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2-[Tris(pyridin-2-yl)methyl]pyridinium *trans*-bis(acetonitrile)tetrachloridoruthenate(III) acetonitrile monosolvate

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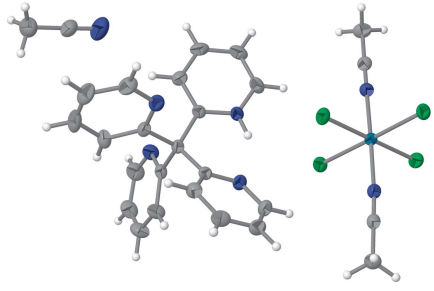
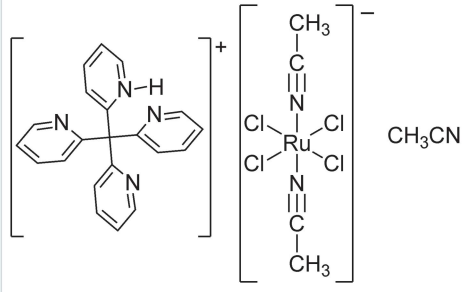
The asymmetric unit of the title compound, $[(C_5H_4N)_3C(C_5H_5N)][RuCl_4(CH_3CN)_2]\cdot CH_3CN$, contains one 2-[tris(pyridin-2-yl)methyl]pyridinium cation, one *trans*-bis(acetonitrile)tetrachloridoruthenate(III) anion and one acetonitrile solvent molecule. The Ru^{III} ion is coordinated by four Cl^- anions in the equatorial plane and by two acetonitrile ligands in the axial positions, forming a distorted octahedral geometry. The cation, the monoprotonated species of tetrakis(pyridin-2-yl)methane, forms an intramolecular N—H···N hydrogen bond between the pyridinium ring and one of the pyridine rings. The complex anions are linked to each other *via* C—H···Cl hydrogen bonds, forming an undulating sheet parallel to the *ac* plane. A C—H···N hydrogen bond between the cation and the anion is also observed. The solvate acetonitrile molecule forms C—H···N and C—H···Cl hydrogen bonds, respectively, with the cation and the anion.

3D view



Chemical scheme



Structure description

We have investigated the synthesis and properties of tetrakis(pyridin-2-yl)methane (py_4C) over the last decade (Matsumoto *et al.*, 2003, 2004). In the course of our studies on py_4C, we are interested in the ruthenium complex with py_4C because of the fascinating properties of ruthenium polypyridine complexes (Juris *et al.*, 1988; Balzani *et al.*, 1996). Although we did not obtain the desired ruthenium complex, we obtained single crystals of the title compound instead. This is the first report of the crystal structure including the monoprotonated py_4C cation, $[(py_4C)\cdot H]^+$.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2	0.87 (2)	1.87 (2)	2.615 (2)	143.3 (19)
C22—H18···Cl1^{i}	0.98	2.69	3.5521 (19)	146
C22—H19···Cl4^{i}	0.98	2.78	3.5972 (19)	142
C24—H21···Cl1^{ii}	0.98	2.77	3.7393 (18)	172
C24—H22···Cl2^{iii}	0.98	2.77	3.6346 (18)	147
C24—H23···N4^{ii}	0.98	2.65	3.606 (2)	165
C6—H5···N7	0.95	2.45	3.248 (3)	142
C26—H26···Cl4^{iv}	0.98	2.84	3.749 (3)	154

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

The asymmetric unit consists of one molecule of $[(py_4C)\cdot H]^+$, one molecule of *trans*-bis(acetonitrile)tetrachloridoruthenate(III), $[RuCl_4(CH_3CN)_2]^-$, and one acetonitrile molecule (Fig. 1). It should be noted that an intramolecular N—H···N hydrogen bond is formed in the cation (Fig. 1 and Table 1). Although py_4C often takes a highly symmetric part in the crystal structure, the cation shows an unsymmetrical structure, where atom C1 occupies a general position. On the other hand, the structure of $[RuCl_4(CH_3CN)_2]^-$ resembles those in previous reports (Gheller *et al.*, 1995; Appelbaum *et al.*, 1999; Jabłońska-Wawrzycka *et al.*, 2013). The Ru^{III} ion adopts an octahedral coordination geometry, with four Cl atoms occupying equatorial positions and two acetonitrile molecules in the axial positions. The Ru^{III} and four Cl atoms essentially lie in a plane and two acetonitrile molecules are approximately perpendicular to the $RuCl_4$ plane. The average Ru—Cl and Ru—N bond lengths are 2.36 and 2.02 Å, respectively.

