

catena-Poly[[[tetraaquapraseodymium(III)]-di- μ -nicotinato- κ^2 O:N; κ^2 O:N-disilver(I)-di- μ -nicotinato- κ^2 N:O; κ^2 N:O] perchlorate monohydrate]

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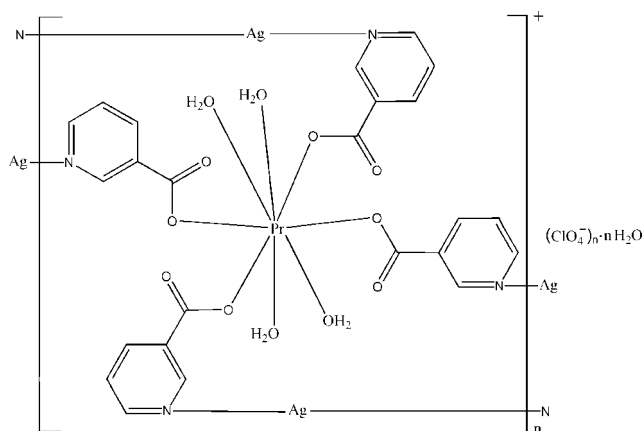
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.035$ Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 13.5.

In the title compound, $[\text{Ag}_2\text{Pr}(\text{C}_6\text{H}_4\text{NO}_2)_4(\text{H}_2\text{O})_4]\text{ClO}_4 \cdot n\text{H}_2\text{O}$, the Pr^{III} atom, lying on a twofold rotation axis, has a distorted square-antiprismatic coordination geometry, defined by four O atoms from four nicotinate (nic) ligands and four water molecules. The Ag^I atom is coordinated in an almost linear fashion by two pyridyl N atoms from two nicotinate ligands. The linear coordination is augmented by weak interactions with three O atoms from one perchlorate anion, one uncoordinated water molecule and one carboxylate group. Two Pr atoms link two $\{\text{Ag}(\text{nic})_2\}^+$ units into a ring, which is further extended into an infinite zigzag chain by sharing the Pr atoms. These chains are further connected into a three-dimensional network *via* weak $\text{Ag} \cdots \text{O}$ interactions, $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, $\text{Ag} \cdots \text{Ag}$ interactions [$3.357(2)$ Å] and $\pi-\pi$ interactions between the pyridyl rings [centroid-centroid distance = $3.685(4)$ Å].

Related literature

For general background, see: Cheng *et al.* (2007a,b); Luo *et al.* (2006, 2007).



Experimental

Crystal data

$[\text{Ag}_2\text{Pr}(\text{C}_6\text{H}_4\text{NO}_2)_4(\text{H}_2\text{O})_4]\text{ClO}_4 \cdot n\text{H}_2\text{O}$
 $M_r = 1034.59$
 Orthorhombic, *Cmca*
 $a = 35.396(3)$ Å
 $b = 12.3733(10)$ Å
 $c = 15.2324(13)$ Å
 $V = 6671.2(10)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 2.76$ mm⁻¹
 $T = 273(2)$ K
 $0.30 \times 0.25 \times 0.22$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.453$, $T_{\text{max}} = 0.552$
 16336 measured reflections
 3065 independent reflections
 2478 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.097$
 $S = 1.06$
 3065 reflections
 227 parameters
 27 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.56$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.87$ e Å⁻³

Table 1

Selected bond lengths (Å).

Pr1—O3 ⁱ	2.390 (14)	Ag1—N1	2.175 (18)
Pr1—O1W	2.477 (14)	Ag1—O4 ⁱⁱ	2.777 (16)
Pr1—O2W	2.495 (14)	Ag1—O5	2.81 (3)
Pr1—O1	2.504 (13)	Ag1—O3W	2.90 (2)
Ag1—N2	2.165 (18)		

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

Table 2

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—H1W ⁱⁱⁱ ···O2 ⁱⁱⁱ	0.88	1.79	2.67 (2)	179
O1W—H2W ^{iv} ···O4 ^{iv}	0.97	1.68	2.63 (2)	163
O2W—H3W ^v ···O2 ^v	1.00	1.77	2.77 (2)	176
O2W—H4W ^{vi} ···O2 ^{vi}	0.83	1.95	2.76 (2)	162
O3W—H5W ^{vii} ···O1W ^{vii}	0.82	2.15	2.91 (2)	157

Symmetry codes: (iii) $-x + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x, -y + 1, -z + 1$; (v) $-x + \frac{1}{2}, y + \frac{1}{2}, z$; (vi) $x, -y + 2, -z + 1$; (vii) $x, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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: HY2177).

