

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

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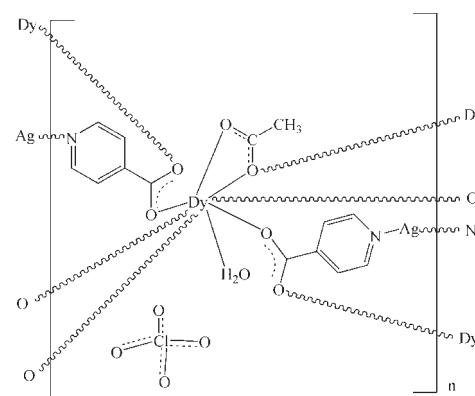
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; disorder in main residue; R factor = 0.023; wR factor = 0.056; data-to-parameter ratio = 10.8.

In the title three-dimensional heterometallic complex, $\{[\text{AgDy}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]\text{ClO}_4\}_n$, the Dy(III) ion is eight-coordinated by four O atoms from four different isonicotinate ligands, three O atoms from two different acetate ligands and one O atom of water molecule. The two-coordinate Ag^I ion is bonded to two N atoms from two different isonicotinate anions. These metal coordination units are connected by bridging isonicotinate and acetate ligands, generating a three-dimensional network. The coordinated water molecules link the carboxylate group and the acetate ligand by O—H···O hydrogen bonding. The perchlorate anion is disordered over two sites with site occupancy factors 0.508 (12) and 0.492 (12) and the methyl group of the acetate ligand is disordered over two positions of equal occupancy.

Related literature

For the applications of lanthanide–transition metal heterometallic complexes with bridging multifunctional organic ligands in ion exchange, magnetism, bimetallic catalysis and as luminescent probes, see: Cheng *et al.* (2006); Kuang *et al.* (2007); Peng *et al.* (2008); Zhu *et al.* (2009).



Experimental

Crystal data

$[\text{AgDy}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]\text{ClO}_4$	$\beta = 92.845$ (1)°
$M_r = 691.08$	$V = 1947.2$ (3) Å ³
Monoclinic, $P2_1/c$	$Z = 4$
$a = 16.1682$ (15) Å	Mo $K\alpha$ radiation
$b = 15.1020$ (14) Å	$\mu = 5.01$ mm ⁻¹
$c = 7.9846$ (7) Å	$T = 296$ K

$0.23 \times 0.20 \times 0.19$ mm

Data collection

Bruker APEXII area-detector diffractometer	9904 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	3486 independent reflections
$T_{\min} = 0.328$, $T_{\max} = 0.386$	3112 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.056$	$\Delta\rho_{\text{max}} = 0.66$ e Å ⁻³
$S = 1.04$	$\Delta\rho_{\text{min}} = -0.76$ e Å ⁻³
3486 reflections	
322 parameters	
158 restraints	

	H atoms treated by a mixture of independent and constrained refinement
	$\Delta\rho_{\text{max}} = 0.66$ e Å ⁻³
	$\Delta\rho_{\text{min}} = -0.76$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H2W···O2 ⁱ	0.79 (3)	2.21 (4)	2.925 (4)	150 (5)
O1W—H1W···O5 ⁱⁱ	0.79 (3)	2.05 (4)	2.813 (4)	161 (5)

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: ZQ2015).

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. E* **63**, 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. A* **64**, 112–122.
- Zhu, L.-C., Zhao, Z.-G. & Yu, S.-J. (2009). *Acta Cryst. E* **65**, m1105.

supplementary materials

Acta Cryst. (2009). E65, m1595-m1596 [doi:10.1107/S1600536809046637]

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

L.-C. 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 luminescent probe(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 which is presented in this article.

