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Crystal structure of *catena*-poly[[[aquabis(dimethylformamide-κO)magnesium(II)]-μ_3-(2,2′-bipyridine-5,5′-dicarboxylato-$\kappa^5 O^2$:$O^{2'}$:N,N':O^5)-[dichloridoplatinum(II)]] dimethylformamide monosolvate]

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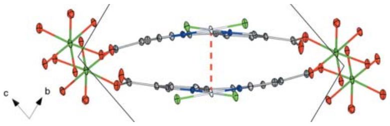
The title compound, $\{[MgPtCl_2(C_{12}H_6N_2O_4)(C_3H_7NO)_2(H_2O)]\cdot C_3H_7NO\}_n$, is a one-dimensional coordination polymer. The structure consists of Pt-functionalized bipyridine ligands connected by Mg^{II} cations, as well as coordinating and non-coordinating solvent molecules. The Pt^{II} cation is coordinated by the two N atoms of the bipyridine moiety and two Cl atoms in a square-planar fashion. This coordination induces an in-plane bend along the bipyridine backbone of approximately 10° from the linear ideal of a conjugated π-system. Likewise, the coordination to the Mg^{II} cation induces a significant bowing of the plane of the bipyridine of about 12°, giving it a distinct curved appearance. The carboxylate groups of the bipyridine ligand exhibit moderate rotations relative to their parent pyridine rings. The Mg^{II} cation has a fairly regular octahedral coordination polyhedron, in which three vertices are occupied by O atoms from the carboxylate groups of three different bipyridine ligands. The remaining three vertices are occupied by the O atoms of two dimethylformamide (DMF) molecules and one water molecule. The one-dimensional chains are oriented in the $[01\overline{1}]$ direction, and non-coordinating DMF molecules can be found in the space between the chains. The shortest intermolecular O⋯H contacts are 2.844 (4) and 2.659 (4) Å, suggesting moderate hydrogen-bonding interactions. In addition, there is a short intermolecular Pt⋯Pt contact of 3.491 (1) Å, indicating a Pt stacking interaction. Some structure-directing contribution from the hydrogen bonding and Pt⋯Pt interaction is probable. However, the crystal packing seems to be directed primarily by van der Waals interactions.



1. Chemical context

Metal–organic frameworks (MOFs) are porous materials that have attracted significant attention over the last two decades. The materials are formed from inorganic and organic components, typically a cationic unit linked by an organic ligand commonly referred to as a linker. Incorporating a catalytically active site in the linker of a porous MOF has the potential to create a heterogenous catalyst with the same selectivity often associated with homogenous catalysts. To this end, there are two main strategies for incorporating the active species. One method is to add the active species to the MOF after the frameworks has been formed, so called post-synthetic modification. The other option is to functionalize the linker either before or during the MOF synthesis (Cohen, 2017).

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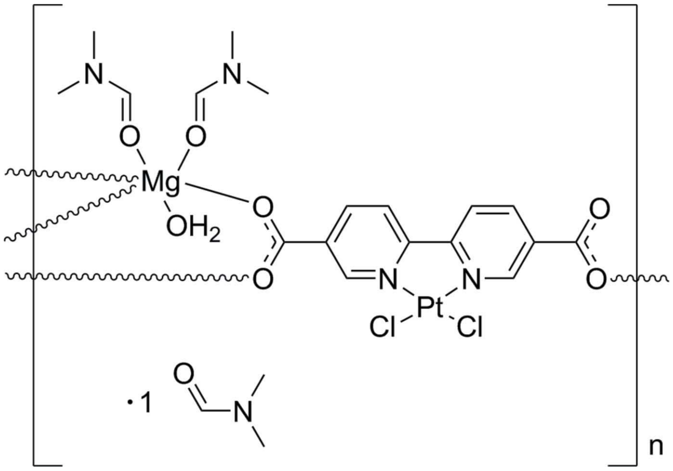
The title compound is an unexpected byproduct from the synthesis of the functionalized linker (2,2′-bipyridine-5,5′-dicarboxcylic acid)tetrachloridoplatinum(IV). 2,2′-bipyridine-5,5′-dicarboxcylic acid is highly suitable for incorporation in the UiO-67 MOF, where it can partially substitute the biphenyl linker of the parent structure (Cavka *et al.*, 2008). Furthermore, the N atoms of the bipyridine linker can be used to anchor and functionalize the linker with *e.g.* Pt or other noble metals. The Pt site of the target linker is interesting in a catalytic context. Pt has a rich redox chemistry and is know to readily switch between oxidation states Pt^{II} and Pt^{IV}, thus providing an active site for *e.g.* C—H activation. The target linker and its successful inclusion in the UiO-67 MOF has been reported in the literature (Øien *et al.*, 2015).



2. Structural commentary

The asymmetric unit of the title compound comprises a Mg^{II} cation coordinated by two dimethylformamide (DMF) molecules and one water molecule, as well as a bipyridine moiety with two Cl atoms and Pt^{II} in a square-planar coordination. In addition, the asymmetric unit contains a DMF solvent molecule that does not coordinate to the rest of the structure (Fig. 1). The Mg^{II} cation is octahedrally coordinated, with the vertices occupied by O atoms from two DMF molecules, one water molecule and three carboxylate groups from three different bipyridine moieties.

