addenda and errata

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Poly[[di- μ_3 -nicotinato- μ_3 -oxalato-samarium(III)silver(I)] dihydrate]. Corrigendum

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The title of the paper by Zhu, Zhao & Yu [*Acta Cryst.* (2009), E**65**, m1105] is corrected.

In the paper by Zhu *et al.* (2009), the chemical name given in the *Title* should be 'Poly[[tetra- μ_3 -nicotinato- μ_4 -oxalato- μ_2 -oxalato-disamarium(III)disilver(I)] tetrahydrate]'. The revised scheme is shown below.



References

Zhu, L.-C., Zhao, Z.-G. & Yu, S.-J. (2009). Acta Cryst. E65, m1105.

V = 1769.4 (2) Å³

Mo $K\alpha$ radiation

 $0.23 \times 0.20 \times 0.19 \text{ mm}$

8972 measured reflections

3171 independent reflections

2995 reflections with $I > 2\sigma(I)$

 $\mu = 4.45 \text{ mm}^-$

T = 296 K

 $R_{\rm int} = 0.027$

Z = 4

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Poly[[di- μ_3 -nicotinato- μ_3 -oxalato-samarium(III)silver(I)] dihvdrate]

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.006 Å; R factor = 0.023; wR factor = 0.052; data-to-parameter ratio = 12.5.

In the title three-dimensional heterometallic complex, $\{[AgSm(C_6H_4NO_2)_2(C_2O_4)] \cdot 2H_2O\}_n$, the Sm^{III} ion is eightcoordinated by four O atoms from four different nicotinate ligands and four O atoms from two different oxalate ligands. The three-coordinate Ag^I ion is bonded to two N atoms from two different nicotinate anions and one O atom from an oxalate anion. These metal coordination units are connected by bridging nicotinate and oxalate ligands, generating a threedimensional network. The uncoordinated water molecules link the carboxylate groups *via* $O-H \cdots O$ hydrogen bonding. The crystal structure is further stabilized by hydrogen bonds between the water molecules.

Related literature

For theapplications of lanthanide-transition metal heterometallic complexes with bridging multifunctional organic ligands, see: Cheng et al. (2006); Kuang et al. (2007); Luo et al. (2007); Peng et al. (2008).



Experimental

Crystal data

 $[AgSm(C_6H_4NO_2)_2(C_2O_4)]\cdot 2H_2O$ $M_r = 626.49$ Monoclinic, $P2_1/c$ a = 9.7145 (9) Åb = 22.3444 (15) Å c = 9.1726 (6) Å $\beta = 117.295 (1)^{\circ}$

Data collection

Bruker APEXII area-detector diffractometer Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\min} = 0.374, T_{\max} = 0.429$

Refinement

ŀ

V 5

3

$R[F^2 > 2\sigma(F^2)] = 0.023$	254 parameters
$vR(F^2) = 0.052$	H-atom parameters constrained
S = 1.12	$\Delta \rho_{\rm max} = 0.84 \ {\rm e} \ {\rm \AA}^{-3}$
171 reflections	$\Delta \rho_{\rm min} = -0.65 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
O1W−H1W···O7 ⁱ	0.86	2.10	2.960 (5)	175
$O1W - H2W \cdot \cdot \cdot O2W$	0.86	2.06	2.892 (7)	161
$O2W - H4W \cdots O1W^{i}$	0.87	1.92	2.780 (7)	171

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

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: SHELXL97.

The authors acknowledge South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2185).

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supporting information

Acta Cryst. (2009). E65, m1105 [doi:10.1107/S1600536809032115]

Poly[[di-µ₃-nicotinato-µ₃-oxalato-samarium(III)silver(I)] dihydrate]

Li-Cai Zhu, Zhen-Gang Zhao and Shu-Juan Yu

S1. Comment

In the past few years, lanthanide-transition metal heterometallic complexs with bridging multifunctionnal organic ligands have generated much interest, not only because of their impressive topological structures, but also due to their versatile applications in ion exchange, magnetism, bimetallic catalysis and luminescent probe (Cheng *et al.*, 2006; Kuang *et al.*, 2007; Luo *et al.*, 2007; Luo *et al.*, 2008). As an extension of this research, we report here the structure of the title compound, a new heterometallic coordination polymer.