In the crystal, the anions form an undulating sheet parallel to the *ac* plane *via* C—H···Cl hydrogen bonds (C22—H18···Cl1^{i}, C22—H19···Cl4^{i}, C24—H21···Cl1^{ii} and C24—H22···Cl2^{iii}; symmetry codes as in Table 1). A C—H···N hydrogen bond between $[(py_4C)\cdot H]^+$ and $[RuCl_4(CH_3CN)_2]^-$ is also formed (C24—H23···N4^{ii}; Table 1). The acetonitrile solvent molecule forms C—H···N and C—H···Cl hydrogen bonds (C6—H5···N7 and C26—H26···Cl4^{iv}; Table 1), respectively, with $[(py_4C)\cdot H]^+$ and $[RuCl_4(CH_3CN)_2]^-$.

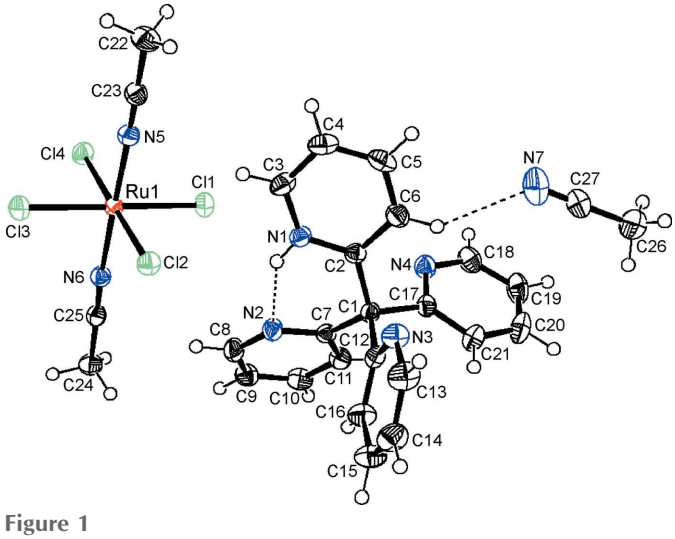


Figure 1
A view of the molecular components of the title compound, showing the atom-labelling and displacement ellipsoids drawn at the 50% probability level for non-H atoms. The intramolecular N—H···N hydrogen bond and the C—H···N hydrogen bond are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_{21}H_{17}N_4)[RuCl_4(C_2H_3N)_2]\cdot C_2H_3N$
M_r	691.42
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	200
a, b, c (Å)	7.6796 (3), 30.3330 (14), 13.1153 (6)
β (°)	100.194 (2)
V (Å^3)	3006.9 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.91
Crystal size (mm)	0.2 × 0.2 × 0.1
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.739, 0.913
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28746, 6815, 6043
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.648
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.059, 1.06
No. of reflections	6815
No. of parameters	359
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.25

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *SIR92* (Altomare *et al.*, 1994), *SHELXL2017* (Sheldrick, 2015), *Yadokari-XG 2009* (Wakita, 2001) and *ORTEP-3 for Windows* (Farrugia, 2012), *CrystalStructure* (Rigaku, 2011) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