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supplementary materials

Acta Cryst. (2009). E65, m208-m209 [doi:10.1107/S1600536809001718]

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B. Guan, C.-H. Zhang and W.-D. Song

Comment

Nicotinic acid is a multifunctional bridging ligand possessing of O and N donors, which can thus be utilized to construct lanthanide–transition heterometallic complexes, *via* carboxylate O atoms binding to lanthanides and N atoms binding to transition metal ions such as Ag^I or Cu^I (Cheng *et al.*, 2007a,b; Luo *et al.*, 2006, 2007). On the basis of above considerations, we chose nicotinic acid, Pr^{III} and Ag^I metal ions as building blocks. A new one-dimensional 4 d–4f coordination polymer was obtained from the hydrothermal treatment of Pr₆O₁₁, AgNO₃, perchloric acid and nicotinic acid in water.

In the title compound (Fig. 1), the Pr^{III} atom, lying on a twofold rotation axis, has a distorted square-antiprismatic coordination geometry, defined by four O atoms from four nicotinate (nic) ligands and four water molecules. The perchlorate anion lies on a mirror plane and the uncoordinated water molecule lies on a twofold rotation axis. The Ag^I atom is coordinated in an almost linear fashion by two pyridyl N atoms from two nic ligands. The linear coordination are augmented by weak Ag \cdots O interactions with one O atom from the ClO₄⁻ anion, one O atom from the uncoordinated water molecule and one carboxylate O atom from the nic ligand (Table 1). The Ag atom also exhibits an argentophilic interaction, with an Ag \cdots Ag distance of 3.357 (1) Å. The pyridyl rings of the nic ligands coordinating to the Ag atom are almost coplanar and have a dihedral angle of 1.74 (2)°. Two Pr atoms link two Ag(nic)₂⁺ units into a ring, which are further extended into an infinite zigzag chain by sharing the common Pr atoms (Fig. 2). These chains are further connected into a three-dimensional network *via* the weak Ag \cdots O interactions, O—H \cdots O hydrogen bonds (Table 2), weak Ag \cdots Ag interactions and π – π interactions occurring between the pyridyl rings of neighboring nic ligands [centroid–centroid distance = 3.685 (4) Å].

Experimental

A mixture of Pr₆O₁₁ (0.170 g, 0.5 mmol), AgNO₃ (0.169 g, 1 mmol), nicotinic acid (0.123 g, 1 mmol), HClO₄ (0.12 ml) and H₂O (10 ml) was placed in a 23 ml Teflon-lined reactor, which was heated to 433 K for 3 d and then cooled to room temperature at a rate of 10 K h⁻¹. The pale-purple plate crystals obtained were washed with water and dried in air (yield 46% based on Pr).

Refinement

H atoms on C atoms were positioned geometrically and treated as riding on the parent C atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecules were located in difference Fourier maps and fixed in the refinements, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest residual electron density was found 1.09 Å from atom Pr1 and the deepest hole 0.76 Å from atom Cl1.

Figures

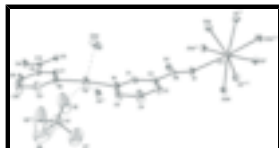


Fig. 1. The asymmetric unit of the title compound, extended to show the Pr and Ag coordination environments. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1/2 - x, 3/2 - y, 1 - z$; (ii) $x, 1/2 + y, 3/2 - z$; (iii) $1/2 - x, y, 1/2 - z$; (viii) $x, 3/2 - y, -1/2 + z$; (ix) $-x, y, z$.]