In the title compound (Fig. 1), there are one Dy(III) ion, one Ag(I) ion, two halves of acetate ligand, two isonicotinate ligands, one coordinated water molecule, and one perchlorate anion in the asymmetric unit. Each Dy(III) ion is eight-coordinated by four O atoms from four different isonicotinate ligands [Dy—O distances ranging from 2.297 (3) to 2.348 (3) Å], and three O atoms from two different acetate ligands [Dy—O distances ranging from 2.394 (3) to 2.484 (3) Å], and one O atom of water molecule [Dy—O distances 2.414 (3) Å]. The O—Dy—O bond angles are in the range from 52.70 (10) to 155.05 (10) °. The Dy center can be described as having a bicapped trigonal prism coordination geometry. The two-coordinate Ag(I) ion is bonded to two N atoms from two different isonicotinate anions [Ag—N distances 2.163 (4) Å]. Thus the Ag(I) ion is in a somewhat linear configuration with N1—Ag1—N2 angle 165.40 (17) °. These metal coordination units are 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). The perchlorate anion is disordered over two sites with site occupancy factors 0.508 (12) and 0.492 (12). The methyl group of the acetate ligand is disordered over two positions of equal occupancy (0.5:0.5).

Experimental

A mixture of AgNO₃(0.057 g, 0.33 mmol), Dy₂O₃(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. Colorless block 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 anion is disordered over two sites with site occupancy factors 0.508 (12) and 0.492 (12). The methyl group of the acetate ligand is disordered over two positions of equal occupancy (0.5:0.5).

supplementary materials

Figures

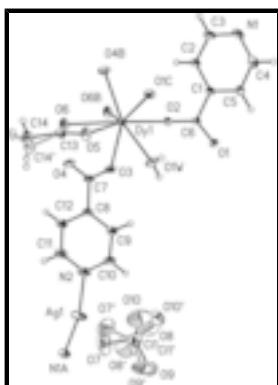


Fig. 1. The molecular structure showing the atomic-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Symmetry codes: (A) $1 + x, 1.5 - y, -1/2 + z$; (B) $1 - x, 1 - y, 2 - z$; (C) $x, 1.5 - y, 1/2 + z$.

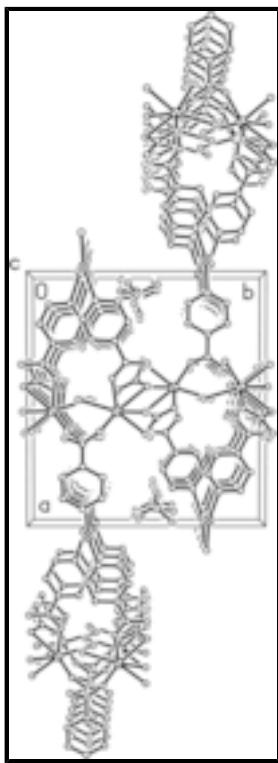


Fig. 2. A view of the three-dimensional structure of the title compound. Hydrogen atoms are omitted for clarity.

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

Crystal data

$[\text{AgDy}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_3\text{O}_2)(\text{H}_2\text{O})]\text{ClO}_4$

$F_{000} = 1316$

$M_r = 691.08$

$D_x = 2.357 \text{ Mg m}^{-3}$

Monoclinic, $P2_1/c$

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

Hall symbol: -P 2ybc

Cell parameters from 5589 reflections

$a = 16.1682 (15) \text{ \AA}$

$\theta = 2.7\text{--}27.8^\circ$

$b = 15.1020 (14) \text{ \AA}$

$\mu = 5.01 \text{ mm}^{-1}$

$c = 7.9846 (7) \text{ \AA}$

$T = 296 \text{ K}$

$\beta = 92.8450(10)^\circ$
 $V = 1947.2(3) \text{ \AA}^3$
 $Z = 4$

Data collection

Bruker APEXII area-detector diffractometer
 Radiation source: fine-focus sealed tube
 Monochromator: graphite
 $T = 296 \text{ K}$
 φ and ω scan
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.328, T_{\max} = 0.386$
 9904 measured reflections