In the title compound (Fig. 1), there are one Sm^{III} ion, one Ag^I ion, two halves of oxalate ligand, two nicotinate ligands, and two lattice water molecules in the asymmetric unit. Each Sm^{III} ion is eight-coordinated by four O atoms from four different nicotinate ligands, and four O atoms of two different oxalate ligands. The Sm center can be described as having a bicapped trigonal prism coordination geometry. The three-coordinate Ag^I ion is bonded to two N atoms from two different nicotinate anions and one O atom from an oxalate anion. Thus the Ag^I ion is in a T-shaped configuration. These metal coordination units are connected by bridging nicotinate and oxalate ligands, generating a three-dimensional network (Fig. 2). The uncoordinated water molecules link the carboxylate groups by O—H…O hydrogen bonding (Table 1). The crystal structure is further stabilized by hydrogen bonds.

S2. Experimental

A mixture of AgNO₃ (0.057 g, 0.33 mmol), Sm_2O_3 (0.116 g, 0.33 mmol), nicotinic acid (0.164 g, 1.33 mmol), oxalic acid (0.119 g, 1.33 mmol), H_2O (7 ml), and $HClO_4$ (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. Colorless block crystals suitable for X-ray analysis were obtained.

S3. Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2$ $U_{eq}(C)$. H atoms of water molecules were found from difference Fourier maps and included in the refinements with a restraint of O—H = 0.86 - 0.87 Å and $U_{iso}(H) = 1.5$ $U_{eq}(O)$. The largest residual electron density in the final difference map was located at a distance of 0.82 Å from Ag2 atom and was meaningless.



Figure 1

The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Symmetry codes included in the atomic labels: (A) 2-x, 2-y, 1-z; (B) 1-x, 2-y, -z; (C) 1+x, y, z; (D) x, 1.5-y, -0.5+z; (E) 2-x, 0.5+y, 0.5-z.



Figure 2

A view of the three-dimensional structure of the title compound; dotted lines denote hydrogen bonds.

Poly[[di-µ₃-nicotinato-µ₃-oxalato-samarium(III)silver(I)] dihydrate]

Crystal data	
$[AgSm(C_6H_4NO_2)_2(C_2O_4)] \cdot 2H_2O$	F(000) = 1196
$M_r = 626.49$	$D_{\rm x} = 2.352 {\rm ~Mg} {\rm ~m}^{-3}$
Monoclinic, $P2_1/c$	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6346 reflections
a = 9.7145 (9) Å	$\theta = 2.4 - 27.8^{\circ}$
b = 22.3444 (15) Å	$\mu = 4.45 \text{ mm}^{-1}$
c = 9.1726 (6) Å	T = 296 K
$\beta = 117.295 (1)^{\circ}$	Block, colorless
V = 1769.4 (2) Å ³	$0.23 \times 0.20 \times 0.19 \text{ mm}$
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer Radiation source: fine-focus sealed tube Graphite monochromator φ and ω scans Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996) $T_{\min} = 0.374, T_{\max} = 0.429$ <i>Refinement</i>	8972 measured reflections 3171 independent reflections 2995 reflections with $I > 2\sigma(I)$ $R_{int} = 0.027$ $\theta_{max} = 25.2^{\circ}, \ \theta_{min} = 2.4^{\circ}$ $h = -5 \rightarrow 11$ $k = -26 \rightarrow 26$ $l = -10 \rightarrow 10$
Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.052$ S = 1.12 3171 reflections 254 parameters 0 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 $w = 1/[\sigma^2(F_o^2) + (0.0174P)^2 + 1.7329P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.002$ $\Delta\rho_{max} = 0.84$ e Å ⁻³ $\Delta\rho_{min} = -0.65$ e Å ⁻³ Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), Fc*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4} Extinction coefficient: 0.00351 (16)