A solution of ruthenium(III) chloride n-hydrate (100 mg) in ethanol (6 ml) and water (4 ml) was refluxed for 4 h. Tetrakis(pyridin-2-yl)methane (324 mg) in ethanol (120 ml) was added to the refluxing solution and the reflux was continued for additional 4 h. After cooling to room temperature, the solvents were evaporated and dried under vacuum. Acetonitrile (50 ml) was added to the residue and the insoluble substances were removed by filtration. Brown prisms (70 mg, 21%) appeared from the filtrate by slow evaporation at room temperature. Although the residue obtained from the reaction mixture might have included the desired ruthenium complex, acetonitrile molecules coordinating the ruthenium ion resulted in formation of the title compound. Analysis calculated for $C_{27}H_{26}Cl_4N_7Ru$: C 46.90, H 3.79, N 14.18%; found: C 46.86, H 3.78, N 14.24%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N—H atom H1 was located in a difference Fourier map and refined freely. The CH hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Funding information

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full crystallographic data

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Crystal data

$(C_{21}H_{17}N_4)[RuCl_4(C_2H_3N)_2]\cdot C_2H_3N$
M_r = 691.42
Monoclinic, $P2_1/n$
a = 7.6796 (3) Å
b = 30.3330 (14) Å
c = 13.1153 (6) Å
β = 100.194 (2)°
V = 3006.9 (2) Å^3
Z = 4
$F(000)$ = 1396
D_x = 1.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 21524 reflections
θ = 3.0–27.4°
μ = 0.91 mm^{-1}
T = 200 K
Prism, brown
0.2 × 0.2 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.739, T_{max} = 0.913
28746 measured reflections
6815 independent reflections
6043 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.4°, θ_{min} = 3.0°
h = −9→9
k = −39→38
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.059
S = 1.06
6815 reflections
359 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 1.1697P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.13693 (2)	0.17595 (2)	0.31885 (2)	0.02132 (4)
Cl1	0.23972 (6)	0.23538 (2)	0.22993 (3)	0.03010 (9)
Cl2	0.04670 (5)	0.22761 (2)	0.43493 (3)	0.02920 (9)
Cl3	0.02924 (6)	0.11680 (2)	0.40743 (3)	0.03249 (9)
Cl4	0.22432 (6)	0.12549 (2)	0.20175 (3)	0.02980 (9)
N1	0.03878 (19)	0.32851 (4)	0.29181 (11)	0.0257 (3)
H1	0.119 (3)	0.3148 (7)	0.3352 (16)	0.037 (6)*
N2	0.33833 (18)	0.32182 (4)	0.42140 (11)	0.0282 (3)
N3	0.00392 (19)	0.42519 (5)	0.44106 (11)	0.0325 (3)
N4	0.3292 (2)	0.41845 (5)	0.19756 (11)	0.0308 (3)
N5	−0.10403 (19)	0.18046 (4)	0.22930 (11)	0.0271 (3)
N6	0.37875 (19)	0.17269 (4)	0.41090 (11)	0.0257 (3)
N7	−0.1595 (3)	0.49066 (7)	0.10578 (18)	0.0695 (6)
C1	0.2296 (2)	0.39335 (5)	0.35306 (12)	0.0229 (3)
C2	0.0678 (2)	0.37197 (5)	0.28477 (12)	0.0235 (3)
C3	−0.1004 (2)	0.30712 (6)	0.23517 (14)	0.0330 (4)
H2	−0.113620	0.276230	0.242896	0.040*
C4	−0.2220 (2)	0.33032 (6)	0.16662 (14)	0.0367 (4)
H3	−0.319864	0.315804	0.125818	0.044*
C5	−0.1990 (2)	0.37557 (7)	0.15810 (13)	0.0363 (4)
H4	−0.282418	0.392278	0.111461	0.044*
C6	−0.0557 (2)	0.39630 (6)	0.21712 (13)	0.0315 (4)
H5	−0.041347	0.427264	0.211507	0.038*
C7	0.3840 (2)	0.36092 (5)	0.38549 (11)	0.0228 (3)
C8	0.4657 (2)	0.29287 (6)	0.45778 (14)	0.0330 (4)
H6	0.432529	0.265062	0.481619	0.040*
C9	0.6437 (2)	0.30171 (6)	0.46217 (14)	0.0330 (4)
H7	0.731354	0.280592	0.488755	0.040*
C10	0.6897 (2)	0.34202 (6)	0.42687 (14)	0.0331 (4)
H8	0.810860	0.349216	0.429875	0.040*
C11	0.5595 (2)	0.37222 (6)	0.38685 (13)	0.0289 (3)
H9	0.589818	0.399919	0.361057	0.035*
C12	0.1711 (2)	0.41119 (5)	0.45254 (12)	0.0246 (3)
C13	−0.0499 (3)	0.44280 (7)	0.52414 (15)	0.0412 (4)
H10	−0.168848	0.452695	0.516620	0.049*
C14	0.0566 (3)	0.44738 (7)	0.61927 (15)	0.0414 (4)
H11	0.013023	0.460603	0.675424	0.050*
C15	0.2287 (3)	0.43228 (7)	0.63130 (14)	0.0420 (4)
H12	0.305565	0.434512	0.696352	0.050*
C16	0.2875 (2)	0.41376 (6)	0.54648 (13)	0.0349 (4)
H13	0.405156	0.403048	0.552629	0.042*

