

Poly[[$(\mu_2$ -acetato- $\kappa^3 O, O':O')$ aquabis(μ_3 -isonicotinato- $\kappa^3 O:O':N$)samarium(III)-silver(I)] perchlorate]

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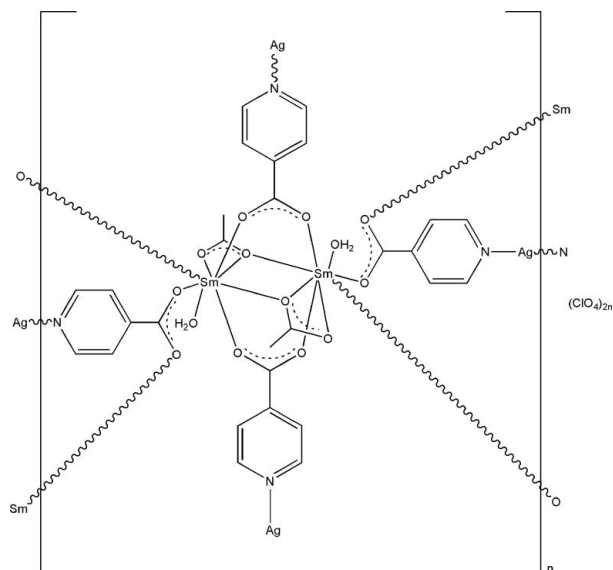
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.007$ Å; disorder in main residue; R factor = 0.026; wR factor = 0.064; data-to-parameter ratio = 11.0.

The title compound, $\{[AgSm(C_6H_4NO_2)_2(CH_3CO_2)(H_2O)]ClO_4\}_n$, is a three-dimensional heterobimetallic complex constructed from a repeating dimeric unit. Only half of the dimeric moiety is found in the asymmetric unit; the unit cell is completed by crystallographic inversion symmetry. The Sm^{III} ion is eight-coordinated by four O atoms of four different isonicotinate ligands, three O atoms of two different acetate ligands, and one O atom of a water molecule. The two-coordinate Ag^I ion is bonded to two N atoms of two different isonicotinate anions, thereby connecting the disamarium units. In addition, the isonicotinate ligands also act as bridging ligands, generating a three-dimensional network. The coordinated water molecules link the carboxylate group and acetate ligands by $O-H \cdots O$ hydrogen bonding. Another $O-H \cdots O$ hydrogen bond is observed in the crystal structure. The perchlorate ion is disordered over two sites with site-occupancy factors of 0.560 (11) and 0.440 (11), whereas the methyl group of the acetate ligand is disordered over two sites with site-occupancy factors of 0.53 (5) and 0.47 (5).

Related literature

For background to lanthanide–transition metal heterometallic complexes, see: Cheng *et al.* (2006); Kuang *et al.* (2007); Peng *et al.* (2008); Zhu *et al.* (2009).



Experimental

Crystal data

$[AgSm(C_6H_4NO_2)_2(C_2H_3O_2)(H_2O)]ClO_4$
 $M_r = 678.94$
 Monoclinic, $P2_1/c$
 $a = 16.1703$ (15) Å
 $b = 15.1042$ (14) Å
 $c = 7.9858$ (7) Å

$\beta = 92.845$ (1) $^\circ$
 $V = 1948.0$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.19$ mm⁻¹
 $T = 296$ K
 $0.22 \times 0.20 \times 0.19$ mm

Data collection

Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.414$, $T_{max} = 0.451$

9927 measured reflections
 3512 independent reflections
 2957 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.064$
 $S = 1.07$
 3512 reflections
 320 parameters
 158 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.85$ e Å⁻³
 $\Delta\rho_{min} = -0.59$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H2W \cdots O6^i$	0.81 (4)	1.98 (4)	2.785 (4)	171 (6)
$O1W-H1W \cdots O2^{ii}$	0.81 (4)	2.22 (3)	2.921 (5)	146 (5)

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2297).

