

Poly[[μ_2 -acetato-aquadi- μ_3 -isonicotinato-erbium(III)silver(I)] perchlorate]

Li-Cai Zhu

School of Chemistry and Environment, South China Normal University, Guangzhou 510631, People's Republic of China

Correspondence e-mail: licai Zhu1977@yahoo.com.cn

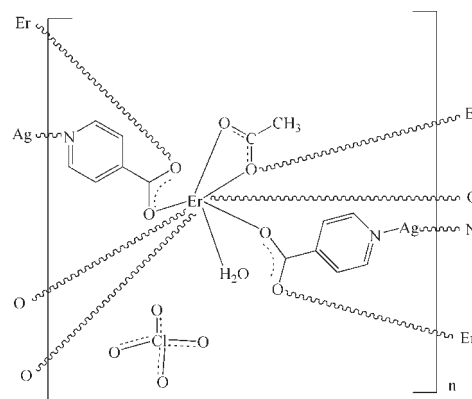
Received 4 November 2009; accepted 14 November 2009

 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; disorder in main residue; R factor = 0.025; wR factor = 0.057; data-to-parameter ratio = 10.7.

In the title three-dimensional heterometallic complex, $\{[\text{AgEr}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]\text{ClO}_4\}_n$, the eight-coordinate Er^{III} ion adopts a distorted bicapped trigonal-prismatic geometry, being coordinated by four O atoms from four different isonicotinate ligands, three O atoms from two different acetate ligands and one O atom of the water molecule. The two-coordinate Ag^{I} ion is surrounded by two N atoms from two different isonicotinate anions in a slightly bent configuration. These building blocks are connected by bridging isonicotinate and acetate ligands, generating a three-dimensional network. This structure is consolidated by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding between the coordinated water molecule and a carboxylate group of the acetate ligand. The perchlorate anion is disordered over two sites with site-occupancy factors of 0.526 (13) and 0.474 (13), while the methyl group of the acetate ligand is equally disordered over two sites.

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

$[\text{AgEr}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]\text{ClO}_4$
 $M_r = 695.84$
 Monoclinic, $P2_1/c$
 $a = 16.1952$ (11) Å
 $b = 14.8673$ (11) Å
 $c = 7.8938$ (6) Å

$\beta = 91.783$ (1)°
 $V = 1899.7$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.62$ mm⁻¹
 $T = 296$ K
 $0.23 \times 0.20 \times 0.19$ mm

Data collection

Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.285$, $T_{\text{max}} = 0.344$

9611 measured reflections
 3423 independent reflections
 3009 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.057$
 $S = 1.05$
 3423 reflections
 320 parameters
 158 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.76$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.04$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H2W}\cdots\text{O4}^{\text{i}}$	0.82 (4)	2.19 (3)	2.891 (5)	145 (5)
$\text{O1W}-\text{H1W}\cdots\text{O6}^{\text{ii}}$	0.81 (4)	1.99 (4)	2.786 (5)	167 (6)

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

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: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

The author acknowledges South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2280).

References

- Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc, Madison, Wisconsin, USA.
- Cheng, J.-W., Zhang, J., Zheng, S.-T., Zhang, M.-B. & Yang, G.-Y. (2006). *Angew. Chem. Int. Ed.* **45**, 73–77.
- Kuang, D.-Z., Feng, Y.-L., Peng, Y.-L. & Deng, Y.-F. (2007). *Acta Cryst.* **E63**, m2526–m2527.
- Peng, G., Qiu, Y.-C., Hu, Z.-H., Li, Y.-H., Liu, B. & Deng, H. (2008). *Inorg. Chem. Commun.* **11**, 1409–1411.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Zhu, L.-C., Zhao, Z.-G. & Yu, S.-J. (2009). *Acta Cryst.* **E65**, m1105.

supplementary materials

Acta Cryst. (2009). E65, m1617-m1618 [doi:10.1107/S1600536809048429]

Poly[[μ_2 -acetato-aquadi- μ_3 -isonicotinato-erbium(III)silver(I)] perchlorate]

L.-C. Zhu

Comment

In the past few years, lanthanide-transition metal heterometallic complexes with bridging multifunctional organic ligands gained increasing interest, not only because of their crystal structures, but also due to their applications in ion exchange, magnetism, catalysis and as luminescent material (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 heterometallic coordination polymer, (I), has been determined and is presented in this article.

