

Nd1—O2	2.526 (4)	C10—H10	0.93
Nd1—O3	2.502 (9)	C11—C12	1.485 (8)
Nd1—O5	2.392 (4)	C12—C15	1.355 (8)
Nd1—O6	2.575 (4)	C12—C13	1.431 (8)
Nd1—O9	2.341 (4)	C15—H15	0.93
Nd1—O10	2.526 (4)	C16—C17	1.391 (10)
Nd1—O1W	2.475 (4)	C16—H16	0.93
Nd1—N1i	2.478 (6)	C17—C18	1.366 (11)
Nd1—N7	2.638 (5)	C17—H17	0.93
Nd1—N8	2.725 (5)	C18—C19	1.361 (11)
O4—C6	1.234 (7)	C18—H18	0.93
O5—C6	1.268 (7)	C19—C20	1.419 (9)
O6—C8	1.233 (7)	C19—C21	1.431 (11)
O7—C9	1.229 (8)	C20—C24	1.427 (9)
O8—C11	1.232 (7)	C21—C22	1.330 (12)
O9—C11	1.279 (7)	C21—H21	0.93
O10—C13	1.252 (7)	C22—C23	1.424 (11)
O11—C14	1.222 (7)	C22—H22	0.93
O1W—H1W1	0.85	C23—C25	1.381 (11)
O1W—H1W2	0.85	C23—C24	1.402 (9)
N3—C10	1.351 (8)	C25—C26	1.361 (12)
N3—C9	1.366 (9)	C25—H25	0.93
N3—H3N	0.86	C26—C27	1.391 (9)
N4—C9	1.367 (8)	C26—H26	0.93
N4—C8	1.378 (7)	C27—H27	0.93
N4—H4N	0.86	O1—C1	1.238 (8)
N5—C15	1.345 (8)	O2—C1	1.191 (8)
N5—C14	1.354 (7)	O3—C3	1.307 (8)
N5—H5N	0.86	C1—C2	1.473 (8)
N6—C13	1.368 (7)	C2—C3	1.39
N6—C14	1.371 (7)	C2—C5	1.39
N6—H6N	0.86	C3—N2	1.39
N7—C16	1.305 (9)	N2—C4	1.39
N7—C20	1.375 (8)	N2—H2N	0.86
N8—C27	1.343 (9)	C4—N1	1.39
N8—C24	1.358 (8)	N1—C5	1.39
C6—C7	1.487 (8)	N1—Nd1i	2.478 (6)
C7—C10	1.346 (8)	C5—H5	0.93
C7—C8	1.438 (8)		
O2—Nd1—O3	67.5 (2)	O7—C9—N4	122.9 (7)