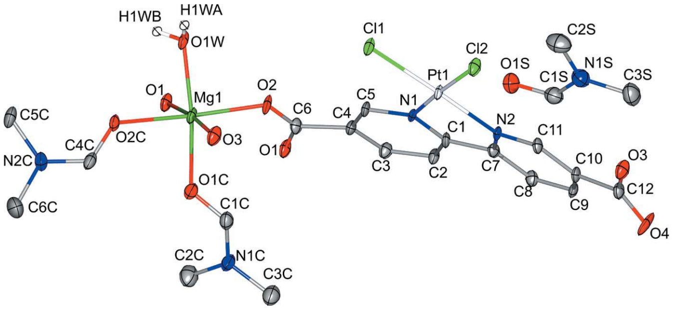


Figure 1
The asymmetric unit of the title compound, with atom labels and 50% probability displacement ellipsoids. H atoms have been omitted for clarity, excluding the H atoms of the coordinating water molecule (H1*WA*/*B*).

Table 1
Selected geometric parameters (Å, °).

Pt1—Cl1	2.3000 (14)	Mg1—O2^{ii}	2.066 (3)
Pt1—Cl2	2.3066 (13)	Mg1—O3^{iii}	2.063 (3)
Pt1—N1	2.020 (3)	Mg1—O1*C*	2.086 (3)
Pt1—N2	2.016 (3)	Mg1—O2*C*	2.155 (3)
Pt1—Pt1^{i}	3.491 (1)	Mg1—O1*W*	2.053 (3)
Mg1—O1	2.030 (3)		
Cl1—Pt1—Cl2	88.94 (5)	N2—Pt1—N1	80.50 (13)
N1—Pt1—Cl1	94.88 (10)	N1—C1—C7	114.8 (4)
N2—Pt1—Cl2	95.66 (10)	N2—C7—C1	114.8 (4)

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

The carboxylate groups coordinate to the cation in a monodentate fashion, thus each bipyridine moiety coordinates to three different Mg^{II} cations. The fourth O atom of the carboxylate groups (O4) is uncoordinating, and has a more pronounced displacement ellipsoid when compared to the coordinating O atoms O1, O2 and O3. Moderate torsion angles of 12.56 (29)° and 12.29 (25)° can be observed for the two carboxylate groups relative to their parent pyridine rings.

One Pt^{II} and two Cl atoms are coordinated by the N atoms of the bipyridine ligand in a square-planar coordination. This type of coordination is commonly observed in complexes with Pt^{II} and other transition metals with a d^8 electron configuration (Krogmann, 1969). The square plane itself is regular with an r.m.s. deviation from the flat plane of only 0.013 Å. Angles of 88.94 (5) and 80.50 (13)° are observed for Cl1—Pt1—Cl2 and N1—Pt1—N2, respectively. Notably, the Pt—Cl bonds are slightly longer (∼2.30 Å) than the Pt—N bonds (∼2.02 Å). This indicates that there is a stronger *trans* effect from the bipyridine ligand than the Cl atoms. The bond lengths and angles (Table 1) are consistent with other similar structures (Hazell *et al.*, 1986; Kato & Ikemori, 2003; Kato *et al.*, 2006; Hazell, 2004; Maheshwari *et al.*, 2007).

The bipyridine backbone exhibits a distinct bowing relative to the plane of the molecule (Figs. 2 and 3) as well as an in-plane bend (Fig. 4). The bowing has been calculated to 12.74 (20)° by comparing the angle between the least-squares planes of the pyridine rings. Deviations from the ideal 120° for the N1—C1—C7 and C1—C7—N2 angles give an estimation of the in-plane bending of about 10°. Such in-plane bending and bowing has been observed in several similar, albeit non-coordinating, bipyridine compounds (Hazell *et al.*, 1986; Kato & Ikemori, 2003; Kato *et al.*, 2006; Hazell, 2004; Maheshwari *et al.*, 2007). However, it is likely that the distortion of the bipyridine is influenced by the coordination to Mg as well as the intermolecular Pt···Pt interaction.

3. Supramolecular features

The title compound forms one-dimensional chains comprising two bipyridine linkers and two Mg^{II} cations with associated coordinating solvent molecules as the repeating unit. These

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2$C^{\rm iv}$	0.87	2.05	2.844 (4)	151
O1W—H1WB···O4$^{\rm v}$	0.87	1.80	2.659 (4)	168

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

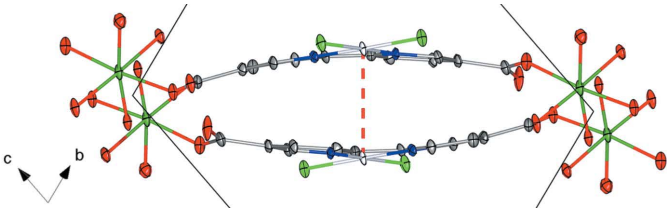


Figure 3
Detailed view of the title compound viewed along the *a* axis, with 50% probability displacement ellipsoids. H atoms, non-coordinating solvent molecules and non-O atoms of coordinating solvent molecules have been omitted for clarity. The Pt···Pt interaction is indicated by a red dashed line. The second bipyridine moiety is generated by the symmetry operation ($-x + 2$, $-y + 1$, $-z + 1$).

chains are oriented in the [01$\overline{1}$] direction (Fig. 1). DMF solvent molecules can be found between the chains, oriented side-on to the plane of the bipyridine linker. Hydrogen-bonding interactions (Table 2) are found between the coordinating water molecule O2W and atoms O2C and O4 of neighboring DMF and bipyridine moieties. The donor–acceptor distances are 2.844 (4) and 2.659 (4) Å, indicating moderately strong bonds. There is also a short intermolecular Pt···Pt contact of 3.491 (1) Å, indicating a Pt stacking interaction between pairs of bipyridine ligands in the chain. These types of stacking interactions are common in square-planar complexes of metals in a d^8 electronic configuration (Krogmann, 1969). The hydrogen bonding and Pt···Pt stacking interaction are likely to contribute to the overall structure and crystal packing.