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 $(Å^2)$

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Sm1	0.85715 (2)	0.991315 (8)	0.11767 (2)	0.01683 (8)	
Ag2	0.82067 (4)	0.852371 (14)	0.48309 (5)	0.04794 (12)	
01	0.8835 (3)	0.94402 (11)	0.3695 (3)	0.0275 (6)	
N1	0.6254 (4)	0.88411 (15)	0.5163 (4)	0.0346 (8)	
C4	0.3834 (4)	0.93617 (16)	0.4147 (4)	0.0231 (8)	
C3	0.4789 (5)	0.88129 (19)	0.6648 (5)	0.0368 (10)	
Н3	0.4696	0.8681	0.7560	0.044*	
C1	0.5154 (4)	0.91951 (17)	0.4047 (5)	0.0291 (9)	
H1	0.5291	0.9334	0.3166	0.035*	
C2	0.6042 (5)	0.86566 (19)	0.6441 (5)	0.0382 (10)	
H2	0.6788	0.8410	0.7221	0.046*	
C6	0.2586 (4)	0.97226 (16)	0.2811 (4)	0.0222 (8)	
C5	0.3662 (5)	0.91690 (17)	0.5490 (4)	0.0293 (9)	
Н5	0.2795	0.9279	0.5608	0.035*	
O3	0.2900 (3)	0.99674 (11)	0.1769 (3)	0.0284 (6)	

O2	0.1309 (3)	0.97383 (13)	0.2834 (3)	0.0313 (6)
N2	0.9619 (4)	0.78296 (14)	0.4537 (4)	0.0332 (8)
C7	0.9364 (4)	0.72618 (16)	0.4792 (5)	0.0287 (8)
H7	0.8605	0.7184	0.5117	0.034*
C9	1.1309 (5)	0.6899 (2)	0.4136 (5)	0.0390 (10)
H9	1.1876	0.6589	0.3994	0.047*
C8	1.0722 (5)	0.79305 (19)	0.4069 (5)	0.0408 (10)
H8	1.0903	0.8322	0.3859	0.049*
O7	0.6156 (3)	0.93618 (11)	0.0496 (3)	0.0253 (6)
C10	1.0169 (4)	0.67816 (16)	0.4599 (4)	0.0239 (8)
C12	1.1588 (5)	0.7483 (2)	0.3889 (6)	0.0490 (12)
H12	1.2365	0.7573	0.3600	0.059*
C13	0.9793 (4)	0.96697 (16)	0.5028 (4)	0.0207 (7)
08	1.0418 (3)	0.94114 (11)	0.6386 (3)	0.0255 (6)
O6	0.3580 (3)	0.94430 (11)	-0.0787 (3)	0.0280 (6)
O1W	0.6113 (6)	0.69616 (19)	0.5607 (5)	0.0925 (14)
H1W	0.6115	0.6576	0.5630	0.139*
H2W	0.5551	0.7081	0.6053	0.139*
O2W	0.4884 (7)	0.7331 (2)	0.7801 (6)	0.1179 (19)
H3W	0.4044	0.7508	0.7119	0.177*
H4W	0.5226	0.7525	0.8720	0.177*
C11	0.9771 (4)	0.61643 (15)	0.4922 (4)	0.0236 (8)
04	0.8882 (3)	0.61157 (11)	0.5557 (3)	0.0322 (6)
O5	1.0350 (3)	0.57246 (12)	0.4552 (3)	0.0353 (7)
C14	0.4919 (4)	0.96531 (16)	-0.0083 (4)	0.0216 (8)