O2—Nd1—O5	71.6 (1)	N3—C9—N4	114.1 (6)
O2—Nd1—O6	123.5 (1)	C7—C10—N3	123.2 (6)
O2—Nd1—O9	127.7 (1)	C7—C10—H10	118.4
O2—Nd1—O10	71.8 (1)	N3—C10—H10	118.4
O2—Nd1—O1W	136.6 (2)	O8—C11—O9	124.9 (6)
O2—Nd1—N7	70.6 (2)	O8—C11—C12	118.8 (6)
O2—Nd1—N8	111.7 (2)	O9—C11—C12	116.3 (5)
O3—Nd1—O5	138.7 (2)	C15—C12—C13	117.4 (5)
O3—Nd1—O6	133.6 (3)	C15—C12—C11	119.2 (5)
O3—Nd1—O9	68.6 (3)	C13—C12—C11	123.3 (5)
O3—Nd1—O10	76.5 (3)	O10—C13—N6	116.8 (5)
O3—Nd1—O1W	138.2 (3)	O10—C13—C12	126.6 (5)
O3—Nd1—N7	87.9 (3)	N6—C13—C12	116.6 (5)
O3—Nd1—N8	65.6 (3)	O11—C14—N5	122.8 (6)
O5—Nd1—O6	67.9 (1)	O11—C14—N6	122.0 (6)
O5—Nd1—O9	139.7 (2)	N5—C14—N6	115.2 (5)
O5—Nd1—O10	85.9 (1)	N5—C15—C12	122.7 (5)
O5—Nd1—O1W	78.2 (2)	N5—C15—H15	118.7
O5—Nd1—N7	83.8 (2)	C12—C15—H15	118.7
O5—Nd1—N8	138.8 (2)	N7—C16—C17	123.6 (7)
O6—Nd1—O9	72.6 (1)	N7—C16—H16	118.2
O6—Nd1—O10	67.7 (1)	C17—C16—H16	118.2
O6—Nd1—O1W	69.0 (1)	C18—C17—C16	119.1 (8)
O6—Nd1—N7	138.2 (2)	C18—C17—H17	120.5
O6—Nd1—N8	124.8 (2)	C16—C17—H17	120.5
O9—Nd1—O10	71.5 (1)	C19—C18—C17	120.1 (7)
O9—Nd1—O1W	95.5 (2)	C19—C18—H18	120.0
O9—Nd1—N7	133.8 (2)	C17—C18—H18	120.0
O9—Nd1—N8	72.8 (2)	C18—C19—C20	118.1 (7)
O10—Nd1—O1W	136.7 (2)	C18—C19—C21	123.4 (7)
O10—Nd1—N7	142.5 (2)	C20—C19—C21	118.5 (8)
O10—Nd1—N8	135.1 (2)	N7—C20—C19	121.5 (7)
O1W—Nd1—N7	75.78 (16)	N7—C20—C24	119.0 (6)
O1W—Nd1—N8	72.93 (16)	C19—C20—C24	119.5 (6)
N7—Nd1—N8	61.14 (16)	C22—C21—C19	121.9 (7)
O9—Nd1—N1[i]	80.8 (3)	C22—C21—H21	119.1
O5—Nd1—N1[i]	124.7 (3)	C19—C21—H21	119.1
O1W—Nd1—N1[i]	147.5 (3)	C21—C22—C23	120.8 (7)
N1[i]—Nd1—O3	14.1 (3)	C21—C22—H22	119.6
N1[i]—Nd1—O10	73.0 (3)	C23—C22—H22	119.6
N1[i]—Nd1—O2	53.4 (2)	C25—C23—C24	118.0 (7)
N1[i]—Nd1—O6	137.7 (4)	C25—C23—C22	122.0 (7)
N1[i]—Nd1—N7	83.6 (4)	C24—C23—C22	119.9 (8)
N1[i]—Nd1—N8	75.1 (3)	N8—C24—C23	122.7 (7)
C6—O5—Nd1	140.6 (4)	N8—C24—C20	117.9 (5)
C8—O6—Nd1	123.2 (4)	C23—C24—C20	119.4 (6)
C11—O9—Nd1	137.2 (4)	C26—C25—C23	119.8 (7)
C13—O10—Nd1	130.2 (4)	C26—C25—H25	120.1