Block, colorless
 $0.23 \times 0.20 \times 0.19 \text{ mm}$
 3486 independent reflections
 3112 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\max} = 25.2^\circ$
 $\theta_{\min} = 1.9^\circ$
 $h = -15 \rightarrow 19$
 $k = -18 \rightarrow 17$
 $l = -8 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.056$
 $S = 1.04$
 3486 reflections
 322 parameters
 158 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
 $w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 3.5237P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.66 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.76 \text{ e \AA}^{-3}$
 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)
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supplementary materials

Dy1	0.454540 (11)	0.616178 (12)	1.04948 (2)	0.01852 (7)	
Ag1	0.97316 (3)	0.73989 (4)	0.60071 (7)	0.06665 (17)	
O1	0.35829 (18)	0.81592 (19)	0.7190 (4)	0.0300 (7)	
O2	0.38143 (17)	0.68117 (19)	0.8281 (4)	0.0263 (7)	
O3	0.5762 (2)	0.6330 (2)	0.9080 (5)	0.0401 (9)	
O4	0.63060 (19)	0.49745 (19)	0.8632 (5)	0.0403 (9)	
O5	0.5347 (2)	0.6149 (2)	1.3147 (4)	0.0360 (8)	
O6	0.54781 (19)	0.4970 (2)	1.1607 (4)	0.0320 (7)	
O1W	0.4979 (2)	0.7687 (2)	1.0758 (4)	0.0358 (8)	
H1W	0.518 (3)	0.795 (3)	1.002 (6)	0.054*	
H2W	0.475 (3)	0.800 (3)	1.139 (6)	0.054*	
N1	0.0943 (2)	0.7527 (3)	0.9981 (6)	0.0404 (10)	
N2	0.8576 (3)	0.6967 (3)	0.6991 (6)	0.0500 (12)	
C1	0.2516 (3)	0.7494 (3)	0.8695 (5)	0.0231 (9)	
C2	0.2116 (3)	0.6710 (3)	0.9112 (6)	0.0312 (11)	
H1	0.2372	0.6165	0.8967	0.037*	
C3	0.1336 (3)	0.6753 (3)	0.9741 (7)	0.0388 (12)	
H2	0.1072	0.6229	1.0008	0.047*	
C4	0.1333 (3)	0.8284 (4)	0.9589 (7)	0.0446 (13)	
H3	0.1068	0.8821	0.9760	0.054*	
C5	0.2109 (3)	0.8294 (3)	0.8945 (6)	0.0335 (11)	
H4	0.2358	0.8828	0.8680	0.040*	
C6	0.3367 (2)	0.7495 (3)	0.8008 (5)	0.0202 (9)	
C7	0.6332 (3)	0.5809 (3)	0.8637 (6)	0.0303 (10)	
C8	0.7113 (3)	0.6231 (3)	0.8058 (6)	0.0293 (10)	
C9	0.7156 (3)	0.7123 (3)	0.7613 (7)	0.0410 (13)	
H7	0.6693	0.7486	0.7668	0.049*	
C10	0.7894 (3)	0.7458 (4)	0.7088 (8)	0.0489 (15)	
H8	0.7917	0.8053	0.6791	0.059*	
C11	0.8533 (3)	0.6108 (4)	0.7457 (9)	0.0568 (17)	
H5	0.9009	0.5763	0.7427	0.068*	
C12	0.7818 (3)	0.5719 (3)	0.7975 (7)	0.0428 (13)	
H6	0.7810	0.5123	0.8264	0.051*	
C13	0.5697 (3)	0.5411 (3)	1.2898 (5)	0.0276 (10)	
C14	0.6271 (11)	0.5015 (17)	1.421 (3)	0.045 (4)	0.50
H14A	0.6719	0.5418	1.4467	0.068*	0.50
H14B	0.6487	0.4468	1.3804	0.068*	0.50
H14C	0.5976	0.4905	1.5203	0.068*	0.50
C14'	0.6444 (10)	0.5127 (17)	1.393 (3)	0.045 (4)	0.50
H14D	0.6503	0.5488	1.4915	0.068*	0.50
H14E	0.6926	0.5191	1.3282	0.068*	0.50
H14F	0.6385	0.4518	1.4246	0.068*	0.50
Cl1	0.9165 (8)	0.9620 (9)	0.7618 (15)	0.0633 (8)	0.492 (12)
O7	0.9742 (9)	0.8934 (9)	0.785 (2)	0.138 (7)	0.492 (12)
O8	0.8752 (9)	0.9496 (8)	0.6037 (14)	0.105 (5)	0.492 (12)
O9	0.9544 (10)	1.0465 (9)	0.761 (2)	0.074 (5)	0.492 (12)
O10	0.8556 (9)	0.9600 (10)	0.8849 (19)	0.139 (7)	0.492 (12)
Cl1'	0.9216 (7)	0.9553 (8)	0.7502 (15)	0.0633 (8)	0.508 (12)
O7'	0.9307 (9)	0.8895 (9)	0.8748 (17)	0.125 (6)	0.508 (12)