4. Synthesis and crystallization

2,2′-Bipyridine-5,5′-dicarboxylic acid, was synthesized according to literature methods (Szeto *et al.*, 2008). Dimethylformamide (DMF) was supplied by Sigma–Aldrich and dried before use. K_2PtCl_6 and 35%$_{\rm wt}$ HCl were used as received from Sigma–Aldrich.

The title compound was synthesized by dissolving 16.3 mg (0.067 mmol) 2,2′-bipyridine-5,5′-dicarboxylic acid, 65.3 mg (0.134 mmol) K_2PtCl_6 and three drops of 35% HCl in 4 ml of DMF. The mixture was heated in a closed glass vial in a convection oven at 323 K for 48 h, followed by 24 h at 343 K and finally 48 h at 353 K. This procedure yielded clusters of yellow needle-shaped crystals suitable for single crystal X-ray diffraction, as well as a yet unidentified red compound.

Note that the synthesis procedure does not include a source of Mg, despite its inclusion as cation in the title compound. The initial structural solution included K$^+$ as the cation. However, the refinement of this initial model indicated several problems. First of all, a fully deprotonated organic ligand (L^{2-}) and just one K$^+$ cation would imply a charge imbalance in the structure. Secondly, the model had unrealistic displacement ellipsoids for the metal species as well as an unusual weighting scheme. Lastly, the metal-to-oxygen bond lengths were significantly shorter than expected for K—O bonds in an

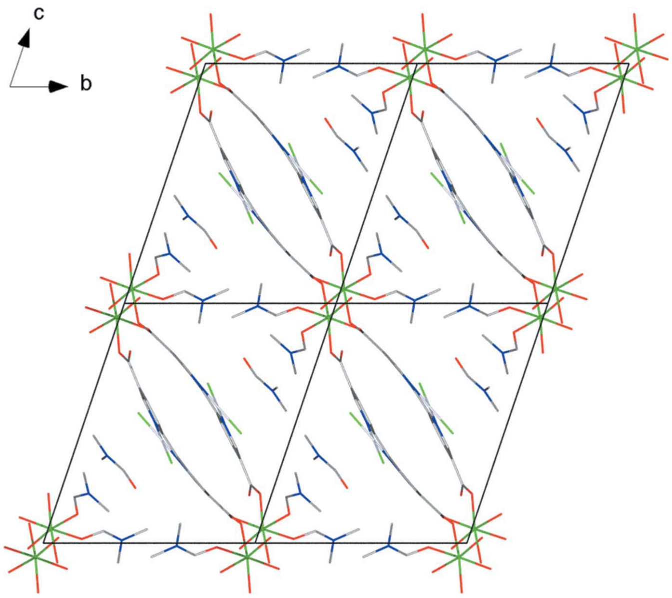


Figure 2
Packing diagram of the title compound, viewed along the *a* axis. H atoms have been omitted for clarity.

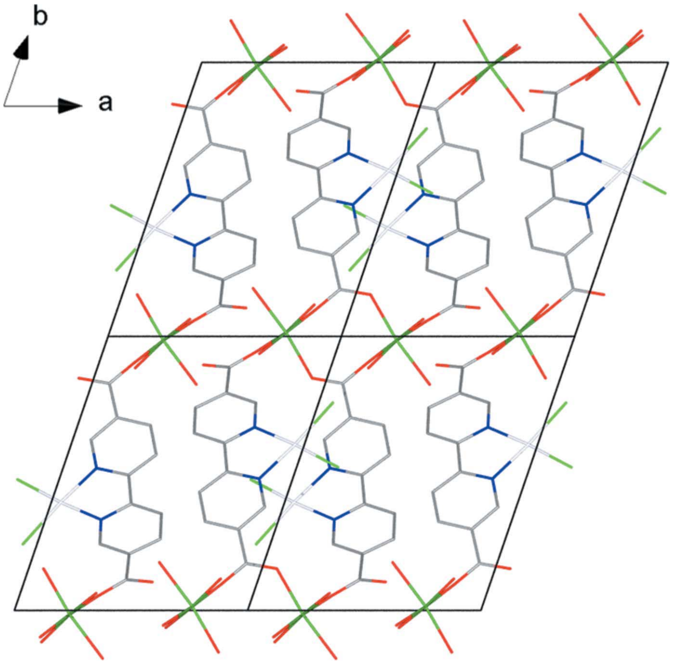


Figure 4
Packing diagram of the title compound, viewed along the *c* axis. H atoms, non-coordinating solvent molecules and non-O atoms of coordinating solvent molecules have been omitted for clarity.