Nd1—O1W—H1W1	117.9	C23—C25—H25	120.1
Nd1—O1W—H1W2	107.8	C25—C26—C27	119.5 (8)
H1W1—O1W—H1W2	107.7	C25—C26—H26	120.2
C10—N3—C9	122.5 (6)	C27—C26—H26	120.2
C10—N3—H3N	118.7	N8—C27—C26	122.6 (7)
C9—N3—H3N	118.7	N8—C27—H27	118.7
C9—N4—C8	126.9 (6)	C26—C27—H27	118.7
C9—N4—H4N	116.5	C1—O2—Nd1	143.9 (5)
C8—N4—H4N	116.5	C3—O3—Nd1	135.9 (6)
C15—N5—C14	122.6 (5)	O2—C1—O1	120.4 (8)
C15—N5—H5N	118.7	O2—C1—C2	119.1 (7)
C14—N5—H5N	118.7	O1—C1—C2	120.5 (8)
C13—N6—C14	125.4 (5)	C3—C2—C5	120.0
C13—N6—H6N	117.3	C3—C2—C1	124.7 (6)
C14—N6—H6N	117.3	C5—C2—C1	115.3 (6)
C16—N7—C20	117.7 (6)	O3—C3—N2	113.1 (6)
C16—N7—Nd1	120.3 (4)	O3—C3—C2	126.9 (6)
C20—N7—Nd1	121.9 (4)	N2—C3—C2	120.0
C27—N8—C24	117.3 (6)	C4—N2—C3	120.0
C27—N8—Nd1	122.7 (4)	C4—N2—H2N	120.0
C24—N8—Nd1	119.9 (4)	C3—N2—H2N	120.0
O4—C6—O5	123.3 (6)	N2—C4—N1	120.0
O4—C6—C7	118.8 (5)	N2—C4—Nd1[i]	175.4 (3)
O5—C6—C7	117.9 (5)	N1—C4—Nd1[i]	55.6 (3)
C10—C7—C8	117.7 (6)	C5—N1—C4	120.0
C10—C7—C6	119.6 (5)	C5—N1—Nd1[i]	143.1 (4)
C8—C7—C6	122.7 (5)	C4—N1—Nd1[i]	96.8 (4)
O6—C8—N4	118.1 (5)	N1—C5—C2	120.0
O6—C8—C7	126.6 (5)	N1—C5—H5	120.0
N4—C8—C7	115.3 (5)	C2—C5—H5	120.0
O7—C9—N3	123.0 (7)		
O9—Nd1—O5—C6	21.5 (8)	C9—N3—C10—C7	−0.6 (11)
O1W—Nd1—O5—C6	106.0 (7)	Nd1—O9—C11—O8	−131.1 (6)
N1[i]—Nd1—O5—C6	−99.5 (8)	Nd1—O9—C11—C12	50.7 (8)
O3—Nd1—O5—C6	−97.6 (8)	O8—C11—C12—C15	−30.9 (9)
O10—Nd1—O5—C6	−33.4 (6)	O9—C11—C12—C15	147.5 (6)
O2—Nd1—O5—C6	−105.6 (7)	O8—C11—C12—C13	153.3 (6)
O6—Nd1—O5—C6	34.1 (6)	O9—C11—C12—C13	−28.4 (9)
N7—Nd1—O5—C6	−177.3 (7)	Nd1—O10—C13—N6	−156.8 (4)
N8—Nd1—O5—C6	152.1 (6)	Nd1—O10—C13—C12	24.7 (9)
C4[i]—Nd1—O5—C6	−104.4 (7)	C14—N6—C13—O10	179.7 (6)
O9—Nd1—O6—C8	125.4 (5)	C14—N6—C13—C12	−1.7 (9)
O5—Nd1—O6—C8	−46.1 (4)	C15—C12—C13—O10	177.3 (6)
O1W—Nd1—O6—C8	−131.5 (5)	C11—C12—C13—O10	−6.8 (10)
N1[i]—Nd1—O6—C8	71.6 (6)	C15—C12—C13—N6	−1.2 (8)
O3—Nd1—O6—C8	90.9 (5)	C11—C12—C13—N6	174.7 (5)
O10—Nd1—O6—C8	48.7 (4)	C15—N5—C14—O11	178.8 (7)