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supplementary materials

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Poly[[$(\mu_2$ -acetato- $\kappa^3 O, O':O')$ aquabis(μ_3 -isonicotinato- $\kappa^3 O:O':N$)samarium(III)silver(I)] perchlorate]

L.-C. Zhu and S.-M. Zhu

Comment

In the past few years, lanthanide-transition metal heterometallic complexes with bridging multifunctional organic ligands are of increasing interest not only because of their impressive topological structures, but also due to their versatile applications in ion exchange, magnetism, bimetallic catalysis and as luminescent probes (Cheng *et al.*, 2006; Kuang *et al.*, 2007; Peng *et al.*, 2008; Zhu *et al.*, 2009). As an extension of this research, the structure of the title compound, a new heterobimetallic coordination polymer, (I), has been determined which is presented in this article.

The polymer of the title compound displays a three-dimensional heterometallic coordination framework constructed from the repeating dimeric unit. Only half of the dimeric unit is found in the asymmetric unit whose center is a crystallographic center of inversion (Fig. 1). The asymmetric unit of the title compound, contains one of the Sm^{III} and Ag^I ions each, two halves of the acetate ligands, two isonicotinate ligands and one coordinated water molecule. The Sm^{III} ion is eight-coordinated by four O atoms of four different isonicotinate ligands, three O atoms of two different acetate ligands and one O atom of a water molecule. The Sm center can therefore be described as adopting a bicapped trigonal prismatic coordination geometry. The two-coordinate Ag^I ion is bonded to two N atoms of two different isonicotinate anions. The Ag^I ion shows an almost linear coordination with N1—Ag1—N2 being 166.2 (2) °. These metal coordination units are additionally connected by bridging isonicotinate and acetate ligands, generating a three-dimensional network (Fig. 2). The coordinated water molecules link the carboxylate group and acetate ligand by O—H···O hydrogen bonding (Table 1). Another O—H···O hydrogen bond is observed in the crystal structure.

Experimental

A mixture of AgNO₃ (0.057 g, 0.33 mmol), Sm₂O₃ (0.116 g, 0.33 mmol), isonicotinic acid (0.164 g, 1.33 mmol), CH₃COONa (0.057 g, 0.7 mmol), H₂O (7 ml), and HClO₄ (0.257 mmol, pH 2) was sealed in a 20 ml Teflon-lined reaction vessel at 443 K for 6 days then slowly cooled to room temperature. The product was collected by filtration, washed with water and air-dried (yield: 45% based on Sm). Yellow block shaped crystals suitable for X-ray analysis were obtained.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 or 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$. H atoms of water molecules were found from difference Fourier maps and refined isotropically with a restraint of O—H = 0.82 Å. The perchlorate ion was disordered over two sites with site occupancy factors 0.560 (11) and 0.440 (11), whereas the methyl group of the acetate ligand was disordered over two sites with site occupancy factors 0.53 (5) and 0.47 (5).

Figures

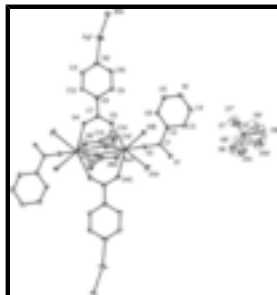


Fig. 1. Molecular structure showing displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry codes: (A) $1 - x, 1/2 + y, 2.5 - z$; (B) $x, 1.5 - y, 1/2 + z$; (C) $2 - x, 2 - y, 2 - z$.

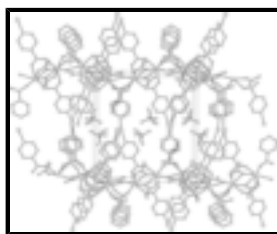


Fig. 2. A view of the three-dimensional structure of the title compound. Hydrogen atoms are omitted for clarity.