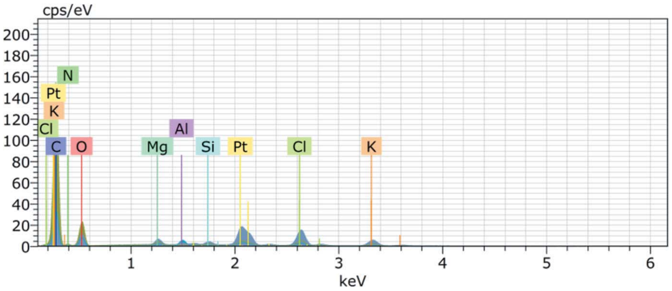


Figure 5
Energy-dispersive X-ray spectroscopy (EDX) spectrum of the title compound.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[MgPtCl_2(C_{12}H_6N_2O_4)(C_3H_7NO)_2(H_2O)]\cdot C_3H_7NO$
M_r	769.79
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	9.224 (4), 12.083 (6), 13.673 (7)
α, β, γ (°)	69.206 (14), 80.361 (17), 69.054 (14)
V (Å^3)	1329.1 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.56
Crystal size (mm)	0.2 × 0.1 × 0.09
Data collection	
Diffractometer	Bruker PHOTON CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.518, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31765, 4615, 4405
R_{int}	0.057
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.028, 0.074, 1.09
No. of reflections	4615
No. of parameters	352
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.92, −2.42

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2014), *ChemBioDraw Ultra* (Cambridge Soft, 2012) and *publCIF* (Westrip, 2010).

octahedral environment when applying the bond-valence method (Brown & Altermatt, 1985). Thus we hypothesized that the coordination polymer must contain a contamination from the synthesis. The correct cation would likely be a divalent metal that is commonly encountered in organic chemistry, often exhibits octahedral coordination, and most importantly has a short metal-to-oxygen bond. Based on these criteria, the cation of the initial model was replaced with Mg, which solved the aforementioned refinement issues. Subsequent energy-dispersive X-ray spectroscopy (EDX) confirmed the presence of Mg in the sample (Fig. 5). The source of the contamination is likely from a batch of DMF incorrectly dried over $MgSO_4$.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically at distances of 0.87 (OH), 0.95 (CH) and 0.98 Å (CH_3) and refined using a riding model with $U_{iso}(H) = 1.2\ U_{eq}(CH)$ and $U_{iso}(H) = 1.5U_{eq}(OH\ and\ CH_3)$.

Acknowledgements

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Funding information

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supporting information

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Crystal structure of *catena*-poly[[[aquabis(dimethylformamide-κ*O*)magnesium(II)]-μ_3-(2,2′-bipyridine-5,5′-dicarboxylato-κ^5O^2:$O^{2\prime}$:*N*,*N*′:O^5)-[dichloridoplatinum(II)]] dimethylformamide monosolvate]

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *DIAMOND* (Brandenburg, 2014) and *ChemBioDraw Ultra* (Cambridge Soft, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

catena-Poly[[[aquabis(dimethylformamide-κ*O*)magnesium(II)]-μ_3-(2,2′-bipyridine-5,5′-dicarboxylato-κ^5O^2:$O^{2\prime}$:*N*,*N*′:O^5)-[dichloridoplatinum(II)]] dimethylformamide monosolvate]

Crystal data

$[MgPtCl_2(C_{12}H_6N_2O_4)$
$(C_3H_7NO)_2(H2O)]\cdot C_3H_7NO$
$M_r = 769.79$
Triclinic, $P\bar{1}$
$a = 9.224\ (4)$ Å
$b = 12.083\ (6)$ Å
$c = 13.673\ (7)$ Å
$\alpha = 69.206\ (14)°$
$\beta = 80.361\ (17)°$
$\gamma = 69.054\ (14)°$
$V = 1329.1\ (11)$ Å^3

$Z = 2$
$F(000) = 756$
$D_x = 1.923$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9986 reflections
$\theta = 2.4–24.8°$
$\mu = 5.56$ mm^{-1}
$T = 100$ K
Needle, clear yellow
0.2 × 0.1 × 0.09 mm

Data collection

Bruker PHOTON CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)
$T_{min} = 0.518$, $T_{max} = 0.745$

