Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[aqua[μ_3-*N*′-(carboxymethyl)-ethylenediamine-*N*,*N*,*N*′-triacetato]-samarium(III)]

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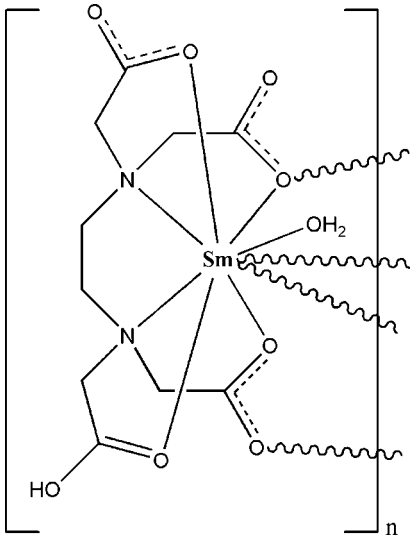
Received 31 August 2008; accepted 25 September 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.028; wR factor = 0.064; data-to-parameter ratio = 12.8.

In the title coordination polymer, $[Sm(C_{10}H_{13}N_2O_8)(H_2O)]_n$, each samarium(III) centre is nine-coordinated by six O and two N atoms from three *N*′-(carboxymethyl)ethylenediamine-*N*,*N*,*N*′-triacetate ligands and one O atom of a water molecule, forming polymeric chains running parallel to the *a* axis. The packing is governed by intermolecular O—H···O hydrogen-bonding interactions.

Related literature

For the corresponding neodymium polymeric complex, see: Huang *et al.* (2008). For related literature, see: Dakanali *et al.* (2003); Kitaura *et al.* (2002); Rowsell *et al.* (2004).



Experimental

Crystal data

$[Sm(C_{10}H_{13}N_2O_8)(H_2O)]$
M_r = 457.60
Orthorhombic, *Pbca*
a = 6.6506 (7) Å
b = 14.7051 (16) Å
c = 25.967 (3) Å
V = 2539.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.68 mm^{-1}
T = 296 (2) K
0.23 × 0.19 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.355, T_{max} = 0.433
13066 measured reflections
2637 independent reflections
2289 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.064
S = 1.03
2637 reflections
206 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −1.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2^{i}	0.82	1.66	2.474 (4)	170
O1W—H1W···O6^{ii}	0.820 (10)	2.02 (2)	2.771 (4)	152.8 (18)
O1W—H2W···O8^{iii}	0.823 (10)	2.10 (2)	2.928 (4)	177.1 (15)

Symmetry codes: (i) $-x+\frac{5}{2}, y+\frac{1}{2}, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge Hezhou University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2243).

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supporting information

Acta Cryst. (2008). E**64**, m1348 [doi:10.1107/S1600536808031036]

Poly[aqua[μ_3-*N*′-(carboxymethyl)ethylenediamine-*N*,*N*,*N*′-triacetato]-samarium(III)]

Guo-Yong Zhou, Gui-Rong Wu, Zhi-Yong Deng and Xing-Tian Chen

S1. Comment

Research on metal–organic frameworks has been expanding rapidly, due to their interesting structural motifs (Dakanali *et al.*, 2003) and other potential applications (Kitaura *et al.*, 2002; Rowsell *et al.*, 2004) in molecular-based materials. Ethylenediaminetetraacetic acid (H_4edta) is a good example of a bridging ligand that can link metal centres into extended networks. Herein, we report a new samarium complex obtained by the hydrothermal treatment of Sm_2O_3 and H_4edta in the presence of $HClO_4$.

The samarium(III) metal centre is nine-coordinated by six oxygen and two nitrogen atoms from three different N′-(carboxymethyl)ethylenediamine-N,N,N′-triacetato ligands and one water molecule (Fig. 1) to form a polymeric chain running parallel to the crystallographic *a* axis (Fig. 2). The Sm···Sm separations between adjacent metal centres are 4.2461 (6) and 6.6506 (8) Å. The polymeric chains self-assemble *via* intermolecular O—H···O hydrogen bonding interactions (Table 1) to form a three-dimensional supramolecular network. The title compound is isostructural with the corresponding neodymium polymeric complex (Huang *et al.*, 2008).