Poly[[$(\mu_2$ -acetato- $\kappa^3O,O':O')$ aquabis(μ_3 - isonicotinato- $\kappa^3O:O':N$)samarium(III)silver(I)] perchlorate]

Crystal data

[AgSm(C₆H₄NO₂)₂(C₂H₃O₂)(H₂O)]ClO₄

$M_r = 678.94$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 16.1703$ (15) Å

$b = 15.1042$ (14) Å

$c = 7.9858$ (7) Å

$\beta = 92.845$ (1)°

$V = 1948.0$ (3) Å³

$Z = 4$

$F(000) = 1300$

$D_x = 2.315$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3844 reflections

$\theta = 2.5$ – 27.3 °

$\mu = 4.19$ mm⁻¹

$T = 296$ K

Block, yellow

$0.22 \times 0.20 \times 0.19$ mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scan

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.414$, $T_{\max} = 0.451$

9927 measured reflections

3512 independent reflections

2957 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 25.2$ °, $\theta_{\min} = 1.9$ °

$h = -17 \rightarrow 19$

$k = -17 \rightarrow 18$

$l = -7 \rightarrow 9$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.064$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 0.0621P]$
3512 reflections	where $P = (F_o^2 + 2F_c^2)/3$
320 parameters	$(\Delta/\sigma)_{\max} = 0.001$
158 restraints	$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sm1	0.952467 (14)	0.883640 (13)	1.04772 (3)	0.02097 (9)	
Ag1	0.52807 (3)	1.23823 (4)	1.39951 (7)	0.06436 (17)	
C1	0.8319 (3)	0.7509 (3)	0.7966 (5)	0.0243 (10)	
C2	0.7476 (3)	0.7501 (3)	0.8658 (6)	0.0255 (10)	
C3	0.7080 (3)	0.6710 (3)	0.8907 (6)	0.0357 (12)	
H3	0.7332	0.6178	0.8639	0.043*	
C4	0.6304 (3)	0.6710 (3)	0.9558 (7)	0.0465 (14)	
H4	0.6042	0.6171	0.9726	0.056*	
C5	0.6303 (3)	0.8222 (3)	0.9692 (6)	0.0388 (12)	
H5	0.6037	0.8747	0.9948	0.047*	
C6	0.7077 (3)	0.8270 (3)	0.9062 (6)	0.0331 (11)	
H6	0.7328	0.8816	0.8911	0.040*	
C7	0.8665 (3)	1.0831 (3)	1.1375 (7)	0.0367 (12)	
C8	0.7883 (3)	1.1243 (3)	1.1940 (6)	0.0310 (11)	
C9	0.7177 (3)	1.0739 (3)	1.2021 (7)	0.0414 (13)	
H9	0.7186	1.0143	1.1728	0.050*	
C10	0.6466 (4)	1.1114 (4)	1.2534 (8)	0.0529 (16)	