31765 measured reflections
4615 independent reflections
4405 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -10\rightarrow10$
$k = -14\rightarrow14$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.074$
$S = 1.09$
4615 reflections
352 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 1.4382P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.92$ e Å^{-3}
$\Delta\rho_{min} = -2.42$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
Pt1	0.96005 (2)	0.60542 (2)	0.56892 (2)	0.01206 (8)
Cl1	1.17780 (12)	0.52245 (9)	0.66544 (8)	0.0179 (2)
Cl2	1.06049 (12)	0.75785 (9)	0.45784 (8)	0.0178 (2)
Mg1	0.75731 (15)	0.01424 (12)	1.05885 (10)	0.0146 (3)
O1	0.8504 (3)	0.0973 (3)	0.9186 (2)	0.0170 (6)
O2	1.0637 (3)	0.1526 (3)	0.8926 (2)	0.0191 (6)
O3	0.6600 (4)	0.9454 (3)	0.2053 (2)	0.0210 (7)
O4	0.4507 (4)	0.8962 (3)	0.1999 (2)	0.0305 (8)
O1C	0.8374 (3)	0.1152 (3)	1.1211 (2)	0.0205 (6)
O2C	0.5514 (3)	0.1750 (3)	1.0171 (2)	0.0172 (6)
O1W	0.6744 (3)	−0.0626 (3)	0.9774 (2)	0.0167 (6)
H1WA	0.6049	−0.1000	1.0028	0.025*
H1WB	0.6456	−0.0055	0.9174	0.025*
N1	0.8564 (4)	0.4808 (3)	0.6630 (3)	0.0105 (7)
N2	0.7619 (4)	0.6682 (3)	0.4934 (3)	0.0117 (7)
N1C	1.0118 (4)	0.1352 (4)	1.2069 (3)	0.0226 (8)
N2C	0.3786 (4)	0.3657 (3)	1.0119 (3)	0.0244 (8)
C1	0.7083 (5)	0.5059 (4)	0.6397 (3)	0.0137 (8)
C2	0.6205 (5)	0.4317 (4)	0.6998 (3)	0.0146 (8)
H2	0.5144	0.4540	0.6859	0.017*
C3	0.6879 (5)	0.3246 (4)	0.7803 (3)	0.0165 (9)
H3	0.6298	0.2717	0.8215	0.020*
C4	0.8419 (5)	0.2961 (4)	0.7994 (3)	0.0137 (8)
C5	0.9213 (5)	0.3777 (4)	0.7419 (3)	0.0147 (8)
H5	1.0247	0.3606	0.7586	0.018*
C6	0.9253 (5)	0.1716 (4)	0.8792 (3)	0.0147 (8)
C7	0.6553 (5)	0.6113 (4)	0.5438 (3)	0.0133 (8)
C8	0.5117 (5)	0.6468 (4)	0.5021 (3)	0.0155 (9)
H8	0.4370	0.6076	0.5391	0.019*
C9	0.4788 (5)	0.7396 (4)	0.4065 (3)	0.0151 (8)

H9	0.3803	0.7661	0.3778	0.018*
C10	0.5910 (5)	0.7938 (4)	0.3526 (3)	0.0144 (8)
C11	0.7305 (5)	0.7576 (3)	0.3990 (3)	0.0127 (8)
H11	0.8060	0.7966	0.3634	0.015*
C12	0.5650 (5)	0.8877 (4)	0.2425 (3)	0.0168 (9)
C1C	0.9292 (5)	0.0737 (4)	1.1917 (3)	0.0207 (9)
H1C	0.9411	−0.0084	1.2386	0.025*
C2C	1.0120 (6)	0.2562 (5)	1.1336 (4)	0.0316 (11)
H2CA	0.9431	0.2807	1.0769	0.047*
H2CB	1.1178	0.2512	1.1044	0.047*
H2CC	0.9753	0.3186	1.1702	0.047*
C3C	1.1173 (6)	0.0797 (5)	1.2919 (4)	0.0294 (11)
H3CA	1.2248	0.0591	1.2634	0.044*
H3CB	1.0986	0.0033	1.3402	0.044*
H3CC	1.0997	0.1393	1.3295	0.044*
C4C	0.4982 (5)	0.2652 (4)	1.0503 (3)	0.0212 (9)
H4C	0.5468	0.2621	1.1077	0.025*
C5C	0.3018 (5)	0.3840 (4)	0.9197 (4)	0.0250 (10)
H5CA	0.3560	0.3146	0.8919	0.038*
H5CB	0.3041	0.4629	0.8661	0.038*
H5CC	0.1937	0.3867	0.9391	0.038*
C6C	0.3190 (7)	0.4667 (5)	1.0579 (5)	0.0389 (14)
H6CA	0.2148	0.4698	1.0898	0.058*
H6CB	0.3138	0.5465	1.0031	0.058*
H6CC	0.3884	0.4514	1.1116	0.058*
O1S	0.3963 (4)	0.6539 (3)	0.7698 (3)	0.0312 (8)
N1S	0.3595 (5)	0.8390 (4)	0.6353 (3)	0.0270 (9)
C1S	0.3216 (6)	0.7374 (4)	0.6968 (4)	0.0266 (10)
H1S	0.2290	0.7298	0.6826	0.032*
C2S	0.5037 (7)	0.8550 (6)	0.6488 (5)	0.0377 (14)
H2SA	0.5607	0.8737	0.5810	0.056*
H2SB	0.5677	0.7779	0.6977	0.056*
H2SC	0.4795	0.9242	0.6768	0.056*
C3S	0.2617 (6)	0.9344 (5)	0.5520 (4)	0.0344 (12)
H3SA	0.2239	1.0142	0.5664	0.052*
H3SB	0.1731	0.9096	0.5482	0.052*
H3SC	0.3222	0.9438	0.4851	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01192 (11)	0.00874 (11)	0.01110 (11)	−0.00185 (7)	−0.00702 (7)	0.00337 (7)
Cl1	0.0156 (5)	0.0152 (5)	0.0185 (5)	−0.0041 (4)	−0.0110 (4)	0.0037 (4)
Cl2	0.0181 (5)	0.0143 (5)	0.0167 (5)	−0.0071 (4)	−0.0068 (4)	0.0047 (4)
Mg1	0.0143 (7)	0.0117 (7)	0.0126 (7)	−0.0027 (6)	−0.0079 (5)	0.0040 (5)
O1	0.0173 (15)	0.0150 (15)	0.0134 (15)	−0.0046 (13)	−0.0072 (12)	0.0039 (12)
O2	0.0138 (15)	0.0148 (15)	0.0200 (16)	−0.0026 (12)	−0.0116 (12)	0.0072 (12)
O3	0.0221 (17)	0.0205 (16)	0.0153 (15)	−0.0075 (14)	−0.0065 (13)	0.0032 (12)