Atomic displacement parameters (\mathring{A}^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.01410 (11)	0.01776 (12)	0.01771 (11)	0.00069 (7)	0.00649 (8)	0.00163 (7)
Ag2	0.0358 (2)	0.02335 (18)	0.0903 (3)	0.00795 (13)	0.0338 (2)	0.00929 (16)
01	0.0327 (16)	0.0290 (14)	0.0187 (12)	-0.0129 (12)	0.0100 (12)	-0.0031 (10)
N1	0.0243 (18)	0.0306 (19)	0.046 (2)	0.0061 (14)	0.0134 (16)	0.0060 (15)
C4	0.021 (2)	0.026 (2)	0.0181 (17)	-0.0007 (15)	0.0052 (15)	0.0010 (14)
C3	0.044 (3)	0.042 (3)	0.024 (2)	0.010 (2)	0.0148 (19)	0.0092 (17)
C1	0.023 (2)	0.032 (2)	0.032 (2)	0.0064 (16)	0.0126 (17)	0.0080 (17)
C2	0.032 (3)	0.037 (2)	0.034 (2)	0.0069 (19)	0.005 (2)	0.0100 (18)
C6	0.0167 (19)	0.0244 (19)	0.0190 (17)	0.0007 (15)	0.0027 (15)	-0.0008 (14)
C5	0.026 (2)	0.035 (2)	0.027 (2)	0.0038 (17)	0.0124 (17)	0.0024 (17)
03	0.0231 (15)	0.0376 (16)	0.0205 (13)	0.0005 (11)	0.0066 (11)	0.0056 (11)
O2	0.0161 (14)	0.0495 (17)	0.0254 (14)	0.0082 (12)	0.0070 (11)	0.0042 (12)
N2	0.0314 (19)	0.0210 (17)	0.048 (2)	0.0001 (14)	0.0188 (16)	0.0057 (15)
C7	0.024 (2)	0.023 (2)	0.041 (2)	0.0007 (16)	0.0171 (18)	0.0021 (16)
C9	0.036 (3)	0.037 (3)	0.053 (3)	0.0067 (19)	0.029 (2)	0.005 (2)
C8	0.044 (3)	0.031 (2)	0.053 (3)	-0.0032 (19)	0.026 (2)	0.010 (2)
O7	0.0179 (14)	0.0232 (13)	0.0326 (14)	0.0020 (11)	0.0097 (11)	0.0017 (11)
C10	0.022 (2)	0.0234 (19)	0.0251 (18)	0.0017 (15)	0.0098 (16)	-0.0018 (15)
C12	0.041 (3)	0.051 (3)	0.071 (3)	-0.002 (2)	0.040 (3)	0.011 (2)

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C13	0.0181 (19)	0.0234 (19)	0.0239 (19)	0.0007 (14)	0.0126 (16)	0.0006 (14)
08	0.0291 (15)	0.0218 (13)	0.0221 (13)	0.0012 (11)	0.0088 (11)	0.0022 (10)
O6	0.0179 (14)	0.0271 (14)	0.0371 (15)	-0.0011 (11)	0.0109 (12)	-0.0066 (11)
O1W	0.120 (4)	0.060 (3)	0.108 (3)	0.008 (3)	0.062 (3)	-0.012 (2)
O2W	0.147 (5)	0.100 (4)	0.106 (4)	0.027 (4)	0.056 (4)	0.012 (3)
C11	0.024 (2)	0.0162 (18)	0.0233 (18)	0.0018 (14)	0.0045 (16)	-0.0033 (14)
04	0.0308 (16)	0.0235 (14)	0.0488 (17)	-0.0014 (11)	0.0239 (14)	0.0039 (12)
05	0.0417 (18)	0.0265 (15)	0.0296 (14)	0.0111 (12)	0.0092 (13)	-0.0050 (11)
C14	0.021 (2)	0.025 (2)	0.0208 (18)	-0.0003 (15)	0.0115 (16)	-0.0035 (14)

Geometric parameters (Å, °)