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H10	0.5991	1.0767	1.2566	0.064*	
C11	0.7115 (3)	1.2455 (3)	1.2903 (8)	0.0475 (15)	
H11	0.7096	1.3048	1.3216	0.057*	
C12	0.7843 (3)	1.2127 (3)	1.2376 (7)	0.0431 (14)	
H12	0.8304	1.2490	1.2310	0.052*	
O1	0.8543 (2)	0.68433 (19)	0.7172 (4)	0.0336 (8)	
O2	0.87650 (19)	0.81870 (18)	0.8220 (4)	0.0288 (7)	
O3	0.8699 (2)	1.0005 (2)	1.1391 (5)	0.0493 (11)	
O4	0.9236 (2)	1.1345 (2)	1.0941 (5)	0.0472 (11)	
O5	0.9496 (2)	0.99873 (19)	0.8377 (4)	0.0375 (8)	
O6	0.9636 (2)	1.1151 (2)	0.6844 (4)	0.0400 (9)	
N1	0.5915 (3)	0.7460 (3)	0.9955 (6)	0.0420 (11)	
N2	0.6427 (3)	1.1970 (3)	1.2995 (6)	0.0467 (12)	
O1W	0.9949 (3)	0.72899 (19)	1.0725 (4)	0.0411 (9)	
H2W	1.012 (3)	0.698 (2)	0.999 (5)	0.062*	
H1W	0.974 (3)	0.696 (2)	1.138 (5)	0.062*	
C13	0.9284 (3)	1.0421 (3)	0.7094 (6)	0.0305 (11)	
C14	0.8508 (14)	1.0157 (19)	0.608 (3)	0.048 (4)	0.47 (5)
H14A	0.8496	0.9525	0.5953	0.071*	0.47 (5)
H14B	0.8506	1.0432	0.5000	0.071*	0.47 (5)
H14C	0.8031	1.0345	0.6656	0.071*	0.47 (5)
C14'	0.8691 (14)	1.0029 (16)	0.577 (3)	0.048 (4)	0.53 (5)
H14D	0.8380	1.0496	0.5221	0.071*	0.53 (5)
H14E	0.8318	0.9631	0.6293	0.071*	0.53 (5)
H14F	0.8997	0.9712	0.4966	0.071*	0.53 (5)
Cl1	0.58196 (10)	0.45830 (10)	0.2449 (2)	0.0586 (4)	0.440 (11)
O7	0.5413 (12)	0.5414 (9)	0.242 (2)	0.091 (8)	0.440 (11)
O8	0.6274 (10)	0.4512 (9)	0.3969 (14)	0.107 (6)	0.440 (11)
O9	0.5293 (9)	0.3894 (8)	0.216 (2)	0.123 (6)	0.440 (11)
O10	0.6425 (9)	0.4616 (9)	0.1148 (18)	0.124 (6)	0.440 (11)
Cl1'	0.58196 (10)	0.45830 (10)	0.2449 (2)	0.0586 (4)	0.560 (11)
O7'	0.5434 (8)	0.5371 (7)	0.201 (2)	0.080 (5)	0.560 (11)
O8'	0.6654 (5)	0.4696 (6)	0.2946 (18)	0.101 (4)	0.560 (11)
O9'	0.5408 (9)	0.4196 (8)	0.3857 (15)	0.139 (6)	0.560 (11)
O10'	0.5760 (8)	0.3951 (8)	0.1174 (13)	0.116 (5)	0.560 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.02057 (14)	0.01549 (13)	0.02745 (14)	-0.00121 (9)	0.00717 (9)	-0.00001 (9)
Ag1	0.0295 (3)	0.0884 (4)	0.0776 (4)	0.0140 (2)	0.0260 (2)	-0.0008 (3)
C1	0.023 (3)	0.024 (2)	0.026 (2)	-0.0023 (19)	0.0013 (19)	0.0000 (19)
C2	0.023 (3)	0.026 (2)	0.028 (3)	-0.0038 (19)	0.0054 (19)	-0.0029 (19)
C3	0.031 (3)	0.028 (3)	0.049 (3)	-0.004 (2)	0.013 (2)	-0.005 (2)
C4	0.034 (3)	0.041 (3)	0.066 (4)	-0.010 (3)	0.011 (3)	0.002 (3)
C5	0.026 (3)	0.040 (3)	0.051 (3)	0.008 (2)	0.012 (2)	0.002 (2)
C6	0.029 (3)	0.024 (2)	0.047 (3)	0.002 (2)	0.014 (2)	0.001 (2)
C7	0.031 (3)	0.025 (2)	0.056 (3)	0.001 (2)	0.019 (2)	0.002 (2)