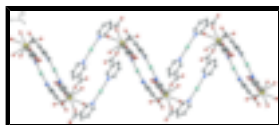


Fig. 2. View of the zigzag chain in the title compound.

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Crystal data

[Ag₂Pr(C₆H₄NO₂)₄(H₂O)₄]ClO₄·H₂O

$M_r = 1034.59$

Orthorhombic, *Cmca*

Hall symbol: -C 2bc 2

$a = 35.396$ (3) Å

$b = 12.3733$ (10) Å

$c = 15.2324$ (13) Å

$V = 6671.2$ (10) Å³

$Z = 8$

$F_{000} = 4032$

$D_x = 2.060$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3121 reflections

$\theta = 1.4$ – 28°

$\mu = 2.76$ mm⁻¹

$T = 273$ (2) K

Plate, pale purple

$0.30 \times 0.25 \times 0.22$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

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

$T_{\min} = 0.453$, $T_{\max} = 0.552$

16336 measured reflections

3065 independent reflections

2478 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

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

$\theta_{\min} = 2.2^\circ$

$h = -28 \rightarrow 42$

$k = -13 \rightarrow 14$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 31.5675P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3065 reflections	$(\Delta/\sigma)_{\max} < 0.001$
227 parameters	$\Delta\rho_{\max} = 1.56 \text{ e } \text{\AA}^{-3}$
27 restraints	$\Delta\rho_{\min} = -0.86 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pr1	0.2500	1.08315 (12)	0.2500	0.0216 (5)
Ag1	0.11088 (6)	0.60988 (15)	0.56463 (12)	0.0439 (6)
C2	0.1570 (6)	0.8876 (17)	0.4208 (13)	0.031 (5)
C6	0.1963 (6)	0.9230 (16)	0.3979 (13)	0.027 (4)
C3	0.1260 (7)	0.943 (2)	0.3901 (17)	0.048 (6)
H3	0.1292	1.0038	0.3555	0.058*
C1	0.1508 (6)	0.7976 (18)	0.4725 (13)	0.033 (5)
H1	0.1716	0.7607	0.4945	0.040*
C4	0.0904 (8)	0.908 (2)	0.411 (2)	0.067 (9)
H4	0.0692	0.9439	0.3899	0.081*
C5	0.0867 (7)	0.816 (2)	0.4631 (18)	0.054 (7)
H5	0.0625	0.7927	0.4782	0.065*
N1	0.1163 (5)	0.7608 (15)	0.4925 (12)	0.040 (5)
O1	0.2002 (4)	0.9976 (12)	0.3439 (9)	0.035 (3)
O2	0.2235 (4)	0.8725 (12)	0.4344 (9)	0.033 (3)
N2	0.1025 (5)	0.4681 (15)	0.6456 (12)	0.037 (4)
C7	0.1323 (6)	0.4144 (16)	0.6770 (14)	0.032 (5)
H7	0.1563	0.4385	0.6610	0.038*
C11	0.0685 (8)	0.434 (2)	0.669 (2)	0.057 (8)
H11	0.0474	0.4718	0.6489	0.069*
Cl1	0.0000	0.6849 (10)	0.5898 (10)	0.080 (4)
O7	0.0000	0.803 (3)	0.588 (4)	0.150 (19)
O6	0.0000	0.647 (5)	0.685 (4)	0.25 (4)
C8	0.1300 (6)	0.3255 (16)	0.7316 (13)	0.030 (5)
C9	0.0945 (7)	0.292 (2)	0.7558 (19)	0.057 (8)
H9	0.0914	0.2344	0.7941	0.069*
C10	0.0631 (8)	0.346 (3)	0.723 (3)	0.082 (12)
H10	0.0388	0.3232	0.7362	0.098*
C12	0.1652 (6)	0.2676 (16)	0.7619 (13)	0.028 (4)
O3	0.1962 (4)	0.3019 (12)	0.7341 (9)	0.032 (3)
O4	0.1611 (4)	0.1878 (13)	0.8104 (11)	0.044 (4)
O1W	0.2180 (4)	0.9435 (12)	0.1603 (9)	0.035 (4)
H1W	0.2373	0.9195	0.1295	0.053*
H2W	0.1996	0.8918	0.1807	0.053*
O2W	0.2515 (5)	1.1653 (13)	0.3996 (10)	0.046 (4)
H3W	0.2615	1.2394	0.4110	0.069*