C17	0.2905 (2)	0.43121 (5)	0.28908 (12)	0.0253 (3)
C18	0.3850 (3)	0.44934 (6)	0.13796 (15)	0.0375 (4)
H14	0.414699	0.440486	0.073710	0.045*
C19	0.4017 (3)	0.49347 (6)	0.16468 (17)	0.0431 (5)
H15	0.440902	0.514366	0.119743	0.052*
C20	0.3602 (3)	0.50621 (6)	0.25791 (17)	0.0420 (5)
H16	0.369078	0.536291	0.278364	0.050*
C21	0.3050 (2)	0.47458 (5)	0.32215 (15)	0.0337 (4)
H17	0.277691	0.482619	0.387538	0.040*
C22	−0.4196 (2)	0.18499 (7)	0.11958 (15)	0.0366 (4)
H18	−0.483352	0.209827	0.143506	0.055*
H19	−0.483417	0.157542	0.127168	0.055*
H20	−0.411174	0.189300	0.046559	0.055*
C23	−0.2424 (2)	0.18244 (5)	0.18128 (13)	0.0276 (3)
C24	0.6850 (2)	0.17443 (6)	0.53247 (14)	0.0324 (4)
H21	0.690383	0.199937	0.578794	0.049*
H22	0.779032	0.176740	0.491025	0.049*
H23	0.700991	0.147313	0.573680	0.049*
C25	0.5133 (2)	0.17341 (5)	0.46386 (13)	0.0256 (3)
C26	−0.0305 (4)	0.56800 (8)	0.0851 (2)	0.0668 (7)
H24	−0.122484	0.590094	0.088294	0.100*
H25	0.008716	0.570030	0.018113	0.100*
H26	0.070138	0.573380	0.140994	0.100*
C27	−0.1013 (3)	0.52436 (7)	0.09689 (17)	0.0506 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02089 (7)	0.02070 (7)	0.02179 (7)	0.00083 (5)	0.00222 (5)	0.00059 (4)
Cl1	0.0362 (2)	0.02404 (18)	0.0321 (2)	0.00159 (16)	0.01156 (16)	0.00320 (15)
Cl2	0.0315 (2)	0.02802 (19)	0.02932 (19)	0.00249 (16)	0.00885 (16)	−0.00262 (15)
Cl3	0.0360 (2)	0.0302 (2)	0.0315 (2)	−0.00501 (17)	0.00631 (17)	0.00562 (16)
Cl4	0.0355 (2)	0.02499 (18)	0.02973 (19)	0.00138 (16)	0.00792 (16)	−0.00290 (15)
N1	0.0234 (7)	0.0236 (6)	0.0290 (7)	0.0004 (5)	0.0014 (6)	−0.0024 (5)
N2	0.0242 (7)	0.0238 (6)	0.0351 (8)	0.0011 (5)	0.0008 (6)	0.0022 (5)
N3	0.0287 (7)	0.0374 (8)	0.0320 (7)	0.0041 (6)	0.0072 (6)	−0.0055 (6)
N4	0.0360 (8)	0.0285 (7)	0.0290 (7)	0.0016 (6)	0.0085 (6)	0.0018 (6)
N5	0.0268 (7)	0.0268 (7)	0.0269 (7)	0.0004 (6)	0.0027 (6)	−0.0002 (5)
N6	0.0265 (7)	0.0235 (6)	0.0271 (7)	0.0007 (5)	0.0046 (6)	0.0002 (5)
N7	0.0874 (17)	0.0433 (11)	0.0750 (15)	−0.0007 (11)	0.0065 (13)	0.0190 (10)
C1	0.0233 (7)	0.0206 (7)	0.0247 (7)	0.0006 (6)	0.0037 (6)	−0.0004 (6)
C2	0.0244 (7)	0.0250 (7)	0.0214 (7)	0.0010 (6)	0.0050 (6)	−0.0024 (6)
C3	0.0272 (8)	0.0306 (8)	0.0398 (10)	−0.0034 (7)	0.0020 (7)	−0.0085 (7)
C4	0.0275 (9)	0.0465 (10)	0.0336 (9)	−0.0012 (8)	−0.0014 (7)	−0.0113 (8)
C5	0.0312 (9)	0.0483 (11)	0.0266 (8)	0.0094 (8)	−0.0023 (7)	0.0012 (7)
C6	0.0326 (9)	0.0317 (8)	0.0293 (8)	0.0037 (7)	0.0028 (7)	0.0025 (7)
C7	0.0236 (7)	0.0228 (7)	0.0218 (7)	0.0014 (6)	0.0032 (6)	−0.0022 (6)
C8	0.0319 (9)	0.0245 (8)	0.0399 (10)	0.0014 (7)	−0.0014 (7)	0.0045 (7)

