

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

Department of Chemistry and Biology Engineering, Hezhou University, Hezhou, Guangxi Zhuang Autonomous Region 542800, People's Republic of China

Correspondence e-mail: gyzhou@yahoo.cn

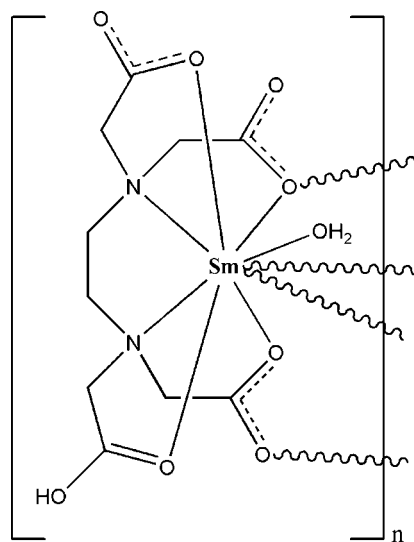
Received 31 August 2008; accepted 25 September 2008

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.028; wR factor = 0.064; data-to-parameter ratio = 12.8.

In the title coordination polymer, $[\text{Sm}(\text{C}_{10}\text{H}_{13}\text{N}_2\text{O}_8)(\text{H}_2\text{O})]_n$, 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 $\text{O}-\text{H}\cdots\text{O}$ 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

$[\text{Sm}(\text{C}_{10}\text{H}_{13}\text{N}_2\text{O}_8)(\text{H}_2\text{O})]$
 $M_r = 457.60$
 Orthorhombic, $Pbca$
 $a = 6.6506$ (7) Å
 $b = 14.7051$ (16) Å
 $c = 25.967$ (3) Å

$V = 2539.5$ (5) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 4.68$ mm⁻¹
 $T = 296$ (2) K
 $0.23 \times 0.19 \times 0.18$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

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
 $\Delta\rho_{\text{max}} = 0.94$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4-H4 \cdots O2 ⁱ	0.82	1.66	2.474 (4)	170
O1W-H1W \cdots O6 ⁱⁱ	0.820 (10)	2.02 (2)	2.771 (4)	152.8 (18)
O1W-H2W \cdots 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).

References

- Bruker (2004). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dakanali, M., Kefalas, E. T., Raptopoulou, C. P., Terzis, A., Mavromoustakos, T. & Salifoglou, A. (2003). *Inorg. Chem.* **42**, 2531–2537.
- Huang, X.-H., Xu, X.-H., Pan, W.-B. & Zeng, R.-H. (2008). *Acta Cryst.* **E64**, m1194.
- Kitaura, R., Fujimoto, K., Noro, S., Kondo, M. & Kitagawa, S. (2002). *Angew. Chem. Int. Ed.* **41**, 133–135.
- Rowsell, J. L. C., Millward, A. R., Park, K. S. & Yaghi, O. M. (2004). *J. Am. Chem. Soc.* **126**, 5666–5667.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m1348 [doi:10.1107/S1600536808031036]

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

G.-Y. Zhou, G.-R. Wu, Z.-Y. Deng and X.-T. Chen

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 ($H_4\text{edta}$) 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 $H_4\text{edta}$ 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 $\text{Sm}\cdots\text{Sm}$ separations between adjacent metal centres are 4.2461 (6) and 6.6506 (8) Å. The polymeric chains self-assemble *via* intermolecular $\text{O}\cdots\text{H}\cdots\text{O}$ 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).

Experimental

A mixture of Sm_2O_3 (0.5 mmol), ethylenediaminetetraacetic acid ($H_4\text{edta}$) (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 dried in air.

Refinement

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

Figures

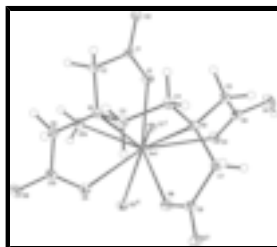


Fig. 1. The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown as 30% probability displacement ellipsoids. Symmetry codes: (i: $1+x, y, z$; ii: $2-x, 1-y, 1-z$).

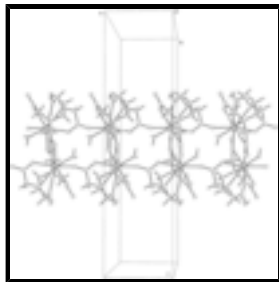


Fig. 2. The one-dimensional polymeric chain of the title compound.

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

Crystal data

[Sm(C₁₀H₁₃N₂O₈)(H₂O)]

$M_r = 457.60$

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) Å³

$Z = 8$

$F_{000} = 1784$

$D_x = 2.394$ 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

$T = 296$ (2) K

Block, colourless

$0.23 \times 0.19 \times 0.18$ mm

Data collection

Bruker APEXII area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 26.5^\circ$

$\theta_{\min} = 1.6^\circ$

$h = -8 \rightarrow 5$

$k = -16 \rightarrow 18$

$l = -32 \rightarrow 32$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.064$

$S = 1.03$

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 $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

2637 reflections $\Delta\rho_{\max} = 0.94 \text{ e } \text{\AA}^{-3}$
 206 parameters $\Delta\rho_{\min} = -1.21 \text{ e } \text{\AA}^{-3}$
 3 restraints Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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)

supplementary materials

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 (\AA^2)

	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 (\AA , $^\circ$)

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)

supplementary materials

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 ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4 \cdots O2 ^{iv}	0.82	1.66	2.474 (4)	170
O1W—H1W \cdots O6 ⁱⁱ	0.820 (10)	2.02 (2)	2.771 (4)	152.8 (18)
O1W—H2W \cdots O8 ^v	0.823 (10)	2.10 (2)	2.928 (4)	177.1 (15)

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

Fig. 2