C8	0.027 (3)	0.030 (2)	0.037 (3)	0.005 (2)	0.013 (2)	0.003 (2)
C9	0.034 (3)	0.028 (3)	0.063 (4)	-0.005 (2)	0.017 (3)	-0.004 (3)
C10	0.031 (3)	0.047 (3)	0.083 (5)	-0.009 (3)	0.019 (3)	0.005 (3)
C11	0.035 (3)	0.034 (3)	0.075 (4)	0.006 (2)	0.021 (3)	-0.009 (3)
C12	0.029 (3)	0.028 (3)	0.073 (4)	0.000 (2)	0.017 (3)	-0.003 (3)
O1	0.0282 (19)	0.0250 (16)	0.049 (2)	-0.0004 (14)	0.0150 (15)	-0.0096 (15)
O2	0.0237 (18)	0.0259 (16)	0.0371 (19)	-0.0067 (14)	0.0060 (14)	-0.0072 (14)
O3	0.044 (2)	0.0207 (17)	0.086 (3)	0.0039 (16)	0.038 (2)	0.0031 (17)
O4	0.039 (2)	0.0222 (17)	0.083 (3)	0.0019 (15)	0.036 (2)	0.0050 (17)
O5	0.050 (2)	0.0264 (16)	0.0346 (19)	-0.0114 (16)	-0.0101 (16)	0.0089 (15)
O6	0.053 (3)	0.0338 (18)	0.033 (2)	-0.0138 (17)	-0.0029 (16)	0.0100 (15)
N1	0.026 (3)	0.048 (3)	0.054 (3)	-0.004 (2)	0.014 (2)	0.002 (2)
N2	0.028 (3)	0.046 (3)	0.067 (3)	0.011 (2)	0.017 (2)	0.003 (2)
O1W	0.065 (3)	0.0229 (17)	0.037 (2)	0.0084 (18)	0.0223 (19)	0.0043 (15)
C13	0.035 (3)	0.030 (2)	0.026 (3)	-0.005 (2)	0.001 (2)	0.001 (2)
C14	0.047 (6)	0.048 (6)	0.048 (6)	-0.008 (5)	-0.007 (5)	0.003 (4)
C14'	0.047 (6)	0.048 (6)	0.048 (6)	-0.008 (5)	-0.007 (5)	0.003 (4)
C11	0.0610 (11)	0.0449 (8)	0.0692 (11)	0.0000 (8)	-0.0030 (8)	-0.0018 (8)
O7	0.097 (11)	0.085 (10)	0.090 (10)	0.023 (8)	0.000 (7)	-0.016 (7)
O8	0.130 (10)	0.104 (8)	0.083 (8)	0.032 (8)	-0.039 (7)	-0.001 (7)
O9	0.129 (10)	0.092 (8)	0.143 (11)	-0.067 (7)	-0.032 (8)	0.025 (7)
O10	0.130 (10)	0.120 (9)	0.125 (10)	0.036 (8)	0.045 (8)	0.001 (7)
C11'	0.0610 (11)	0.0449 (8)	0.0692 (11)	0.0000 (8)	-0.0030 (8)	-0.0018 (8)
O7'	0.071 (7)	0.071 (7)	0.100 (8)	0.030 (5)	0.024 (6)	0.043 (6)
O8'	0.065 (6)	0.079 (6)	0.158 (9)	-0.003 (5)	-0.016 (6)	-0.012 (6)
O9'	0.164 (10)	0.131 (8)	0.128 (8)	-0.020 (7)	0.068 (7)	0.039 (7)
O10'	0.127 (9)	0.122 (8)	0.097 (7)	0.022 (7)	-0.017 (6)	-0.058 (6)

Geometric parameters (Å, °)

Sm1—O2	2.345 (3)	C9—C10	1.364 (7)
Sm1—O3	2.352 (3)	C9—H9	0.9300
Sm1—O4 ⁱ	2.367 (3)	C10—N2	1.346 (6)
Sm1—O1 ⁱⁱ	2.371 (3)	C10—H10	0.9300
Sm1—O5	2.414 (3)	C11—N2	1.337 (7)
Sm1—O1W	2.440 (3)	C11—C12	1.364 (7)
Sm1—O6 ⁱ	2.476 (3)	C11—H11	0.9300
Sm1—O5 ⁱ	2.521 (3)	C12—H12	0.9300
Sm1—C13 ⁱ	2.892 (5)	O1—Sm1 ^{iv}	2.371 (3)
Sm1—Sm1 ⁱ	3.9263 (5)	O4—Sm1 ⁱ	2.367 (3)
Ag1—N2	2.148 (4)	O5—C13	1.249 (5)
Ag1—N1 ⁱⁱⁱ	2.149 (4)	O5—Sm1 ⁱ	2.521 (3)
C1—O1	1.252 (5)	O6—C13	1.262 (5)
C1—O2	1.264 (5)	O6—Sm1 ⁱ	2.476 (3)
C1—C2	1.495 (6)	N1—Ag1 ^v	2.149 (4)
C2—C3	1.375 (6)	O1W—H2W	0.81 (4)
C2—C6	1.375 (6)	O1W—H1W	0.81 (4)