Sm1—O5 ⁱ	2.340 (3)	N2—C7	1.334 (5)
Sm1—O2 ⁱⁱ	2.414 (2)	N2—C8	1.342 (5)
Sm1—O4 ⁱⁱⁱ	2.420 (3)	C7—C10	1.386 (5)
Sm1—O3 ^{iv}	2.424 (2)	С7—Н7	0.9300
Sm1—O6 ^{iv}	2.425 (2)	C9—C12	1.372 (6)
Sm1—01	2.444 (2)	C9—C10	1.381 (5)
Sm1—O7	2.464 (2)	С9—Н9	0.9300
Sm1—O8 ^v	2.496 (2)	C8—C12	1.366 (6)
Ag2—N2	2.168 (3)	C8—H8	0.9300
Ag2—N1	2.174 (3)	O7—C14	1.251 (4)
Ag2—O1	2.497 (2)	C10—C11	1.498 (5)
O1—C13	1.257 (4)	C12—H12	0.9300
N1—C2	1.344 (5)	C13—O8	1.249 (4)
N1—C1	1.346 (5)	C13—C13 ^v	1.537 (7)
C4—C1	1.378 (5)	O8—Sm1 ^v	2.496 (2)
C4—C5	1.385 (5)	O6—C14	1.249 (4)
C4—C6	1.504 (5)	O6—Sm1 ^{iv}	2.425 (2)
С3—С2	1.361 (6)	O1W—H1W	0.8624
С3—С5	1.376 (5)	O1W—H2W	0.8612
С3—Н3	0.9300	O2W—H3W	0.8629
C1—H1	0.9300	O2W—H4W	0.8667
С2—Н2	0.9300	C11—O4	1.249 (4)
C6—O2	1.251 (4)	C11—O5	1.253 (4)
С6—ОЗ	1.254 (4)	O4—Sm1 ^{vii}	2.420 (3)
С5—Н5	0.9300	O5—Sm1 ^{viii}	2.340 (3)
O3—Sm1 ^{iv}	2.424 (2)	C14C14 ^{iv}	1.559 (7)
O2—Sm1 ^{vi}	2.414 (2)		
O5 ⁱ —Sm1—O2 ⁱⁱ	78.29 (10)	N1—C2—C3	123.2 (4)
O5 ⁱ —Sm1—O4 ⁱⁱⁱ	123.28 (10)	N1—C2—H2	118.4
O2 ⁱⁱ —Sm1—O4 ⁱⁱⁱ	76.96 (9)	C3—C2—H2	118.4
O5 ⁱ —Sm1—O3 ^{iv}	73.05 (9)	O2—C6—O3	126.2 (3)
O2 ⁱⁱ —Sm1—O3 ^{iv}	129.50 (9)	O2—C6—C4	115.9 (3)
O4 ⁱⁱⁱ —Sm1—O3 ^{iv}	85.19 (9)	O3—C6—C4	117.9 (3)
O5 ⁱ —Sm1—O6 ^{iv}	88.09 (10)	C3—C5—C4	119.2 (4)
O2 ⁱⁱ —Sm1—O6 ^{iv}	144.58 (9)	С3—С5—Н5	120.4