O8'	0.9565 (10)	0.9226 (10)	0.6054 (17)	0.139 (6)	0.508 (12)
O9'	0.9612 (10)	1.0334 (9)	0.809 (2)	0.090 (6)	0.508 (12)
O10'	0.8355 (6)	0.9715 (7)	0.720 (2)	0.101 (5)	0.508 (12)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.01576 (11)	0.01481 (11)	0.02554 (12)	0.00081 (7)	0.00650 (8)	0.00006 (8)
Ag1	0.0261 (2)	0.0917 (4)	0.0846 (4)	-0.0148 (2)	0.0267 (2)	0.0028 (3)
O1	0.0256 (16)	0.0230 (16)	0.0424 (19)	0.0016 (13)	0.0128 (14)	0.0096 (14)
O2	0.0190 (15)	0.0247 (15)	0.0357 (18)	0.0039 (12)	0.0055 (13)	0.0049 (13)
O3	0.0302 (19)	0.0227 (17)	0.071 (3)	-0.0018 (13)	0.0332 (18)	-0.0015 (16)
O4	0.0337 (18)	0.0193 (16)	0.070 (2)	-0.0035 (14)	0.0288 (17)	-0.0028 (16)
O5	0.044 (2)	0.0315 (18)	0.0319 (18)	0.0101 (15)	-0.0040 (15)	-0.0092 (14)
O6	0.0376 (18)	0.0270 (16)	0.0304 (17)	0.0082 (14)	-0.0078 (14)	-0.0062 (14)
O1W	0.049 (2)	0.0228 (17)	0.038 (2)	-0.0094 (15)	0.0213 (17)	-0.0029 (14)
N1	0.023 (2)	0.049 (3)	0.051 (3)	0.0021 (18)	0.0138 (19)	-0.003 (2)
N2	0.028 (2)	0.050 (3)	0.074 (3)	-0.009 (2)	0.022 (2)	-0.002 (2)
C1	0.017 (2)	0.028 (2)	0.024 (2)	0.0005 (17)	0.0038 (17)	0.0033 (17)
C2	0.020 (2)	0.026 (2)	0.049 (3)	-0.0004 (18)	0.011 (2)	0.000 (2)
C3	0.025 (2)	0.037 (3)	0.056 (3)	-0.006 (2)	0.017 (2)	-0.001 (2)
C4	0.033 (3)	0.040 (3)	0.062 (4)	0.013 (2)	0.014 (3)	-0.002 (3)
C5	0.027 (2)	0.025 (2)	0.050 (3)	0.0046 (19)	0.012 (2)	0.004 (2)