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H4W	0.2454	1.1409	0.4486	0.069*
O3W	0.1776 (8)	0.5000	0.5000	0.080 (10)
H5W	0.1920	0.5010	0.4583	0.120*
O5	0.0324 (9)	0.643 (3)	0.565 (3)	0.19 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.0227 (9)	0.0223 (8)	0.0199 (8)	0.000	0.0012 (6)	0.000
Ag1	0.0482 (12)	0.0376 (11)	0.0458 (11)	-0.0044 (9)	0.0028 (8)	0.0151 (8)
C2	0.035 (12)	0.033 (11)	0.024 (10)	0.001 (10)	0.006 (9)	0.001 (9)
C6	0.032 (12)	0.025 (10)	0.023 (10)	0.000 (9)	0.005 (9)	-0.004 (8)
C3	0.038 (14)	0.051 (15)	0.054 (15)	0.000 (12)	0.009 (12)	0.023 (12)
C1	0.034 (12)	0.038 (12)	0.028 (10)	-0.003 (10)	0.003 (9)	0.004 (10)
C4	0.035 (15)	0.07 (2)	0.09 (2)	0.003 (14)	0.004 (15)	0.043 (17)
C5	0.034 (14)	0.060 (17)	0.069 (18)	-0.005 (13)	0.012 (12)	0.023 (14)
N1	0.039 (11)	0.040 (11)	0.040 (10)	-0.002 (9)	0.006 (8)	0.014 (9)
O1	0.034 (8)	0.032 (8)	0.037 (8)	0.000 (7)	0.005 (6)	0.013 (7)
O2	0.029 (8)	0.038 (8)	0.031 (8)	0.000 (7)	0.000 (6)	0.005 (7)
N2	0.034 (11)	0.033 (10)	0.045 (11)	0.000 (8)	0.002 (8)	0.010 (8)
C7	0.030 (12)	0.028 (11)	0.037 (12)	-0.006 (9)	0.001 (9)	0.001 (9)
C11	0.037 (15)	0.054 (17)	0.08 (2)	0.006 (12)	0.003 (13)	0.029 (15)
Cl1	0.040 (6)	0.070 (8)	0.130 (11)	0.000	0.000	0.009 (7)
O7	0.17 (5)	0.09 (3)	0.19 (5)	0.000	0.000	0.04 (3)
O6	0.45 (13)	0.14 (5)	0.15 (6)	0.000	0.000	0.02 (4)
C8	0.030 (12)	0.024 (11)	0.036 (12)	-0.002 (9)	0.004 (9)	0.001 (9)
C9	0.034 (14)	0.054 (16)	0.08 (2)	-0.002 (12)	0.005 (13)	0.042 (15)
C10	0.029 (15)	0.08 (2)	0.13 (3)	0.000 (15)	0.004 (17)	0.06 (2)
C12	0.026 (11)	0.028 (11)	0.031 (11)	0.000 (9)	0.003 (8)	-0.005 (9)
O3	0.027 (8)	0.031 (8)	0.037 (8)	-0.005 (6)	0.002 (6)	-0.005 (6)
O4	0.031 (9)	0.044 (10)	0.056 (10)	0.005 (7)	0.007 (7)	0.023 (8)
O1W	0.029 (8)	0.035 (8)	0.041 (9)	-0.006 (6)	0.006 (7)	-0.009 (7)
O2W	0.071 (12)	0.044 (10)	0.024 (8)	-0.021 (9)	0.013 (8)	-0.010 (7)
O3W	0.047 (16)	0.15 (3)	0.040 (14)	0.000	0.000	-0.002 (17)
O5	0.07 (2)	0.14 (3)	0.35 (6)	0.04 (2)	0.07 (3)	0.12 (3)