O4	0.0327 (19)	0.0318 (19)	0.0207 (17)	−0.0173 (15)	−0.0225 (14)	0.0153 (14)
O1C	0.0206 (16)	0.0189 (15)	0.0194 (16)	−0.0039 (13)	−0.0095 (13)	−0.0018 (13)
O2C	0.0181 (15)	0.0121 (14)	0.0163 (15)	−0.0016 (12)	−0.0087 (12)	0.0018 (12)
O1W	0.0152 (15)	0.0135 (15)	0.0148 (15)	−0.0029 (12)	−0.0098 (12)	0.0052 (11)
N1	0.0101 (17)	0.0087 (16)	0.0101 (16)	−0.0001 (14)	−0.0071 (13)	0.0000 (13)
N2	0.0133 (17)	0.0097 (17)	0.0079 (16)	−0.0008 (14)	−0.0055 (13)	0.0012 (13)
N1C	0.025 (2)	0.019 (2)	0.022 (2)	−0.0069 (17)	−0.0112 (16)	−0.0008 (16)
N2C	0.024 (2)	0.0141 (19)	0.029 (2)	0.0016 (16)	−0.0122 (17)	−0.0020 (16)
C1	0.015 (2)	0.0081 (19)	0.012 (2)	0.0018 (16)	−0.0072 (16)	0.0007 (15)
C2	0.013 (2)	0.013 (2)	0.014 (2)	−0.0027 (17)	−0.0063 (16)	0.0014 (16)
C3	0.019 (2)	0.015 (2)	0.013 (2)	−0.0057 (18)	−0.0029 (17)	0.0005 (16)
C4	0.015 (2)	0.010 (2)	0.011 (2)	−0.0001 (17)	−0.0069 (16)	0.0009 (16)
C5	0.017 (2)	0.012 (2)	0.011 (2)	0.0008 (17)	−0.0096 (16)	0.0008 (16)
C6	0.017 (2)	0.012 (2)	0.011 (2)	−0.0039 (17)	−0.0033 (16)	0.0011 (16)
C7	0.019 (2)	0.0083 (19)	0.0097 (19)	−0.0027 (17)	−0.0033 (16)	−0.0001 (15)
C8	0.013 (2)	0.013 (2)	0.017 (2)	−0.0034 (17)	−0.0025 (17)	−0.0009 (17)
C9	0.016 (2)	0.0121 (19)	0.012 (2)	−0.0011 (17)	−0.0098 (16)	0.0020 (16)
C10	0.017 (2)	0.0095 (19)	0.012 (2)	−0.0010 (16)	−0.0072 (16)	0.0021 (15)
C11	0.014 (2)	0.0069 (18)	0.013 (2)	−0.0013 (16)	−0.0037 (16)	0.0011 (15)
C12	0.018 (2)	0.011 (2)	0.016 (2)	−0.0021 (18)	−0.0054 (17)	0.0023 (17)
C1C	0.023 (2)	0.015 (2)	0.019 (2)	−0.0009 (18)	−0.0063 (19)	−0.0012 (18)
C2C	0.031 (3)	0.024 (3)	0.036 (3)	−0.012 (2)	−0.007 (2)	−0.001 (2)
C3C	0.028 (3)	0.027 (3)	0.032 (3)	−0.008 (2)	−0.010 (2)	−0.005 (2)
C4C	0.021 (2)	0.021 (2)	0.019 (2)	−0.0062 (19)	−0.0105 (18)	0.0002 (18)
C5C	0.023 (2)	0.022 (2)	0.021 (2)	−0.001 (2)	−0.0126 (19)	0.0025 (19)
C6C	0.040 (3)	0.025 (3)	0.047 (3)	0.006 (2)	−0.020 (3)	−0.016 (2)
O1S	0.037 (2)	0.0217 (17)	0.0297 (19)	−0.0040 (15)	−0.0119 (15)	−0.0030 (15)
N1S	0.029 (2)	0.022 (2)	0.029 (2)	−0.0078 (18)	−0.0028 (18)	−0.0077 (17)
C1S	0.030 (3)	0.024 (2)	0.028 (3)	−0.008 (2)	−0.002 (2)	−0.011 (2)
C2S	0.036 (3)	0.039 (3)	0.048 (4)	−0.016 (3)	0.002 (3)	−0.023 (3)
C3S	0.042 (3)	0.022 (3)	0.030 (3)	−0.004 (2)	−0.005 (2)	−0.003 (2)

Geometric parameters (Å, º)

Pt1—Cl1	2.3000 (14)	C4—C5	1.378 (6)
Pt1—Cl2	2.3066 (13)	C4—C6	1.527 (5)
Pt1—N1	2.020 (3)	C5—H5	0.9500
Pt1—N2	2.016 (3)	C7—C8	1.392 (6)
Pt1—Pt1^{i}	3.491 (1)	C8—H8	0.9500
Mg1—O1	2.030 (3)	C8—C9	1.381 (6)
Mg1—O2^{ii}	2.066 (3)	C9—H9	0.9500
Mg1—O3^{iii}	2.063 (3)	C9—C10	1.390 (6)
Mg1—O1C	2.086 (3)	C10—C11	1.386 (6)
Mg1—O2C	2.155 (3)	C10—C12	1.525 (6)
Mg1—O1W	2.053 (3)	C11—H11	0.9500
O1—C6	1.245 (5)	C1C—H1C	0.9500
O2—Mg1^{ii}	2.066 (3)	C2C—H2CA	0.9800
O2—C6	1.248 (5)	C2C—H2CB	0.9800