C6	0.016 (2)	0.020 (2)	0.024 (2)	-0.0002 (16)	0.0040 (17)	0.0002 (17)
C7	0.023 (2)	0.028 (2)	0.041 (3)	-0.0069 (19)	0.016 (2)	-0.001 (2)
C8	0.023 (2)	0.026 (2)	0.041 (3)	-0.0048 (18)	0.014 (2)	-0.003 (2)
C9	0.025 (3)	0.029 (3)	0.070 (4)	0.000 (2)	0.017 (2)	0.004 (2)
C10	0.032 (3)	0.036 (3)	0.081 (4)	-0.010 (2)	0.021 (3)	0.007 (3)
C11	0.026 (3)	0.047 (3)	0.100 (5)	0.000 (2)	0.019 (3)	-0.004 (3)
C12	0.027 (3)	0.031 (3)	0.073 (4)	0.001 (2)	0.017 (3)	-0.001 (3)
C13	0.026 (2)	0.032 (2)	0.025 (2)	0.0036 (19)	-0.0008 (19)	-0.0022 (19)
C14	0.046 (6)	0.045 (5)	0.044 (6)	0.006 (5)	-0.012 (5)	-0.003 (4)
C14'	0.046 (6)	0.045 (5)	0.044 (6)	0.006 (5)	-0.012 (5)	-0.003 (4)
Cl1	0.0616 (15)	0.0502 (16)	0.0776 (16)	0.0036 (11)	-0.0019 (11)	-0.0024 (12)
O7	0.145 (10)	0.105 (8)	0.162 (11)	0.076 (7)	-0.030 (8)	-0.017 (7)
O8	0.132 (10)	0.108 (8)	0.072 (7)	-0.039 (7)	-0.042 (7)	0.005 (6)
O9	0.068 (8)	0.060 (7)	0.094 (8)	-0.011 (6)	0.012 (6)	-0.003 (6)
O10	0.135 (10)	0.151 (10)	0.136 (10)	-0.038 (8)	0.054 (8)	-0.009 (8)
Cl1'	0.0616 (15)	0.0502 (16)	0.0776 (16)	0.0036 (11)	-0.0019 (11)	-0.0024 (12)
O7'	0.140 (10)	0.120 (9)	0.112 (8)	-0.019 (7)	-0.017 (7)	0.066 (7)
O8'	0.163 (10)	0.142 (9)	0.119 (9)	0.012 (8)	0.063 (8)	-0.035 (7)
O9'	0.074 (8)	0.082 (9)	0.115 (10)	-0.034 (7)	0.006 (7)	-0.038 (7)
O10'	0.055 (6)	0.088 (7)	0.160 (10)	0.004 (5)	-0.008 (6)	0.008 (7)