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

Pr1—O3 ⁱ	2.390 (14)	N2—C11	1.32 (3)
Pr1—O1W	2.477 (14)	N2—C7	1.34 (3)
Pr1—O2W	2.495 (14)	C7—C8	1.38 (3)
Pr1—O1	2.504 (13)	C7—H7	0.9300
Ag1—N2	2.165 (18)	C11—C10	1.37 (4)
Ag1—N1	2.175 (18)	C11—H11	0.9300
Ag1—O4 ⁱⁱ	2.777 (16)	C11—O5 ^{iv}	1.31 (3)
Ag1—O5	2.81 (3)	Cl1—O5	1.31 (3)
Ag1—O3W	2.90 (2)	Cl1—O7	1.46 (4)
Ag1—Ag1 ⁱⁱⁱ	3.357 (2)	Cl1—O6	1.52 (5)

C2—C3	1.37 (3)	C8—C9	1.37 (3)
C2—C1	1.38 (3)	C8—C12	1.51 (3)
C2—C6	1.50 (3)	C9—C10	1.39 (4)
C6—O1	1.24 (2)	C9—H9	0.9300
C6—O2	1.27 (3)	C10—H10	0.9300
C3—C4	1.37 (4)	C12—O4	1.24 (2)
C3—H3	0.9300	C12—O3	1.25 (2)
C1—N1	1.34 (3)	O1W—H1W	0.88
C1—H1	0.9300	O1W—H2W	0.97
C4—C5	1.39 (4)	O2W—H3W	1.00
C4—H4	0.9300	O2W—H4W	0.83
C5—N1	1.33 (3)	O3W—H5W	0.82
C5—H5	0.9300		
O3 ⁱ —Pr1—O3 ^v	106.9 (7)	C3—C4—H4	120.8
O3 ⁱ —Pr1—O1W	146.7 (5)	C5—C4—H4	120.8
O3 ^v —Pr1—O1W	89.7 (5)	N1—C5—C4	123 (2)
O3 ⁱ —Pr1—O1W ^{vi}	89.7 (5)	N1—C5—H5	118.7
O3 ^v —Pr1—O1W ^{vi}	146.7 (5)	C4—C5—H5	118.7
O1W—Pr1—O1W ^{vi}	91.5 (7)	C5—N1—C1	118 (2)
O3 ⁱ —Pr1—O2W	69.4 (5)	C5—N1—Ag1	122.9 (16)
O3 ^v —Pr1—O2W	82.3 (5)	C1—N1—Ag1	119.1 (15)
O1W—Pr1—O2W	142.9 (5)	C6—O1—Pr1	140.4 (13)
O1W ^{vi} —Pr1—O2W	76.7 (5)	C11—N2—C7	118 (2)
O3 ⁱ —Pr1—O2W ^{vi}	82.3 (5)	C11—N2—Ag1	122.3 (16)
O3 ^v —Pr1—O2W ^{vi}	69.4 (5)	C7—N2—Ag1	119.9 (14)
O1W—Pr1—O2W ^{vi}	76.7 (5)	N2—C7—C8	124 (2)
O1W ^{vi} —Pr1—O2W ^{vi}	142.9 (5)	N2—C7—H7	117.8
O2W—Pr1—O2W ^{vi}	131.9 (7)	C8—C7—H7	117.8
O3 ⁱ —Pr1—O1	139.0 (5)	N2—C11—C10	123 (2)
O3 ^v —Pr1—O1	75.5 (5)	N2—C11—H11	118.7
O1W—Pr1—O1	72.5 (5)	C10—C11—H11	118.7
O1W ^{vi} —Pr1—O1	73.2 (5)	O5 ^{iv} —C11—O5	122 (4)
O2W—Pr1—O1	70.5 (5)	O5 ^{iv} —C11—O7	113.2 (18)
O2W ^{vi} —Pr1—O1	132.8 (5)	O5—C11—O7	113.2 (18)
O3 ⁱ —Pr1—O1 ^{vi}	75.5 (5)	O5 ^{iv} —C11—O6	98 (2)
O3 ^v —Pr1—O1 ^{vi}	139.0 (5)	O5—C11—O6	98 (2)
O1W—Pr1—O1 ^{vi}	73.2 (5)	O7—C11—O6	109 (3)
O1W ^{vi} —Pr1—O1 ^{vi}	72.5 (5)	C9—C8—C7	117 (2)
O2W—Pr1—O1 ^{vi}	132.8 (5)	C9—C8—C12	122.1 (19)
O2W ^{vi} —Pr1—O1 ^{vi}	70.5 (5)	C7—C8—C12	120.9 (19)
O1—Pr1—O1 ^{vi}	129.9 (7)	C8—C9—C10	119 (2)
N2—Ag1—N1	174.6 (7)	C8—C9—H9	120.3
N2—Ag1—Ag1 ⁱⁱⁱ	71.2 (5)	C10—C9—H9	120.3