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C3—C4	1.382 (7)	C13—C14	1.511 (10)
C3—H3	0.9300	C13—C14'	1.511 (9)
C4—N1	1.341 (6)	C13—Sm1 ⁱ	2.892 (5)
C4—H4	0.9300	C14—H14A	0.9600
C5—N1	1.333 (6)	C14—H14B	0.9600
C5—C6	1.373 (6)	C14—H14C	0.9600
C5—H5	0.9300	C14'—H14D	0.9600
C6—H6	0.9300	C14'—H14E	0.9600
C7—O3	1.248 (5)	C14'—H14F	0.9600
C7—O4	1.267 (6)	C11—O9	1.357 (9)
C7—C8	1.500 (6)	C11—O8	1.391 (9)
C8—C9	1.376 (7)	C11—O7	1.417 (10)
C8—C12	1.381 (6)	C11—O10	1.464 (9)
O2—Sm1—O3	105.57 (13)	C5—C6—H6	120.4
O2—Sm1—O4 ⁱ	90.42 (12)	C2—C6—H6	120.4
O3—Sm1—O4 ⁱ	137.99 (11)	O3—C7—O4	125.7 (4)
O2—Sm1—O1 ⁱⁱ	85.29 (11)	O3—C7—C8	116.7 (4)
O3—Sm1—O1 ⁱⁱ	75.00 (10)	O4—C7—C8	117.6 (4)
O4 ⁱ —Sm1—O1 ⁱⁱ	146.13 (10)	C9—C8—C12	118.3 (4)
O2—Sm1—O5	77.05 (10)	C9—C8—C7	119.9 (4)
O3—Sm1—O5	71.54 (12)	C12—C8—C7	121.8 (4)
O4 ⁱ —Sm1—O5	74.83 (12)	C10—C9—C8	119.9 (5)
O1 ⁱⁱ —Sm1—O5	135.91 (12)	C10—C9—H9	120.1
O2—Sm1—O1W	78.25 (13)	C8—C9—H9	120.1
O3—Sm1—O1W	148.79 (11)	N2—C10—C9	122.1 (5)
O4 ⁱ —Sm1—O1W	71.75 (11)	N2—C10—H10	118.9
O1 ⁱⁱ —Sm1—O1W	74.48 (11)	C9—C10—H10	118.9
O5—Sm1—O1W	137.85 (11)	N2—C11—C12	123.4 (5)
O2—Sm1—O6 ⁱ	155.64 (10)	N2—C11—H11	118.3
O3—Sm1—O6 ⁱ	91.24 (14)	C12—C11—H11	118.3
O4 ⁱ —Sm1—O6 ⁱ	88.48 (14)	C11—C12—C8	118.8 (5)
O1 ⁱⁱ —Sm1—O6 ⁱ	82.17 (11)	C11—C12—H12	120.6
O5—Sm1—O6 ⁱ	125.83 (10)	C8—C12—H12	120.6
O1W—Sm1—O6 ⁱ	78.31 (12)	C1—O1—Sm1 ^{iv}	148.9 (3)
O2—Sm1—O5 ⁱ	150.36 (10)	C1—O2—Sm1	137.3 (3)
O3—Sm1—O5 ⁱ	73.42 (13)	C7—O3—Sm1	140.5 (3)
O4 ⁱ —Sm1—O5 ⁱ	73.96 (12)	C7—O4—Sm1 ⁱ	134.8 (3)
O1 ⁱⁱ —Sm1—O5 ⁱ	121.62 (11)	C13—O5—Sm1	160.4 (3)
O5—Sm1—O5 ⁱ	74.62 (12)	C13—O5—Sm1 ⁱ	94.0 (3)
O1W—Sm1—O5 ⁱ	118.44 (13)	Sm1—O5—Sm1 ⁱ	105.38 (12)
O6 ⁱ —Sm1—O5 ⁱ	51.22 (10)	C13—O6—Sm1 ⁱ	95.9 (3)
O2—Sm1—C13 ⁱ	169.71 (12)	C5—N1—C4	117.6 (4)
O3—Sm1—C13 ⁱ	82.55 (14)	C5—N1—Ag1 ^v	123.2 (3)