Geometric parameters (\AA , $^\circ$)

Dy1—O2	2.297 (3)	C2—C3	1.382 (6)
Dy1—O4 ⁱ	2.328 (3)	C2—H1	0.9300

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Dy1—O3	2.330 (3)	C3—H2	0.9300
Dy1—O1 ⁱⁱ	2.348 (3)	C4—C5	1.380 (6)
Dy1—O6 ⁱ	2.394 (3)	C4—H3	0.9300
Dy1—O1W	2.414 (3)	C5—H4	0.9300
Dy1—O5	2.428 (3)	C7—C8	1.509 (6)
Dy1—O6	2.484 (3)	C8—C12	1.381 (6)
Dy1—C13	2.842 (4)	C8—C9	1.395 (6)
Dy1—Dy1 ⁱ	3.9005 (5)	C9—C10	1.381 (6)
Ag1—N2	2.163 (4)	C9—H7	0.9300
Ag1—N1 ⁱⁱⁱ	2.163 (4)	C10—H8	0.9300
O1—C6	1.256 (5)	C11—C12	1.379 (7)
O1—Dy1 ^{iv}	2.348 (3)	C11—H5	0.9300
O2—C6	1.272 (5)	C12—H6	0.9300
O3—C7	1.275 (5)	C13—C14	1.490 (9)
O4—C7	1.261 (5)	C13—C14'	1.490 (9)
O4—Dy1 ⁱ	2.328 (3)	C14—H14A	0.9600
O5—C13	1.269 (5)	C14—H14B	0.9600
O6—C13	1.263 (5)	C14—H14C	0.9600
O6—Dy1 ⁱ	2.394 (3)	C14'—H14D	0.9600
O1W—H1W	0.79 (3)	C14'—H14E	0.9600
O1W—H2W	0.79 (3)	C14'—H14F	0.9600
N1—C3	1.348 (6)	C11—O7	1.399 (12)
N1—C4	1.350 (7)	C11—O8	1.411 (12)
N1—Ag1 ^v	2.163 (4)	C11—O9	1.416 (11)
N2—C10	1.335 (7)	C11—O10	1.426 (12)
N2—C11	1.351 (7)	C11'—O8'	1.401 (12)
C1—C5	1.394 (6)	C11'—O7'	1.408 (12)
C1—C2	1.398 (6)	C11'—O9'	1.411 (11)
C1—C6	1.506 (5)	C11'—O10'	1.420 (11)
O2—Dy1—O4 ⁱ	104.83 (12)	C2—C1—C6	121.9 (4)
O2—Dy1—O3	89.71 (12)	C3—C2—C1	119.1 (4)
O4 ⁱ —Dy1—O3	138.72 (10)	C3—C2—H1	120.4
O2—Dy1—O1 ⁱⁱ	85.79 (11)	C1—C2—H1	120.4
O4 ⁱ —Dy1—O1 ⁱⁱ	74.38 (10)	N1—C3—C2	122.6 (4)
O3—Dy1—O1 ⁱⁱ	146.22 (10)	N1—C3—H2	118.7
O2—Dy1—O6 ⁱ	77.05 (10)	C2—C3—H2	118.7
O4 ⁱ —Dy1—O6 ⁱ	72.23 (11)	N1—C4—C5	122.6 (4)
O3—Dy1—O6 ⁱ	73.89 (11)	N1—C4—H3	118.7
O1 ⁱⁱ —Dy1—O6 ⁱ	136.70 (11)	C5—C4—H3	118.7
O2—Dy1—O1W	78.20 (12)	C4—C5—C1	119.2 (4)
O4 ⁱ —Dy1—O1W	148.29 (11)	C4—C5—H4	120.4
O3—Dy1—O1W	71.91 (11)	C1—C5—H4	120.4
O1 ⁱⁱ —Dy1—O1W	74.40 (11)	O1—C6—O2	124.5 (4)
O6 ⁱ —Dy1—O1W	137.44 (11)	O1—C6—C1	118.2 (3)
O2—Dy1—O5	155.05 (10)	O2—C6—C1	117.3 (3)