supplementary materials

N1—Ag1—Ag1 ⁱⁱⁱ	113.5 (5)	C11—C10—C9	119 (3)
C3—C2—C1	118 (2)	C11—C10—H10	120.5
C3—C2—C6	121.2 (19)	C9—C10—H10	120.5
C1—C2—C6	121 (2)	O4—C12—O3	124.9 (19)
O1—C6—O2	124.6 (19)	O4—C12—C8	117.7 (18)
O1—C6—C2	118.3 (19)	O3—C12—C8	117.4 (18)
O2—C6—C2	117.1 (17)	C12—O3—Pr1 ⁱ	150.2 (13)
C4—C3—C2	120 (2)	Pr1—O1W—H1W	100.1
C4—C3—H3	119.9	Pr1—O1W—H2W	126.4
C2—C3—H3	119.9	H1W—O1W—H2W	118.2
N1—C1—C2	123 (2)	Pr1—O2W—H3W	122.7
N1—C1—H1	118.3	Pr1—O2W—H4W	131.7
C2—C1—H1	118.3	H3W—O2W—H4W	105.6
C3—C4—C5	118 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O2 ^{vi}	0.88	1.79	2.67 (2)	179
O1W—H2W \cdots O4 ⁱⁱⁱ	0.97	1.68	2.63 (2)	163
O2W—H3W \cdots O2 ^{vii}	1.00	1.77	2.77 (2)	176
O2W—H4W \cdots O2 ^{viii}	0.83	1.95	2.76 (2)	162
O3W—H5W \cdots O1W ^{ix}	0.82	2.15	2.91 (2)	157

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

Fig. 1

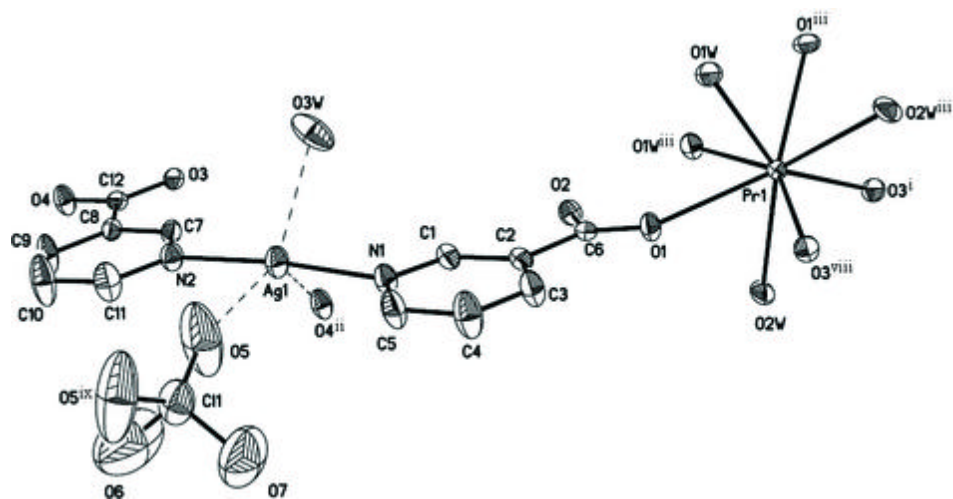


Fig. 2