O2—Nd1—O6—C8	1.2 (5)	C15—N5—C14—N6	−1.8 (10)
N7—Nd1—O6—C8	−97.0 (5)	C13—N6—C14—O11	−177.5 (6)
N8—Nd1—O6—C8	179.0 (4)	C13—N6—C14—N5	3.1 (10)
C4ⁱ—Nd1—O6—C8	30.3 (6)	C14—N5—C15—C12	−1.0 (10)
O5—Nd1—O9—C11	−89.4 (6)	C13—C12—C15—N5	2.5 (9)
O1W—Nd1—O9—C11	−167.6 (6)	C11—C12—C15—N5	−173.6 (6)
N1ⁱ—Nd1—O9—C11	45.0 (6)	C20—N7—C16—C17	−0.5 (10)
O3—Nd1—O9—C11	52.3 (6)	Nd1—N7—C16—C17	−179.3 (6)
O10—Nd1—O9—C11	−30.0 (6)	N7—C16—C17—C18	0.2 (12)
O2—Nd1—O9—C11	17.6 (6)	C16—C17—C18—C19	0.2 (12)
O6—Nd1—O9—C11	−101.6 (6)	C17—C18—C19—C20	−0.2 (11)
N7—Nd1—O9—C11	116.9 (6)	C17—C18—C19—C21	178.3 (8)
N8—Nd1—O9—C11	122.2 (6)	C16—N7—C20—C19	0.5 (9)
C4ⁱ—Nd1—O9—C11	33.9 (6)	Nd1—N7—C20—C19	179.3 (5)
O9—Nd1—O10—C13	−10.0 (5)	C16—N7—C20—C24	179.6 (6)
O5—Nd1—O10—C13	136.0 (5)	Nd1—N7—C20—C24	−1.6 (8)
O1W—Nd1—O10—C13	68.0 (6)	C18—C19—C20—N7	−0.1 (10)
N1ⁱ—Nd1—O10—C13	−95.8 (6)	C21—C19—C20—N7	−178.7 (6)
O3—Nd1—O10—C13	−81.7 (5)	C18—C19—C20—C24	−179.3 (7)
O2—Nd1—O10—C13	−152.0 (5)	C21—C19—C20—C24	2.2 (10)
O6—Nd1—O10—C13	68.3 (5)	C18—C19—C21—C22	−179.8 (8)
N7—Nd1—O10—C13	−149.7 (5)	C20—C19—C21—C22	−1.3 (12)
N8—Nd1—O10—C13	−49.2 (6)	C19—C21—C22—C23	−1.2 (13)
C4ⁱ—Nd1—O10—C13	−124.7 (5)	C21—C22—C23—C25	−176.1 (8)
O9—Nd1—N7—C16	−173.0 (5)	C21—C22—C23—C24	2.8 (12)
O5—Nd1—N7—C16	23.8 (5)	C27—N8—C24—C23	1.0 (10)
O1W—Nd1—N7—C16	103.2 (5)	Nd1—N8—C24—C23	−177.9 (5)
N1ⁱ—Nd1—N7—C16	−102.2 (6)	C27—N8—C24—C20	−176.9 (6)
O3—Nd1—N7—C16	−115.7 (5)	Nd1—N8—C24—C20	4.2 (8)
O10—Nd1—N7—C16	−51.2 (6)	C25—C23—C24—N8	−0.8 (10)
O2—Nd1—N7—C16	−48.8 (5)	C22—C23—C24—N8	−179.7 (7)
O6—Nd1—N7—C16	70.1 (6)	C25—C23—C24—C20	177.1 (7)
N8—Nd1—N7—C16	−178.7 (6)	C22—C23—C24—C20	−1.8 (10)
C4ⁱ—Nd1—N7—C16	−75.8 (5)	N7—C20—C24—N8	−1.8 (9)
O9—Nd1—N7—C20	8.2 (6)	C19—C20—C24—N8	177.3 (6)
O5—Nd1—N7—C20	−155.0 (5)	N7—C20—C24—C23	−179.8 (6)
O1W—Nd1—N7—C20	−75.6 (5)	C19—C20—C24—C23	−0.6 (9)
N1ⁱ—Nd1—N7—C20	79.0 (5)	C24—C23—C25—C26	−0.7 (11)
O3—Nd1—N7—C20	65.6 (5)	C22—C23—C25—C26	178.2 (8)
O10—Nd1—N7—C20	130.0 (4)	C23—C25—C26—C27	1.9 (12)
O2—Nd1—N7—C20	132.4 (5)	C24—N8—C27—C26	0.3 (11)
O6—Nd1—N7—C20	−108.7 (5)	Nd1—N8—C27—C26	179.2 (6)
N8—Nd1—N7—C20	2.5 (4)	C25—C26—C27—N8	−1.8 (12)
C4ⁱ—Nd1—N7—C20	105.4 (5)	O9—Nd1—O2—C1	50.4 (6)
O9—Nd1—N8—C27	2.1 (5)	O5—Nd1—O2—C1	−170.3 (6)
O5—Nd1—N8—C27	−147.0 (5)	O1W—Nd1—O2—C1	−122.0 (6)
O1W—Nd1—N8—C27	−99.4 (6)	N1ⁱ—Nd1—O2—C1	16.0 (8)
N1ⁱ—Nd1—N8—C27	86.9 (6)	O3—Nd1—O2—C1	15.5 (6)