In the title compound (Fig. 1), there are one Er^{III} ion, one Ag^I ion, two halves of an acetate ligand, two isonicotinate ligands, one coordinated water molecule, and one perchlorate anion in the asymmetric unit. Each Er^{III} ion is eight-coordinated by four O atoms from four different isonicotinate ligands [Er—O distances ranging from 2.266 (3) to 2.308 (3) Å], three O atoms from two different acetate ligands [Er—O distances ranging from 2.341 (3) to 2.454 (3) Å], and one O atom of water molecule [Er—O distance 2.369 (3) Å]. The Er center can be described as having a distorted bicapped trigonal-prismatic coordination geometry. The two-coordinated Ag^I ion is bonded to two N atoms from two different isonicotinate anions [Ag—N distances 2.153 (4) and 2.154 (4) Å] and adopts a slight distortion from linearity with an N1—Ag1—N2 angle of 165.44 (19) °. These metal coordination units are connected by bridging isonicotinate and acetate ligands, generating a three-dimensional network (Fig. 2). The coordinated water molecules exhibit O—H···O hydrogen bonding to the uncoordinated O atom of a carboxylate group and to the acetate ligand (Table 1).

Experimental

A mixture of AgNO₃ (0.057 g, 0.33 mmol), Er₂O₃ (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 and then slowly cooled to room temperature. The product was collected by filtration, washed with water and was air-dried. Colorless 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 $U_{iso}(H) = 1.2$ or $1.5 U_{eq}(C)$. H atoms of water molecules were found from difference Fourier maps and refined isotropically with a restraint of O—H = 0.81 - 0.82 Å. The perchlorate anion is disordered over two sites with site occupancy factors 0.526 (13) and 0.474 (13), whereas the methyl group of the acetate ligand is disordered over two sites with site occupancy factors 0.51 (5) and 0.49 (5).

Figures

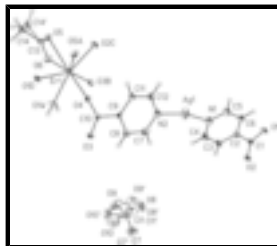


Fig. 1. The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Both disorder components are shown. Symmetry codes: (A) $2 - x, 2 - y, -z$; (B) $x, 1.5 - y, 1/2 + z$; (C) $1 - x, 1/2 + y, 0.5 - z$; (D) $1 + x, 1.5 - y, -1/2 + z$.

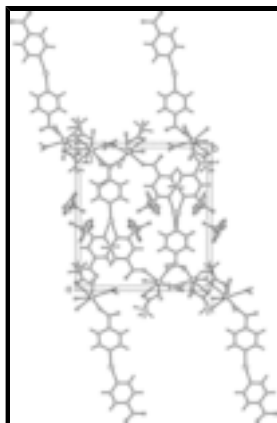


Fig. 2. A view of the three-dimensional arrangement of the title compound. Hydrogen atoms were omitted for clarity.

Poly[[μ_2 -acetato-aquadi- μ_3 -isonicotinato-erbium(III)silver(I)] perchlorate]

Crystal data

[AgEr(C₆H₄NO₂)₂(C₂H₃O₂)(H₂O)]ClO₄

$M_r = 695.84$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 16.1952 (11) \text{ \AA}$

$b = 14.8673 (11) \text{ \AA}$

$c = 7.8938 (6) \text{ \AA}$

$\beta = 91.7830 (10)^\circ$

$V = 1899.7 (2) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1324$

$D_x = 2.433 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4797 reflections