S2. Experimental

A mixture of Sm_2O_3 (0.5 mmol), ethylenediaminetetraacetic acid (H_4edta) (0.5 mmol), $HClO_4$ (0.2 mmol) and H_2O (10 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The crystals obtained were washed with water and dryed in air.

S3. Refinement

Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 Å and H···H = 1.20 Å, each within a standard deviation of 0.01 Å, and with U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed in calculated positions (C—H = 0.97 Å and O—H = 0.82 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C, O).

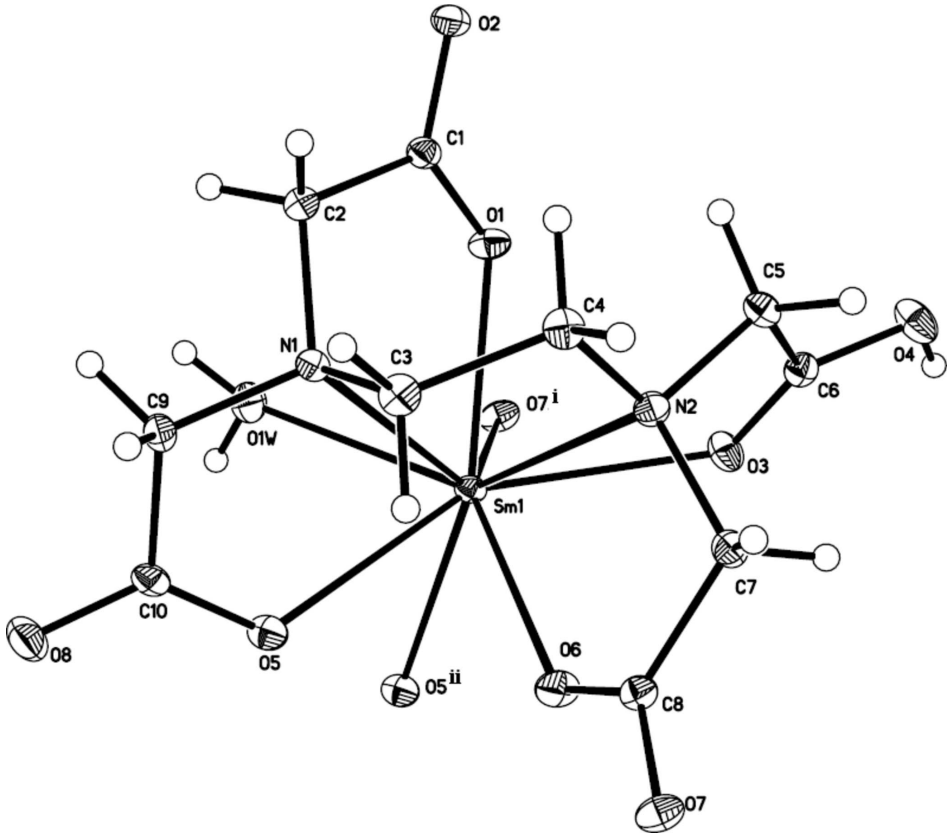

Figure 1

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown as 30% probability displacement ellipsoids. Symmetry codes: (i: 1+*x*, *y*, *z*; ii: 2-*x*, 1-*y*, 1-*z*).