O3—Nd1—N8—C27	75.9 (6)	O10—Nd1—O2—C1	98.0 (6)
O10—Nd1—N8—C27	40.9 (6)	O6—Nd1—O2—C1	143.8 (6)
O2—Nd1—N8—C27	126.6 (5)	N7—Nd1—O2—C1	−80.5 (6)
O6—Nd1—N8—C27	−51.4 (6)	N8—Nd1—O2—C1	−34.2 (6)
N7—Nd1—N8—C27	177.7 (6)	C4ⁱ—Nd1—O2—C1	12.6 (9)
C4ⁱ—Nd1—N8—C27	108.0 (6)	O9—Nd1—O3—C3	−151.4 (14)
O9—Nd1—N8—C24	−179.1 (5)	O5—Nd1—O3—C3	−8.8 (16)
O5—Nd1—N8—C24	31.9 (6)	O1W—Nd1—O3—C3	135.1 (11)
O1W—Nd1—N8—C24	79.4 (5)	N1ⁱ—Nd1—O3—C3	−2 (2)
N1ⁱ—Nd1—N8—C24	−94.3 (6)	O10—Nd1—O3—C3	−76.2 (13)
O3—Nd1—N8—C24	−105.3 (5)	O2—Nd1—O3—C3	−0.5 (12)
O10—Nd1—N8—C24	−140.3 (4)	O6—Nd1—O3—C3	−116.0 (12)
O2—Nd1—N8—C24	−54.6 (5)	N7—Nd1—O3—C3	69.4 (13)
O6—Nd1—N8—C24	127.4 (4)	N8—Nd1—O3—C3	128.4 (14)
N7—Nd1—N8—C24	−3.4 (4)	C4ⁱ—Nd1—O3—C3	1.4 (13)
C4ⁱ—Nd1—N8—C24	−73.2 (5)	Nd1—O2—C1—O1	158.2 (7)
Nd1—O5—C6—O4	168.0 (5)	Nd1—O2—C1—C2	−21.9 (7)
Nd1—O5—C6—C7	−12.1 (9)	O2—C1—C2—C3	10.7 (6)
O4—C6—C7—C10	−19.2 (9)	O1—C1—C2—C3	−169.4 (6)
O5—C6—C7—C10	160.9 (6)	O2—C1—C2—C5	−168.7 (5)
O4—C6—C7—C8	160.7 (6)	O1—C1—C2—C5	11.2 (5)
O5—C6—C7—C8	−19.2 (8)	Nd1—O3—C3—N2	175.8 (8)
Nd1—O6—C8—N4	−137.4 (5)	Nd1—O3—C3—C2	−3.7 (18)
Nd1—O6—C8—C7	44.3 (8)	C5—C2—C3—O3	179.5 (12)
C9—N4—C8—O6	177.5 (7)	C1—C2—C3—O3	0.1 (11)
C9—N4—C8—C7	−4.0 (10)	C5—C2—C3—N2	0.0
C10—C7—C8—O6	178.5 (6)	C1—C2—C3—N2	−179.4 (6)
C6—C7—C8—O6	−1.3 (9)	O3—C3—N2—C4	−179.6 (11)
C10—C7—C8—N4	0.2 (8)	C2—C3—N2—C4	0.0
C6—C7—C8—N4	−179.7 (5)	C3—N2—C4—N1	0.0
C10—N3—C9—O7	175.9 (8)	N2—C4—N1—C5	0.0
C10—N3—C9—N4	−2.7 (11)	N2—C4—N1—Nd1ⁱ	−178.2 (5)
C8—N4—C9—O7	−173.4 (8)	C4—N1—C5—C2	0.0
C8—N4—C9—N3	5.2 (11)	Nd1ⁱ—N1—C5—C2	177.1 (8)
C8—C7—C10—N3	1.9 (10)	C3—C2—C5—N1	0.0
C6—C7—C10—N3	−178.2 (6)	C1—C2—C5—N1	179.4 (6)

Symmetry code: (i) −x+1, −y+1, −z+1.

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H3N⋯O1ⁱⁱ	0.86	2.19	2.877 (13)	136
N3—H3N⋯O2ⁱⁱ	0.86	2.10	2.883 (7)	152
N4—H4N⋯O8ⁱⁱⁱ	0.86	1.91	2.768 (7)	175
N5—H5N⋯O11ⁱᵛ	0.86	1.95	2.786 (7)	164
N6—H6N⋯O4ⁱⁱ	0.86	1.86	2.709 (6)	167

O1*W*—H1*W*1···O4^v	0.85	2.04	2.822 (7)	153
O1*W*—H1*W*2···O11^{vi}	0.85	2.14	2.921 (6)	153

Symmetry codes: (ii) −*x*+1, −*y*, −*z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+2, −*y*+1, −*z*; (v) −*x*, −*y*, −*z*; (vi) *x*−1, *y*, *z*.