O3—Mg1^{iv}	2.063 (3)	C2C—H2CC	0.9800
O3—C12	1.245 (5)	C3C—H3CA	0.9800
O4—C12	1.244 (5)	C3C—H3CB	0.9800
O1C—C1C	1.236 (5)	C3C—H3CC	0.9800
O2C—C4C	1.236 (5)	C4C—H4C	0.9500
O1W—H1WA	0.8696	C5C—H5CA	0.9800
O1W—H1WB	0.8718	C5C—H5CB	0.9800
N1—C1	1.356 (5)	C5C—H5CC	0.9800
N1—C5	1.343 (5)	C6C—H6CA	0.9800
N2—C7	1.354 (5)	C6C—H6CB	0.9800
N2—C11	1.352 (5)	C6C—H6CC	0.9800
N1C—C1C	1.319 (6)	O1S—C1S	1.227 (6)
N1C—C2C	1.451 (6)	N1S—C1S	1.346 (6)
N1C—C3C	1.452 (6)	N1S—C2S	1.461 (7)
N2C—C4C	1.324 (6)	N1S—C3S	1.452 (6)
N2C—C5C	1.460 (6)	C1S—H1S	0.9500
N2C—C6C	1.461 (6)	C2S—H2SA	0.9800
C1—C2	1.382 (6)	C2S—H2SB	0.9800
C1—C7	1.472 (5)	C2S—H2SC	0.9800
C2—H2	0.9500	C3S—H3SA	0.9800
C2—C3	1.385 (6)	C3S—H3SB	0.9800
C3—H3	0.9500	C3S—H3SC	0.9800
C3—C4	1.384 (6)		

Cl1—Pt1—Cl2	88.94 (5)	C9—C8—C7	119.4 (4)
N1—Pt1—Cl1	94.88 (10)	C9—C8—H8	120.3
N1—Pt1—Cl2	175.78 (9)	C8—C9—H9	120.3
N2—Pt1—Cl1	175.36 (9)	C8—C9—C10	119.3 (4)
N2—Pt1—Cl2	95.66 (10)	C10—C9—H9	120.3
N2—Pt1—N1	80.50 (13)	C9—C10—C12	120.9 (4)
O1—Mg1—O2^{ii}	100.05 (13)	C11—C10—C9	118.9 (4)
O1—Mg1—O3^{iii}	174.30 (14)	C11—C10—C12	120.1 (4)
O1—Mg1—O1C	87.00 (13)	N2—C11—C10	121.8 (4)
O1—Mg1—O2C	85.67 (12)	N2—C11—H11	119.1
O1—Mg1—O1W	85.74 (13)	C10—C11—H11	119.1
O2^{ii}—Mg1—O1C	96.54 (13)	O3—C12—C10	117.0 (4)
O2^{ii}—Mg1—O2C	172.91 (13)	O4—C12—O3	127.7 (4)
O3^{iii}—Mg1—O2^{ii}	83.17 (13)	O4—C12—C10	115.3 (4)
O3^{iii}—Mg1—O1C	87.97 (13)	O1C—C1C—N1C	124.9 (4)
O3^{iii}—Mg1—O2C	91.48 (13)	O1C—C1C—H1C	117.6
O1C—Mg1—O2C	87.89 (13)	N1C—C1C—H1C	117.6
O1W—Mg1—O2^{ii}	89.21 (13)	N1C—C2C—H2CA	109.5
O1W—Mg1—O3^{iii}	99.05 (14)	N1C—C2C—H2CB	109.5
O1W—Mg1—O1C	171.43 (13)	N1C—C2C—H2CC	109.5
O1W—Mg1—O2C	87.02 (12)	H2CA—C2C—H2CB	109.5
C6—O1—Mg1	140.5 (3)	H2CA—C2C—H2CC	109.5
C6—O2—Mg1^{ii}	129.6 (3)	H2CB—C2C—H2CC	109.5
C12—O3—Mg1^{iv}	136.2 (3)	N1C—C3C—H3CA	109.5