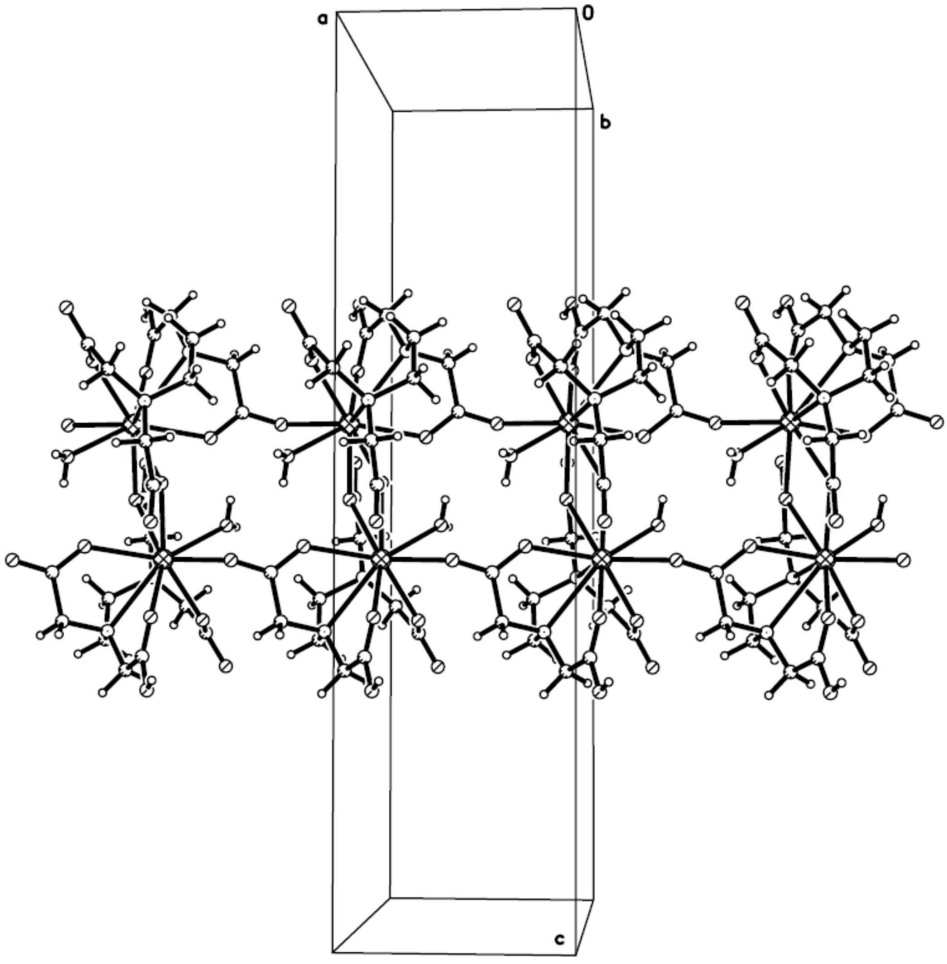

Figure 2

The one-dimensional polymeric chain of the title compound.

Poly[aqua[μ_3-N′-(carboxymethyl)ethylenediamine-N,N,N′-triacetato] samarium(III)]

Crystal data

$[Sm(C_{10}H_{13}N_2O_8)(H_2O)]$
$M_r = 457.60$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 6.6506$ (7) Å
$b = 14.7051$ (16) Å
$c = 25.967$ (3) Å
$V = 2539.5$ (5) Å^3
$Z = 8$
$F(000) = 1784$
$D_x = 2.394$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3600 reflections
$\theta = 1.7$–$28.0°$
$\mu = 4.68$ mm^{-1}
$T = 296$ K
Block, colourless
0.23 × 0.19 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.355$, $T_{max} = 0.433$
13066 measured reflections
2637 independent reflections
2289 reflections with $I > 2\sigma(I)$

R_{int} = 0.035
θ_{max} = 26.5°, θ_{min} = 1.6°
h = −8→5
k = −16→18
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.064
S = 1.03
2637 reflections
206 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 6.2721P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −1.21 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Sm1	1.07590 (3)	0.506856 (12)	0.420681 (7)	0.01387 (8)
C1	1.2133 (6)	0.3523 (3)	0.33453 (14)	0.0168 (8)
C2	1.0904 (6)	0.2870 (3)	0.36651 (15)	0.0186 (8)
H2A	1.0170	0.2467	0.3437	0.022*
H2B	1.1807	0.2500	0.3870	0.022*
C3	0.7461 (6)	0.3440 (3)	0.37554 (15)	0.0197 (8)
H3A	0.6543	0.3739	0.3991	0.024*
H3B	0.6918	0.2843	0.3678	0.024*
C4	0.7586 (6)	0.3985 (3)	0.32648 (14)	0.0193 (8)
H4A	0.8580	0.3713	0.3039	0.023*
H4B	0.6297	0.3965	0.3090	0.023*
C5	0.9165 (6)	0.5334 (3)	0.29164 (15)	0.0186 (8)
H5A	0.8189	0.5486	0.2652	0.022*
H5B	1.0097	0.4893	0.2774	0.022*
C6	1.0293 (6)	0.6179 (3)	0.30788 (15)	0.0178 (8)
C7	0.6310 (6)	0.5491 (3)	0.34790 (15)	0.0199 (9)
H7A	0.5163	0.5205	0.3315	0.024*
H7B	0.6467	0.6091	0.3329	0.024*
C8	0.5880 (6)	0.5592 (3)	0.40475 (15)	0.0166 (8)
C9	0.9173 (6)	0.2796 (3)	0.44879 (15)	0.0194 (9)
H9A	1.0277	0.2369	0.4522	0.023*