$\theta = 2.5\text{--}27.9^\circ$

$\mu = 5.62 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

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

Data collection

Bruker APEXII area-detector diffractometer

3423 independent reflections

Radiation source: fine-focus sealed tube

3009 reflections with $I > 2\sigma(I)$

Monochromator: graphite

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

$T = 296 \text{ K}$

$\theta_{\text{max}} = 25.2^\circ$

φ and ω scan

$\theta_{\text{min}} = 1.9^\circ$

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

$h = -19 \rightarrow 19$

$T_{\min} = 0.285$, $T_{\max} = 0.344$
9611 measured reflections

$k = -17 \rightarrow 17$
 $l = -5 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0218P)^2 + 3.7155P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3423 reflections	$(\Delta/\sigma)_{\max} = 0.002$
320 parameters	$\Delta\rho_{\max} = 0.76 \text{ e } \text{\AA}^{-3}$
158 restraints	$\Delta\rho_{\min} = -1.04 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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)
Er1	0.955305 (12)	0.883792 (13)	0.05025 (3)	0.01689 (8)	
Ag1	0.47352 (3)	0.74056 (4)	0.10055 (8)	0.06366 (18)	
N1	0.3573 (3)	0.6969 (3)	0.1973 (7)	0.0464 (13)	
N2	0.5953 (3)	0.7481 (3)	-0.0007 (6)	0.0378 (11)	
C1	0.1321 (3)	0.5802 (3)	0.3629 (7)	0.0287 (12)	
C2	0.2108 (3)	0.6229 (3)	0.3048 (7)	0.0273 (11)	
C3	0.2810 (3)	0.5718 (4)	0.2968 (8)	0.0427 (15)	
H8	0.2800	0.5114	0.3271	0.051*	
C4	0.3527 (4)	0.6105 (4)	0.2436 (9)	0.0523 (18)	
H7	0.4000	0.5753	0.2397	0.063*	
C5	0.2890 (3)	0.7466 (4)	0.2066 (9)	0.0455 (16)	
H11	0.2914	0.8070	0.1767	0.055*	
C6	0.2147 (3)	0.7121 (4)	0.2589 (8)	0.0378 (14)	
H10	0.1681	0.7485	0.2630	0.045*	

supplementary materials

C7	0.6342 (3)	0.6716 (4)	-0.0395 (8)	0.0438 (15)	
H4	0.6076	0.6171	-0.0221	0.053*	
C8	0.7122 (3)	0.6709 (4)	-0.1041 (7)	0.0340 (13)	
H3	0.7372	0.6167	-0.1315	0.041*	
C9	0.7531 (3)	0.7512 (3)	-0.1281 (6)	0.0199 (10)	
C10	0.8387 (3)	0.7511 (3)	-0.1972 (6)	0.0203 (10)	