O4 ⁱ —Dy1—O5	91.77 (13)	O4—C7—O3	126.4 (4)
O3—Dy1—O5	89.81 (13)	O4—C7—C8	116.7 (4)
O1 ⁱⁱ —Dy1—O5	80.85 (11)	O3—C7—C8	116.9 (4)
O6 ⁱ —Dy1—O5	126.52 (10)	C12—C8—C9	118.5 (4)
O1W—Dy1—O5	77.96 (12)	C12—C8—C7	119.0 (4)
O2—Dy1—O6	149.85 (10)	C9—C8—C7	122.5 (4)
O4 ⁱ —Dy1—O6	73.52 (11)	C10—C9—C8	119.0 (5)
O3—Dy1—O6	74.95 (11)	C10—C9—H7	120.5
O1 ⁱⁱ —Dy1—O6	121.22 (11)	C8—C9—H7	120.5
O6 ⁱ —Dy1—O6	73.84 (12)	N2—C10—C9	122.8 (5)
O1W—Dy1—O6	119.46 (12)	N2—C10—H8	118.6
O5—Dy1—O6	52.70 (10)	C9—C10—H8	118.6
O2—Dy1—C13	169.94 (11)	N2—C11—C12	123.1 (5)
O4 ⁱ —Dy1—C13	83.17 (13)	N2—C11—H5	118.4
O3—Dy1—C13	80.23 (13)	C12—C11—H5	118.4
O1 ⁱⁱ —Dy1—C13	102.45 (12)	C11—C12—C8	118.8 (5)
O6 ⁱ —Dy1—C13	100.12 (12)	C11—C12—H6	120.6
O1W—Dy1—C13	98.28 (13)	C8—C12—H6	120.6
O5—Dy1—C13	26.41 (11)	O6—C13—O5	118.8 (4)
O6—Dy1—C13	26.36 (11)	O6—C13—C14	120.1 (11)
O2—Dy1—Dy1 ⁱ	114.40 (7)	O5—C13—C14	120.6 (11)
O4 ⁱ —Dy1—Dy1 ⁱ	68.41 (7)	O6—C13—C14'	119.0 (11)
O3—Dy1—Dy1 ⁱ	70.39 (7)	O5—C13—C14'	121.4 (12)
O1 ⁱⁱ —Dy1—Dy1 ⁱ	140.97 (7)	C14—C13—C14'	15.6 (17)
O6 ⁱ —Dy1—Dy1 ⁱ	37.71 (7)	O6—C13—Dy1	60.8 (2)
O1W—Dy1—Dy1 ⁱ	139.94 (8)	O5—C13—Dy1	58.3 (2)
O5—Dy1—Dy1 ⁱ	88.82 (7)	C14—C13—Dy1	177.5 (10)
O6—Dy1—Dy1 ⁱ	36.13 (7)	C14'—C13—Dy1	166.7 (9)
C13—Dy1—Dy1 ⁱ	62.43 (9)	C13—C14—H14A	109.5
N2—Ag1—N1 ⁱⁱⁱ	165.40 (17)	C13—C14—H14B	109.5
C6—O1—Dy1 ^{iv}	149.1 (3)	C13—C14—H14C	109.5
C6—O2—Dy1	138.1 (3)	C13—C14'—H14D	109.5
C7—O3—Dy1	134.9 (3)	C13—C14'—H14E	109.5
C7—O4—Dy1 ⁱ	139.1 (3)	H14D—C14'—H14E	109.5
C13—O5—Dy1	95.3 (3)	C13—C14'—H14F	109.5
C13—O6—Dy1 ⁱ	160.5 (3)	H14D—C14'—H14F	109.5
C13—O6—Dy1	92.8 (3)	H14E—C14'—H14F	109.5
Dy1 ⁱ —O6—Dy1	106.16 (12)	O7—C11—O8	107.5 (10)
Dy1—O1W—H1W	123 (4)	O7—C11—O9	112.5 (10)
Dy1—O1W—H2W	119 (4)	O8—C11—O9	107.4 (10)
H1W—O1W—H2W	113 (5)	O7—C11—O10	111.9 (11)
C3—N1—C4	118.2 (4)	O8—C11—O10	107.5 (10)
C3—N1—Ag1 ^v	122.7 (3)	O9—C11—O10	109.7 (10)
C4—N1—Ag1 ^v	119.1 (3)	O8'—C11'—O7'	107.6 (10)

supplementary materials

C10—N2—C11	117.6 (4)	O8'—Cl1'—O9'	111.8 (10)
C10—N2—Ag1	125.7 (4)	O7'—Cl1'—O9'	109.0 (10)
C11—N2—Ag1	116.5 (3)	O8'—Cl1'—O10'	110.8 (10)
C5—C1—C2	118.3 (4)	O7'—Cl1'—O10'	107.9 (10)
C5—C1—C6	119.8 (4)	O9'—Cl1'—O10'	109.6 (10)