H9B	0.7942	0.2447	0.4458	0.023*
C10	0.9064 (6)	0.3372 (3)	0.49695 (15)	0.0173 (8)
N1	0.9459 (5)	0.3332 (2)	0.40114 (12)	0.0164 (7)
N2	0.8138 (5)	0.4946 (2)	0.33643 (12)	0.0173 (7)
O1	1.2293 (4)	0.43367 (18)	0.34962 (10)	0.0207 (6)
O2	1.2980 (5)	0.32419 (18)	0.29435 (10)	0.0235 (7)
O3	1.0724 (4)	0.63138 (19)	0.35307 (11)	0.0232 (7)
O4	1.0758 (5)	0.6717 (2)	0.27029 (11)	0.0292 (7)
H4	1.1182	0.7199	0.2819	0.044*
O5	0.9074 (4)	0.42346 (18)	0.49227 (10)	0.0203 (6)
O6	0.7369 (4)	0.5605 (2)	0.43483 (10)	0.0233 (6)
O7	0.4107 (4)	0.57144 (19)	0.41872 (11)	0.0211 (6)
O8	0.9000 (5)	0.2985 (2)	0.53938 (11)	0.0294 (7)
O1W	1.3250 (5)	0.3977 (2)	0.46232 (11)	0.0271 (7)
H2W	1.350 (8)	0.3428 (10)	0.4613 (15)	0.041*
H1W	1.348 (8)	0.412 (3)	0.4922 (7)	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.01036 (12)	0.01782 (12)	0.01343 (12)	0.00028 (8)	0.00067 (7)	−0.00100 (8)
C1	0.0145 (19)	0.021 (2)	0.0153 (18)	0.0028 (16)	0.0001 (15)	−0.0005 (15)
C2	0.019 (2)	0.0179 (19)	0.019 (2)	0.0032 (17)	0.0014 (16)	0.0000 (16)
C3	0.016 (2)	0.0196 (19)	0.023 (2)	−0.0039 (17)	−0.0008 (18)	−0.0007 (16)
C4	0.017 (2)	0.022 (2)	0.0197 (19)	−0.0027 (16)	−0.0040 (17)	−0.0026 (15)
C5	0.019 (2)	0.022 (2)	0.0152 (19)	−0.0017 (17)	−0.0002 (16)	−0.0008 (16)
C6	0.0142 (19)	0.018 (2)	0.021 (2)	0.0000 (16)	0.0007 (16)	0.0010 (16)
C7	0.016 (2)	0.026 (2)	0.018 (2)	0.0035 (17)	0.0008 (16)	0.0034 (17)
C8	0.014 (2)	0.0157 (18)	0.020 (2)	−0.0015 (15)	0.0019 (16)	−0.0007 (15)
C9	0.025 (2)	0.017 (2)	0.016 (2)	0.0001 (17)	0.0005 (17)	0.0022 (15)
C10	0.0102 (19)	0.024 (2)	0.0176 (19)	−0.0010 (16)	0.0031 (15)	0.0005 (16)
N1	0.0181 (18)	0.0169 (16)	0.0143 (16)	0.0004 (14)	0.0019 (13)	0.0000 (13)
N2	0.0138 (16)	0.0193 (17)	0.0187 (16)	0.0011 (14)	0.0008 (13)	0.0005 (14)
O1	0.0174 (15)	0.0206 (14)	0.0242 (14)	−0.0011 (12)	0.0052 (12)	−0.0055 (12)
O2	0.0319 (18)	0.0201 (14)	0.0186 (14)	0.0006 (13)	0.0078 (12)	−0.0020 (12)
O3	0.0277 (17)	0.0257 (16)	0.0163 (14)	−0.0039 (13)	−0.0037 (12)	0.0008 (12)
O4	0.046 (2)	0.0227 (16)	0.0190 (15)	−0.0149 (15)	0.0017 (14)	0.0007 (12)
O5	0.0218 (16)	0.0184 (14)	0.0209 (15)	−0.0051 (12)	0.0034 (12)	−0.0039 (11)
O6	0.0133 (14)	0.0355 (17)	0.0211 (14)	0.0051 (13)	−0.0039 (12)	−0.0038 (12)
O7	0.0115 (14)	0.0224 (15)	0.0295 (16)	−0.0004 (11)	0.0016 (12)	−0.0047 (12)
O8	0.0337 (19)	0.0355 (18)	0.0189 (15)	0.0007 (15)	0.0027 (13)	0.0061 (13)
O1W	0.0303 (18)	0.0290 (17)	0.0221 (16)	0.0045 (15)	−0.0043 (14)	0.0029 (13)