C11	0.7136 (3)	0.8299 (3)	-0.0871 (7)	0.0309 (12)	
H6	0.7394	0.8851	-0.1018	0.037*	
C12	0.6349 (3)	0.8258 (4)	-0.0237 (7)	0.0359 (13)	
H5	0.6085	0.8792	0.0040	0.043*	
O1	0.0753 (2)	0.6328 (2)	0.4074 (5)	0.0354 (9)	
O2	0.1298 (2)	0.4963 (2)	0.3618 (5)	0.0369 (9)	
O3	0.85978 (19)	0.6842 (2)	-0.2806 (4)	0.0276 (8)	
O4	0.88366 (18)	0.8187 (2)	-0.1684 (4)	0.0237 (7)	
O1W	0.9992 (2)	0.7323 (2)	0.0767 (5)	0.0327 (9)	
H1W	1.017 (3)	0.702 (3)	0.001 (5)	0.049*	
H2W	0.978 (3)	0.697 (3)	0.142 (5)	0.049*	
O6	1.0346 (2)	0.8847 (2)	0.3130 (4)	0.0324 (8)	
O5	1.0476 (2)	1.0034 (2)	0.1567 (4)	0.0289 (8)	
C13	1.0687 (3)	0.9591 (3)	0.2875 (6)	0.0266 (11)	
C14	1.1431 (13)	0.9863 (19)	0.395 (3)	0.040 (4)	0.51 (5)
H14A	1.1728	1.0327	0.3385	0.059*	0.51 (5)
H14B	1.1785	0.9351	0.4129	0.059*	0.51 (5)
H14C	1.1255	1.0082	0.5024	0.059*	0.51 (5)
C14'	1.1264 (15)	1.0028 (19)	0.417 (3)	0.040 (4)	0.49 (5)
H14D	1.1142	1.0659	0.4230	0.059*	0.49 (5)
H14E	1.1824	0.9947	0.3836	0.059*	0.49 (5)
H14F	1.1191	0.9756	0.5255	0.059*	0.49 (5)
C11	0.58069 (12)	0.04095 (12)	0.7436 (3)	0.0642 (5)	0.526 (13)
O7	0.5433 (10)	-0.0457 (8)	0.742 (2)	0.076 (5)	0.526 (13)
O8	0.5249 (9)	0.1082 (9)	0.709 (2)	0.133 (6)	0.526 (13)
O9	0.6203 (10)	0.0528 (9)	0.9021 (14)	0.109 (6)	0.526 (13)
O10	0.6454 (9)	0.0386 (10)	0.6206 (19)	0.134 (7)	0.526 (13)
C11'	0.58069 (12)	0.04095 (12)	0.7436 (3)	0.0642 (5)	0.474 (13)
O7'	0.5399 (11)	-0.0369 (9)	0.691 (2)	0.083 (7)	0.474 (13)
O8'	0.5676 (11)	0.1101 (10)	0.6227 (19)	0.124 (7)	0.474 (13)
O9'	0.5422 (11)	0.0751 (11)	0.8943 (18)	0.134 (7)	0.474 (13)
O10'	0.6643 (6)	0.0289 (8)	0.778 (2)	0.092 (5)	0.474 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01467 (12)	0.01458 (12)	0.02167 (13)	-0.00074 (8)	0.00453 (8)	0.00002 (8)
Ag1	0.0248 (2)	0.0863 (4)	0.0813 (4)	-0.0136 (2)	0.0248 (3)	0.0023 (3)
N1	0.025 (2)	0.047 (3)	0.067 (4)	-0.007 (2)	0.017 (2)	0.000 (3)
N2	0.021 (2)	0.045 (3)	0.048 (3)	-0.003 (2)	0.013 (2)	0.000 (2)
C1	0.028 (3)	0.020 (3)	0.039 (3)	-0.005 (2)	0.012 (2)	-0.003 (2)
C2	0.024 (3)	0.028 (3)	0.031 (3)	-0.005 (2)	0.009 (2)	-0.003 (2)