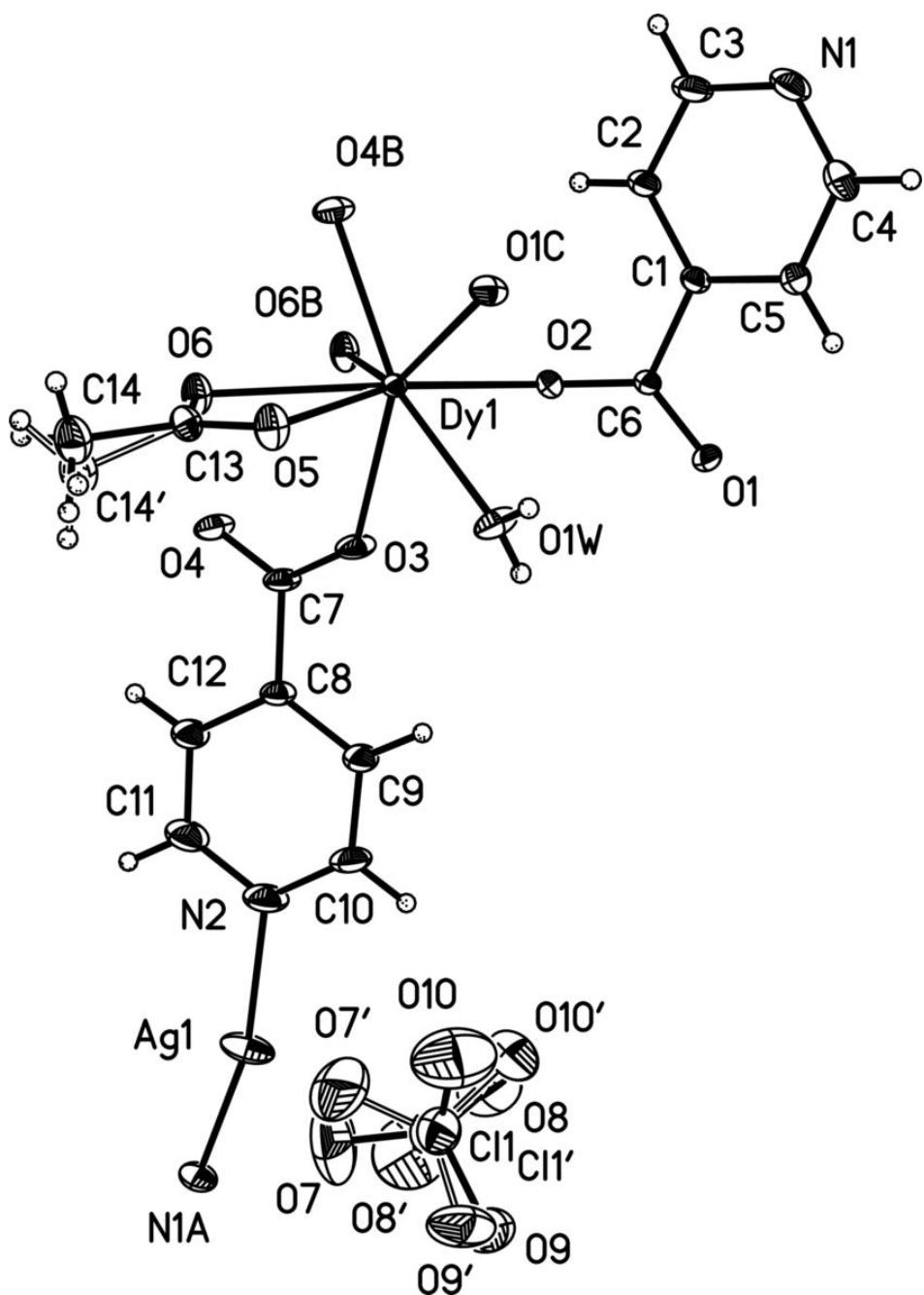
Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, -y+3/2, z+1/2$; (iii) $x+1, -y+3/2, z-1/2$; (iv) $x, -y+3/2, z-1/2$; (v) $x-1, -y+3/2, z+1/2$.

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O1W—H2W ⁱⁱ —O2 ⁱⁱ	0.79 (3)	2.21 (4)	2.925 (4)	150 (5)
O1W—H1W ^{iv} —O5 ^{iv}	0.79 (3)	2.05 (4)	2.813 (4)	161 (5)

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

Fig. 1



supplementary materials

Fig. 2