Geometric parameters (Å, º)

Sm1—O1	2.367 (3)	C5—C6	1.512 (5)
Sm1—O6	2.416 (3)	C5—H5A	0.9700
Sm1—O7^{i}	2.421 (3)	C5—H5B	0.9700

Sm1—O5^{ii}	2.484 (3)	C6—O3	1.224 (5)
Sm1—O5	2.493 (3)	C6—O4	1.294 (5)
Sm1—O3	2.537 (3)	C7—N2	1.486 (5)
Sm1—O1W	2.548 (3)	C7—C8	1.511 (5)
Sm1—N1	2.744 (3)	C7—H7A	0.9700
Sm1—N2	2.803 (3)	C7—H7B	0.9700
C1—O2	1.256 (4)	C8—O7	1.247 (5)
C1—O1	1.263 (5)	C8—O6	1.261 (5)
C1—C2	1.510 (5)	C9—N1	1.479 (5)
C2—N1	1.481 (5)	C9—C10	1.512 (5)
C2—H2A	0.9700	C9—H9A	0.9700
C2—H2B	0.9700	C9—H9B	0.9700
C3—N1	1.494 (5)	C10—O8	1.241 (5)
C3—C4	1.507 (5)	C10—O5	1.274 (5)
C3—H3A	0.9700	O4—H4	0.8200
C3—H3B	0.9700	O5—Sm1^{ii}	2.484 (3)
C4—N2	1.483 (5)	O7—Sm1^{iii}	2.421 (3)
C4—H4A	0.9700	O1W—H2W	0.823 (10)
C4—H4B	0.9700	O1W—H1W	0.820 (10)
C5—N2	1.464 (5)		