C3	0.025 (3)	0.029 (3)	0.075 (5)	0.002 (2)	0.015 (3)	0.001 (3)
C4	0.026 (3)	0.048 (4)	0.084 (5)	0.004 (3)	0.017 (3)	0.000 (3)
C5	0.031 (3)	0.036 (3)	0.071 (5)	-0.009 (3)	0.016 (3)	0.009 (3)
C6	0.027 (3)	0.030 (3)	0.058 (4)	-0.001 (2)	0.015 (3)	0.005 (3)
C7	0.035 (3)	0.036 (3)	0.061 (4)	-0.016 (3)	0.012 (3)	0.002 (3)
C8	0.029 (3)	0.026 (3)	0.048 (4)	-0.003 (2)	0.012 (3)	-0.001 (2)
C9	0.016 (2)	0.023 (3)	0.020 (3)	-0.0031 (19)	0.0016 (19)	-0.0025 (19)
C10	0.018 (2)	0.023 (3)	0.021 (3)	0.0015 (19)	0.0023 (19)	0.002 (2)
C11	0.021 (2)	0.026 (3)	0.046 (3)	-0.004 (2)	0.010 (2)	-0.001 (2)
C12	0.026 (3)	0.035 (3)	0.047 (4)	0.007 (2)	0.012 (3)	0.002 (3)
O1	0.0258 (19)	0.0208 (19)	0.061 (3)	-0.0007 (15)	0.0249 (19)	0.0012 (16)
O2	0.0296 (19)	0.0196 (19)	0.063 (3)	-0.0016 (15)	0.0227 (18)	-0.0038 (17)
O3	0.0246 (17)	0.0214 (18)	0.037 (2)	-0.0021 (14)	0.0110 (16)	-0.0082 (15)
O4	0.0179 (16)	0.0250 (18)	0.0283 (19)	-0.0051 (14)	0.0042 (14)	-0.0058 (14)
O1W	0.045 (2)	0.0204 (18)	0.034 (2)	0.0068 (16)	0.0164 (18)	0.0022 (15)
O6	0.039 (2)	0.033 (2)	0.025 (2)	-0.0065 (16)	-0.0043 (16)	0.0089 (15)
O5	0.0335 (19)	0.0248 (18)	0.028 (2)	-0.0076 (15)	-0.0089 (16)	0.0043 (15)
C13	0.030 (3)	0.023 (3)	0.027 (3)	-0.001 (2)	-0.001 (2)	0.000 (2)
C14	0.038 (6)	0.042 (6)	0.037 (5)	-0.003 (5)	-0.011 (5)	0.000 (4)
C14'	0.038 (6)	0.042 (6)	0.037 (5)	-0.003 (5)	-0.011 (5)	0.000 (4)
Cl1	0.0638 (11)	0.0528 (10)	0.0756 (13)	0.0017 (9)	-0.0046 (10)	-0.0013 (9)
O7	0.071 (8)	0.070 (8)	0.089 (9)	-0.025 (6)	0.001 (6)	-0.009 (6)
O8	0.140 (10)	0.104 (9)	0.153 (11)	0.074 (7)	-0.032 (8)	-0.019 (7)
O9	0.134 (10)	0.110 (8)	0.081 (8)	-0.042 (7)	-0.036 (7)	0.001 (6)
O10	0.133 (10)	0.143 (10)	0.130 (10)	-0.033 (8)	0.052 (8)	-0.008 (8)
Cl1'	0.0638 (11)	0.0528 (10)	0.0756 (13)	0.0017 (9)	-0.0046 (10)	-0.0013 (9)
O7'	0.073 (9)	0.081 (9)	0.096 (10)	-0.033 (7)	0.011 (7)	-0.034 (7)
O8'	0.137 (11)	0.121 (10)	0.113 (10)	-0.009 (8)	-0.012 (8)	0.056 (8)
O9'	0.150 (11)	0.138 (10)	0.118 (10)	0.017 (8)	0.064 (8)	-0.032 (8)
O10'	0.054 (6)	0.077 (7)	0.144 (11)	0.004 (5)	-0.023 (7)	0.009 (7)