O4 ⁱ —Sm1—C13 ⁱ	79.29 (14)	C4—N1—Ag1 ^v	119.2 (3)
O1 ⁱⁱ —Sm1—C13 ⁱ	103.16 (12)	C11—N2—C10	117.5 (4)
O5—Sm1—C13 ⁱ	100.12 (12)	C11—N2—Ag1	126.6 (4)
O1W—Sm1—C13 ⁱ	98.16 (14)	C10—N2—Ag1	115.6 (4)
O6 ⁱ —Sm1—C13 ⁱ	25.73 (11)	Sm1—O1W—H2W	127 (3)
O5 ⁱ —Sm1—C13 ⁱ	25.53 (11)	Sm1—O1W—H1W	121 (3)
O2—Sm1—Sm1 ⁱ	114.86 (7)	H2W—O1W—H1W	106 (4)
O3—Sm1—Sm1 ⁱ	67.80 (8)	O5—C13—O6	118.7 (4)
O4 ⁱ —Sm1—Sm1 ⁱ	70.22 (7)	O5—C13—C14	119.1 (11)
O1 ⁱⁱ —Sm1—Sm1 ⁱ	141.10 (7)	O6—C13—C14	121.0 (11)
O5—Sm1—Sm1 ⁱ	38.26 (8)	O5—C13—C14'	120.4 (10)
O1W—Sm1—Sm1 ⁱ	139.62 (10)	O6—C13—C14'	120.5 (10)
O6 ⁱ —Sm1—Sm1 ⁱ	87.58 (7)	C14—C13—C14'	16.7 (16)
O5 ⁱ —Sm1—Sm1 ⁱ	36.36 (7)	O5—C13—Sm1 ⁱ	60.4 (2)
C13 ⁱ —Sm1—Sm1 ⁱ	61.87 (9)	O6—C13—Sm1 ⁱ	58.4 (2)
N2—Ag1—N1 ⁱⁱⁱ	166.24 (17)	C14—C13—Sm1 ⁱ	165.6 (14)
O1—C1—O2	123.7 (4)	C14'—C13—Sm1 ⁱ	177.6 (12)
O1—C1—C2	118.2 (4)	C13—C14—H14A	109.5
O2—C1—C2	118.1 (4)	C13—C14—H14B	109.5
C3—C2—C6	118.2 (4)	C13—C14—H14C	109.5
C3—C2—C1	120.0 (4)	C13—C14'—H14D	109.5
C6—C2—C1	121.8 (4)	C13—C14'—H14E	109.5
C2—C3—C4	119.6 (4)	H14D—C14'—H14E	109.5
C2—C3—H3	120.2	C13—C14'—H14F	109.5
C4—C3—H3	120.2	H14D—C14'—H14F	109.5
N1—C4—C3	122.2 (5)	H14E—C14'—H14F	109.5
N1—C4—H4	118.9	O9—C11—O8	112.8 (7)
C3—C4—H4	118.9	O9—C11—O7	113.0 (9)
N1—C5—C6	123.2 (4)	O8—C11—O7	108.0 (8)
N1—C5—H5	118.4	O9—C11—O10	110.1 (8)
C6—C5—H5	118.4	O8—C11—O10	106.2 (8)
C5—C6—C2	119.3 (4)	O7—C11—O10	106.5 (8)

Symmetry codes: (i) $-x+2, -y+2, -z+2$; (ii) $x, -y+3/2, z+1/2$; (iii) $-x+1, y+1/2, -z+5/2$; (iv) $x, -y+3/2, z-1/2$; (v) $-x+1, y-1/2, -z+5/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H2W \cdots O6 ^{vi}	0.81 (4)	1.98 (4)	2.785 (4)	171 (6)
O1W—H1W \cdots O2 ⁱⁱ	0.81 (4)	2.22 (3)	2.921 (5)	146 (5)

Symmetry codes: (vi) $-x+2, y-1/2, -z+3/2$; (ii) $x, -y+3/2, z+1/2$.

Fig. 2