O1—Sm1—O6	131.98 (9)	N2—C4—H4B	109.2
O1—Sm1—O7^{i}	76.45 (9)	C3—C4—H4B	109.2
O6—Sm1—O7^{i}	137.16 (10)	H4A—C4—H4B	107.9
O1—Sm1—O5^{ii}	151.34 (10)	N2—C5—C6	109.3 (3)
O6—Sm1—O5^{ii}	76.64 (9)	N2—C5—H5A	109.8
O7^{i}—Sm1—O5^{ii}	79.40 (9)	C6—C5—H5A	109.8
O1—Sm1—O5	123.46 (9)	N2—C5—H5B	109.8
O6—Sm1—O5	68.14 (9)	C6—C5—H5B	109.8
O7^{i}—Sm1—O5	128.46 (9)	H5A—C5—H5B	108.3
O5^{ii}—Sm1—O5	62.91 (10)	O3—C6—O4	124.6 (4)
O1—Sm1—O3	78.03 (9)	O3—C6—C5	121.1 (4)
O6—Sm1—O3	82.03 (9)	O4—C6—C5	114.2 (3)
O7^{i}—Sm1—O3	73.18 (9)	N2—C7—C8	113.8 (3)
O5^{ii}—Sm1—O3	109.41 (9)	N2—C7—H7A	108.8
O5—Sm1—O3	150.11 (9)	C8—C7—H7A	108.8
O1—Sm1—O1W	76.36 (9)	N2—C7—H7B	108.8
O6—Sm1—O1W	138.39 (10)	C8—C7—H7B	108.8
O7^{i}—Sm1—O1W	70.02 (10)	H7A—C7—H7B	107.7
O5^{ii}—Sm1—O1W	81.07 (10)	O7—C8—O6	124.1 (4)
O5—Sm1—O1W	70.48 (10)	O7—C8—C7	118.5 (3)
O3—Sm1—O1W	138.98 (10)	O6—C8—C7	117.2 (3)
O1—Sm1—N1	64.43 (9)	N1—C9—C10	113.6 (3)
O6—Sm1—N1	92.16 (10)	N1—C9—H9A	108.9
O7^{i}—Sm1—N1	130.62 (9)	C10—C9—H9A	108.9
O5^{ii}—Sm1—N1	124.49 (9)	N1—C9—H9B	108.9
O5—Sm1—N1	62.50 (9)	C10—C9—H9B	108.9
O3—Sm1—N1	122.76 (9)	H9A—C9—H9B	107.7

O1W—Sm1—N1	72.34 (10)	O8—C10—O5	122.8 (4)
O1—Sm1—N2	68.30 (10)	O8—C10—C9	118.6 (4)
O6—Sm1—N2	63.86 (9)	O5—C10—C9	118.6 (3)
O7^{i}—Sm1—N2	125.50 (9)	C9—N1—C2	110.3 (3)
O5^{ii}—Sm1—N2	139.87 (9)	C9—N1—C3	108.3 (3)
O5—Sm1—N2	105.71 (9)	C2—N1—C3	110.8 (3)
O3—Sm1—N2	60.04 (9)	C9—N1—Sm1	112.4 (2)
O1W—Sm1—N2	134.02 (10)	C2—N1—Sm1	109.5 (2)
N1—Sm1—N2	66.42 (9)	C3—N1—Sm1	105.3 (2)
O2—C1—O1	122.1 (4)	C5—N2—C4	110.4 (3)
O2—C1—C2	119.3 (3)	C5—N2—C7	109.3 (3)
O1—C1—C2	118.5 (3)	C4—N2—C7	110.2 (3)
N1—C2—C1	113.2 (3)	C5—N2—Sm1	107.8 (2)
N1—C2—H2A	108.9	C4—N2—Sm1	110.6 (2)
C1—C2—H2A	108.9	C7—N2—Sm1	108.5 (2)
N1—C2—H2B	108.9	C1—O1—Sm1	129.5 (2)
C1—C2—H2B	108.9	C6—O3—Sm1	123.3 (3)
H2A—C2—H2B	107.8	C6—O4—H4	109.5
N1—C3—C4	112.6 (3)	C10—O5—Sm1^{ii}	108.9 (2)
N1—C3—H3A	109.1	C10—O5—Sm1	124.3 (2)
C4—C3—H3A	109.1	Sm1^{ii}—O5—Sm1	117.09 (10)
N1—C3—H3B	109.1	C8—O6—Sm1	129.3 (2)
C4—C3—H3B	109.1	C8—O7—Sm1^{iii}	145.0 (3)
H3A—C3—H3B	107.8	Sm1—O1W—H2W	137 (3)
N2—C4—C3	111.9 (3)	Sm1—O1W—H1W	111 (3)
N2—C4—H4A	109.2	H2W—O1W—H1W	104 (4)
C3—C4—H4A	109.2		

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x-1, y, z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O2^{iv}	0.82	1.66	2.474 (4)	170
O1*W*—H1*W*···O6^{ii}	0.82 (1)	2.02 (2)	2.771 (4)	153 (2)
O1*W*—H2*W*···O8^{v}	0.82 (1)	2.10 (2)	2.928 (4)	177 (2)

Symmetry codes: (ii) $-x+2, -y+1, -z+1$; (iv) $-x+5/2, y+1/2, z$; (v) $x+1/2, -y+1/2, -z+1$.