Geometric parameters (Å, °)

Er1—O4	2.266 (3)	C11—C12	1.386 (7)
Er1—O2 ⁱ	2.289 (3)	C11—H6	0.9300
Er1—O1 ⁱⁱ	2.290 (3)	C12—H5	0.9300
Er1—O3 ⁱⁱⁱ	2.308 (3)	O1—Er1 ^v	2.290 (3)
Er1—O5 ^{iv}	2.341 (3)	O2—Er1 ^{vi}	2.289 (3)
Er1—O1W	2.369 (3)	O3—Er1 ^{vii}	2.308 (3)
Er1—O6	2.405 (3)	O1W—H1W	0.81 (4)
Er1—O5	2.454 (3)	O1W—H2W	0.82 (4)
Ag1—N1	2.153 (4)	O6—C13	1.256 (6)
Ag1—N2	2.154 (4)	O5—C13	1.263 (6)
N1—C5	1.336 (7)	O5—Er1 ^{iv}	2.341 (3)
N1—C4	1.337 (8)	C13—C14	1.507 (9)
N2—C12	1.335 (7)	C13—C14'	1.507 (10)
N2—C7	1.341 (7)	C14—H14A	0.9600
C1—O2	1.248 (6)	C14—H14B	0.9600

supplementary materials

C1—O1	1.266 (6)	C14—H14C	0.9600
C1—C2	1.507 (6)	C14'—H14D	0.9600
C2—C3	1.370 (7)	C14'—H14E	0.9600
C2—C6	1.376 (7)	C14'—H14F	0.9600
C3—C4	1.374 (8)	C11—O8	1.368 (9)
C3—H8	0.9300	C11—O10'	1.384 (8)
C4—H7	0.9300	C11—O7'	1.390 (9)
C5—C6	1.382 (7)	C11—O9	1.399 (9)
C5—H11	0.9300	C11—O8'	1.414 (10)
C6—H10	0.9300	C11—O7	1.423 (9)
C7—C8	1.376 (7)	C11—O10	1.451 (9)
C7—H4	0.9300	C11—O9'	1.452 (10)
C8—C9	1.381 (7)	O8—O8'	0.988 (19)
C8—H3	0.9300	O8—O9'	1.557 (19)
C9—C11	1.378 (7)	O9—O10'	1.278 (15)
C9—C10	1.505 (6)	O9—O9'	1.307 (17)
C10—O3	1.246 (5)	O10—O10'	1.280 (17)
C10—O4	1.258 (5)	O10—O8'	1.650 (18)
O4—Er1—O2 ⁱ	104.11 (13)	O4—C10—C9	117.9 (4)
O4—Er1—O1 ⁱⁱ	90.06 (13)	C9—C11—C12	119.1 (5)
O2 ⁱ —Er1—O1 ⁱⁱ	139.15 (12)	C9—C11—H6	120.4
O4—Er1—O3 ⁱⁱⁱ	85.24 (12)	C12—C11—H6	120.4
O2 ⁱ —Er1—O3 ⁱⁱⁱ	73.96 (11)	N2—C12—C11	122.5 (5)
O1 ⁱⁱ —Er1—O3 ⁱⁱⁱ	146.30 (12)	N2—C12—H5	118.7
O4—Er1—O5 ^{iv}	77.04 (11)	C11—C12—H5	118.7
O2 ⁱ —Er1—O5 ^{iv}	71.89 (13)	C1—O1—Er1 ^v	134.9 (3)
O1 ⁱⁱ —Er1—O5 ^{iv}	74.47 (12)	C1—O2—Er1 ^{vi}	138.3 (3)
O3 ⁱⁱⁱ —Er1—O5 ^{iv}	135.93 (12)	C10—O3—Er1 ^{vii}	148.8 (3)
O4—Er1—O1W	78.85 (13)	C10—O4—Er1	139.3 (3)
O2 ⁱ —Er1—O1W	148.19 (12)	Er1—O1W—H1W	125 (4)
O1 ⁱⁱ —Er1—O1W	71.58 (12)	Er1—O1W—H2W	122 (4)
O3 ⁱⁱⁱ —Er1—O1W	74.77 (12)	H1W—O1W—H2W	106 (4)
O5 ^{iv} —Er1—O1W	137.91 (12)	C13—O6—Er1	95.3 (3)
O4—Er1—O6	154.95 (12)	C13—O5—Er1 ^{iv}	160.6 (3)
O2 ⁱ —Er1—O6	92.59 (14)	C13—O5—Er1	92.8 (3)
O1 ⁱⁱ —Er1—O6	89.25 (14)	Er1 ^{iv} —O5—Er1	106.35 (13)
O3 ⁱⁱⁱ —Er1—O6	81.55 (12)	O6—C13—O5	118.7 (4)
O5 ^{iv} —Er1—O6	126.62 (11)	O6—C13—C14	119.6 (11)
O1W—Er1—O6	77.18 (13)	O5—C13—C14	120.8 (11)
O4—Er1—O5	149.53 (11)	O6—C13—C14'	122.6 (12)
O2 ⁱ —Er1—O5	74.51 (12)	O5—C13—C14'	118.3 (12)
O1 ⁱⁱ —Er1—O5	74.32 (12)	O6—C13—Er1	58.3 (2)
O3 ⁱⁱⁱ —Er1—O5	122.10 (12)	O5—C13—Er1	60.6 (2)
O5 ^{iv} —Er1—O5	73.65 (13)	C14—C13—Er1	167.2 (12)