$O4^{iii}$ — $Sm1$ — $O6^{iv}$	136.12 (9)	С4—С5—Н5	120.4
$O3^{iv}$ —Sm1— $O6^{iv}$	75.08 (9)	C6	132.3 (2)
O5 ⁱ —Sm1—O1	137.60 (8)	C6	143.9 (2)
O2 ⁱⁱ —Sm1—O1	74.16 (9)	C7—N2—C8	117.1 (4)
O4 ⁱⁱⁱ —Sm1—O1	80.84 (9)	C7—N2—Ag2	118.6 (3)
O3 ^{iv} —Sm1—O1	148.63 (9)	C8—N2—Ag2	124.2 (3)
O6 ^{iv} —Sm1—O1	96.06 (9)	N2-C7-C10	123.6 (4)
O5 ⁱ —Sm1—O7	144.52 (9)	N2—C7—H7	118.2
O2 ⁱⁱ —Sm1—O7	136.44 (9)	С10—С7—Н7	118.2
O4 ⁱⁱⁱ —Sm1—O7	70.86 (9)	C12—C9—C10	118.5 (4)
O3 ^{iv} —Sm1—O7	76.49 (9)	С12—С9—Н9	120.7
O6 ^{iv} —Sm1—O7	66.61 (8)	С10—С9—Н9	120.7
O1—Sm1—O7	72.42 (8)	N2—C8—C12	122.8 (4)
$O5^{i}$ — $Sm1$ — $O8^{v}$	75.15 (9)	N2—C8—H8	118.6
O2 ⁱⁱ —Sm1—O8 ^v	70.51 (9)	С12—С8—Н8	118.6
$O4^{iii}$ — $Sm1$ — $O8^{v}$	138.13 (9)	C14—O7—Sm1	117.7 (2)
$O3^{iv}$ —Sm1— $O8^{v}$	136.13 (8)	C9—C10—C7	118.1 (4)
$O6^{iv}$ —Sm1— $O8^{v}$	74.44 (8)	C9—C10—C11	123.5 (3)
$O1$ — $Sm1$ — $O8^{v}$	65.62 (8)	C7—C10—C11	118.4 (3)
$O7$ — $Sm1$ — $O8^{v}$	117.85 (8)	C8—C12—C9	119.8 (4)
N2—Ag2—N1	153.35 (12)	C8—C12—H12	120.1
N2—Ag2—O1	104.18 (11)	С9—С12—Н12	120.1
N1—Ag2—O1	100.77 (11)	O8—C13—O1	125.9 (3)
C13—O1—Sm1	116.9 (2)	O8—C13—C13 ^v	117.5 (4)
C13—O1—Ag2	98.2 (2)	O1—C13—C13 ^v	116.6 (4)
Sm1—O1—Ag2	144.02 (10)	C13—O8—Sm1 ^v	115.2 (2)
C2—N1—C1	117.2 (4)	C14—O6—Sm1 ^{iv}	118.5 (2)
C2—N1—Ag2	120.9 (3)	H1W—O1W—H2W	106.9
C1—N1—Ag2	121.7 (3)	H3W—O2W—H4W	106.8
C1—C4—C5	118.1 (3)	O4—C11—O5	123.4 (3)
C1—C4—C6	121.2 (3)	O4—C11—C10	118.0 (3)
C5—C4—C6	120.7 (3)	O5—C11—C10	118.7 (3)
C2—C3—C5	119.1 (4)	C11—O4—Sm1 ^{vii}	112.3 (2)
С2—С3—Н3	120.5	C11—O5—Sm1 ^{viii}	179.0 (3)
С5—С3—Н3	120.5	O6—C14—O7	126.5 (3)
N1-C1-C4	123.1 (4)	O6-C14-C14 ^{iv}	117.3 (4)
N1-C1-H1	118.4	O7—C14—C14 ^{iv}	116.2 (4)
C4—C1—H1	118.4		

Symmetry codes: (i) -*x*+2, *y*+1/2, -*z*+1/2; (ii) *x*+1, *y*, *z*; (iii) *x*, -*y*+3/2, *z*-1/2; (iv) -*x*+1, -*y*+2, -*z*; (v) -*x*+2, -*y*+2, -*z*+1; (vi) *x*-1, *y*, *z*; (vii) *x*, -*y*+3/2, *z*+1/2; (viii) -*x*+2, *y*-1/2, -*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
O1 <i>W</i> —H1 <i>W</i> ···O7 ^{vii}	0.86	2.10	2.960 (5)	175

			supportin	supporting information		
O1 <i>W</i> —H2 <i>W</i> ···O2 <i>W</i>	0.86	2.06	2.892 (7)	161		
$O2W - H4W \cdots O1W^{\text{vii}}$	0.87	1.92	2.780 (7)	171		

Symmetry code: (vii) x, -y+3/2, z+1/2.