C1C—O1C—Mg1	127.8 (3)	N1C—C3C—H3CB	109.5
C4C—O2C—Mg1	129.8 (3)	N1C—C3C—H3CC	109.5
Mg1—O1W—H1WA	124.0	H3CA—C3C—H3CB	109.5
Mg1—O1W—H1WB	107.2	H3CA—C3C—H3CC	109.5
H1WA—O1W—H1WB	109.4	H3CB—C3C—H3CC	109.5
C1—N1—Pt1	114.5 (3)	O2C—C4C—N2C	124.9 (4)
C5—N1—Pt1	126.3 (3)	O2C—C4C—H4C	117.6
C5—N1—C1	119.2 (3)	N2C—C4C—H4C	117.6
C7—N2—Pt1	114.8 (3)	N2C—C5C—H5CA	109.5
C11—N2—Pt1	125.9 (3)	N2C—C5C—H5CB	109.5
C11—N2—C7	119.3 (3)	N2C—C5C—H5CC	109.5
C1C—N1C—C2C	121.3 (4)	H5CA—C5C—H5CB	109.5
C1C—N1C—C3C	121.5 (4)	H5CA—C5C—H5CC	109.5
C2C—N1C—C3C	116.9 (4)	H5CB—C5C—H5CC	109.5
C4C—N2C—C5C	122.1 (4)	N2C—C6C—H6CA	109.5
C4C—N2C—C6C	121.6 (4)	N2C—C6C—H6CB	109.5
C5C—N2C—C6C	116.2 (4)	N2C—C6C—H6CC	109.5
N1—C1—C2	121.1 (4)	H6CA—C6C—H6CB	109.5
N1—C1—C7	114.8 (4)	H6CA—C6C—H6CC	109.5
C2—C1—C7	124.0 (4)	H6CB—C6C—H6CC	109.5
C1—C2—H2	120.2	C1S—N1S—C2S	120.6 (5)
C1—C2—C3	119.6 (4)	C1S—N1S—C3S	121.7 (4)
C3—C2—H2	120.2	C3S—N1S—C2S	117.7 (4)
C2—C3—H3	120.7	O1S—C1S—N1S	125.7 (5)
C4—C3—C2	118.6 (4)	O1S—C1S—H1S	117.1
C4—C3—H3	120.7	N1S—C1S—H1S	117.1
C3—C4—C6	120.0 (4)	N1S—C2S—H2SA	109.5
C5—C4—C3	119.5 (4)	N1S—C2S—H2SB	109.5
C5—C4—C6	120.5 (4)	N1S—C2S—H2SC	109.5
N1—C5—C4	121.8 (4)	H2SA—C2S—H2SB	109.5
N1—C5—H5	119.1	H2SA—C2S—H2SC	109.5
C4—C5—H5	119.1	H2SB—C2S—H2SC	109.5
O1—C6—O2	127.2 (4)	N1S—C3S—H3SA	109.5
O1—C6—C4	116.2 (4)	N1S—C3S—H3SB	109.5
O2—C6—C4	116.4 (3)	N1S—C3S—H3SC	109.5
N2—C7—C1	114.8 (4)	H3SA—C3S—H3SB	109.5
N2—C7—C8	121.2 (4)	H3SA—C3S—H3SC	109.5
C8—C7—C1	123.9 (4)	H3SB—C3S—H3SC	109.5
C7—C8—H8	120.3		

Pt1—N1—C1—C2	−177.5 (3)	C3—C4—C6—O1	4.5 (6)
Pt1—N1—C1—C7	6.2 (4)	C3—C4—C6—O2	−179.7 (4)
Pt1—N1—C5—C4	−177.8 (3)	C5—N1—C1—C2	4.0 (6)
Pt1—N2—C7—C1	−5.4 (4)	C5—N1—C1—C7	−172.3 (3)
Pt1—N2—C7—C8	178.6 (3)	C5—C4—C6—O1	−171.8 (4)
Pt1—N2—C11—C10	179.3 (3)	C5—C4—C6—O2	3.9 (6)
Mg1—O1—C6—O2	69.9 (6)	C6—C4—C5—N1	172.1 (4)
Mg1—O1—C6—C4	−115.0 (4)	C7—N2—C11—C10	0.8 (6)

Mg1^{ii}—O2—C6—O1	22.0 (6)	C7—C1—C2—C3	171.1 (4)
Mg1^{ii}—O2—C6—C4	−153.2 (3)	C7—C8—C9—C10	1.4 (6)
Mg1^{iv}—O3—C12—O4	−33.1 (7)	C8—C9—C10—C11	−3.3 (6)
Mg1^{iv}—O3—C12—C10	145.9 (3)	C8—C9—C10—C12	174.3 (4)
Mg1—O1C—C1C—N1C	158.2 (3)	C9—C10—C11—N2	2.2 (6)
Mg1—O2C—C4C—N2C	172.9 (3)	C9—C10—C12—O3	170.0 (4)
N1—C1—C2—C3	−4.8 (6)	C9—C10—C12—O4	−10.9 (6)
N1—C1—C7—N2	−0.5 (5)	C11—N2—C7—C1	173.2 (3)
N1—C1—C7—C8	175.3 (4)	C11—N2—C7—C8	−2.7 (6)
N2—C7—C8—C9	1.6 (6)	C11—C10—C12—O3	−12.4 (6)
C1—N1—C5—C4	0.6 (6)	C11—C10—C12—O4	166.7 (4)
C1—C2—C3—C4	1.1 (6)	C12—C10—C11—N2	−175.4 (4)
C1—C7—C8—C9	−174.0 (4)	C2C—N1C—C1C—O1C	−5.8 (7)
C2—C1—C7—N2	−176.8 (4)	C3C—N1C—C1C—O1C	180.0 (4)
C2—C1—C7—C8	−0.9 (6)	C5C—N2C—C4C—O2C	−4.1 (7)
C2—C3—C4—C5	3.3 (6)	C6C—N2C—C4C—O2C	177.8 (5)
C2—C3—C4—C6	−173.1 (4)	C2S—N1S—C1S—O1S	2.9 (7)
C3—C4—C5—N1	−4.2 (6)	C3S—N1S—C1S—O1S	−178.7 (4)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*, −*z*+2; (iii) *x*, *y*−1, *z*+1; (iv) *x*, *y*+1, *z*−1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2*C*^{v}	0.87	2.05	2.844 (4)	151
O1*W*—H1*WB*···O4^{vi}	0.87	1.80	2.659 (4)	168

Symmetry codes: (v) −*x*+1, −*y*, −*z*+2; (vi) −*x*+1, −*y*+1, −*z*+1.