O1W—Er1—O5	118.73 (13)	C14'—C13—Er1	177.2 (13)
O6—Er1—O5	52.98 (11)	C13—C14—H14A	109.5
O4—Er1—C13	169.94 (13)	C13—C14—H14B	109.5
O2 ⁱ —Er1—C13	83.95 (14)	C13—C14—H14C	109.5
O1 ⁱⁱ —Er1—C13	79.88 (14)	C13—C14'—H14D	109.5
O3 ⁱⁱⁱ —Er1—C13	102.99 (13)	C13—C14'—H14E	109.5
O5 ^{iv} —Er1—C13	100.25 (13)	H14D—C14'—H14E	109.5
O1W—Er1—C13	97.55 (14)	C13—C14'—H14F	109.5
O6—Er1—C13	26.38 (13)	H14D—C14'—H14F	109.5
O5—Er1—C13	26.64 (12)	H14E—C14'—H14F	109.5
O4—Er1—Er1 ^{iv}	114.47 (8)	O8—C11—O10'	140.3 (9)
O2 ⁱ —Er1—Er1 ^{iv}	68.88 (8)	O8—C11—O7'	104.2 (12)
O1 ⁱⁱ —Er1—Er1 ^{iv}	70.37 (8)	O10'—C11—O7'	113.8 (8)
O3 ⁱⁱⁱ —Er1—Er1 ^{iv}	141.06 (8)	O8—C11—O9	111.5 (8)
O5 ^{iv} —Er1—Er1 ^{iv}	37.84 (8)	O10'—C11—O9	54.6 (7)
O1W—Er1—Er1 ^{iv}	139.44 (9)	O7'—C11—O9	124.9 (10)
O6—Er1—Er1 ^{iv}	88.78 (8)	O10'—C11—O8'	110.7 (8)
O5—Er1—Er1 ^{iv}	35.81 (8)	O7'—C11—O8'	110.1 (9)
C13—Er1—Er1 ^{iv}	62.42 (10)	O9—C11—O8'	124.5 (9)
N1—Ag1—N2	165.44 (19)	O8—C11—O7	112.4 (8)
C5—N1—C4	117.6 (5)	O10'—C11—O7	107.3 (10)
C5—N1—Ag1	126.0 (4)	O9—C11—O7	107.7 (8)
C4—N1—Ag1	116.3 (4)	O8'—C11—O7	126.7 (10)
C12—N2—C7	118.2 (4)	O8—C11—O10	111.8 (8)
C12—N2—Ag1	123.0 (4)	O10'—C11—O10	53.6 (7)
C7—N2—Ag1	118.8 (4)	O7'—C11—O10	97.3 (10)
O2—C1—O1	126.7 (4)	O9—C11—O10	106.3 (7)
O2—C1—C2	116.4 (4)	O8'—C11—O10	70.3 (8)
O1—C1—C2	116.9 (4)	O7—C11—O10	106.7 (8)
C3—C2—C6	118.5 (5)	O8—C11—O9'	66.9 (8)
C3—C2—C1	119.4 (5)	O10'—C11—O9'	109.0 (8)
C6—C2—C1	122.2 (5)	O7'—C11—O9'	108.9 (8)
C2—C3—C4	119.5 (5)	O9—C11—O9'	54.5 (7)
C2—C3—H8	120.2	O8'—C11—O9'	103.8 (8)
C4—C3—H8	120.2	O7—C11—O9'	97.5 (10)
N1—C4—C3	122.7 (5)	O10—C11—O9'	153.4 (9)
N1—C4—H7	118.6	O8'—O8—C11	71.7 (8)
C3—C4—H7	118.6	O8'—O8—O9'	123.3 (13)
N1—C5—C6	122.7 (5)	C11—O8—O9'	59.1 (6)
N1—C5—H11	118.6	O10'—O9—O9'	126.6 (10)
C6—C5—H11	118.6	O10'—O9—C11	62.1 (6)
C2—C6—C5	119.0 (5)	O9'—O9—C11	64.8 (7)
C2—C6—H10	120.5	O10'—O10—C11	60.5 (6)
C5—C6—H10	120.5	O10'—O10—O8'	102.8 (9)
N2—C7—C8	122.2 (5)	C11—O10—O8'	53.8 (5)
N2—C7—H4	118.9	O8—O8'—C11	66.8 (8)

supplementary materials

C8—C7—H4	118.9	O8—O8'—O10	122.7 (11)
C7—C8—C9	119.7 (5)	C11—O8'—O10	55.9 (6)
C7—C8—H3	120.2	O9—O9'—C11	60.7 (5)
C9—C8—H3	120.2	O9—O9'—O8	105.7 (9)
C11—C9—C8	118.2 (4)	C11—O9'—O8	54.0 (5)
C11—C9—C10	121.7 (4)	O9—O10'—O10	126.2 (10)
C8—C9—C10	120.0 (4)	O9—O10'—C11	63.3 (6)
O3—C10—O4	124.5 (4)	O10—O10'—C11	65.9 (6)
O3—C10—C9	117.6 (4)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H2W \cdots O4 ⁱⁱⁱ	0.82 (4)	2.19 (3)	2.891 (5)	145 (5)
O1W—H1W \cdots O6 ^{vii}	0.81 (4)	1.99 (4)	2.786 (5)	167 (6)

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

Fig. 2