C9	0.0274 (8)	0.0340 (9)	0.0353 (9)	0.0089 (7)	−0.0006 (7)	−0.0005 (7)
C10	0.0215 (8)	0.0448 (10)	0.0329 (9)	0.0012 (7)	0.0048 (7)	−0.0018 (8)
C11	0.0267 (8)	0.0315 (8)	0.0292 (8)	−0.0025 (7)	0.0065 (7)	0.0017 (7)
C12	0.0278 (8)	0.0204 (7)	0.0266 (8)	−0.0025 (6)	0.0077 (6)	−0.0015 (6)
C13	0.0364 (10)	0.0474 (11)	0.0422 (10)	0.0079 (9)	0.0135 (8)	−0.0104 (9)
C14	0.0490 (12)	0.0438 (10)	0.0354 (10)	−0.0013 (9)	0.0182 (9)	−0.0105 (8)
C15	0.0464 (11)	0.0515 (11)	0.0274 (9)	−0.0033 (9)	0.0049 (8)	−0.0094 (8)
C16	0.0316 (9)	0.0429 (10)	0.0297 (9)	0.0018 (8)	0.0041 (7)	−0.0059 (7)
C17	0.0246 (8)	0.0223 (7)	0.0290 (8)	0.0014 (6)	0.0045 (6)	0.0019 (6)
C18	0.0394 (10)	0.0412 (10)	0.0338 (9)	0.0013 (8)	0.0113 (8)	0.0097 (8)
C19	0.0416 (11)	0.0348 (10)	0.0548 (12)	−0.0031 (8)	0.0137 (9)	0.0166 (9)
C20	0.0412 (11)	0.0226 (8)	0.0639 (13)	−0.0023 (8)	0.0136 (10)	0.0022 (8)
C21	0.0357 (9)	0.0247 (8)	0.0421 (10)	−0.0010 (7)	0.0110 (8)	−0.0040 (7)
C22	0.0221 (8)	0.0481 (10)	0.0382 (10)	0.0020 (8)	0.0009 (7)	0.0043 (8)
C23	0.0276 (8)	0.0288 (8)	0.0270 (8)	0.0003 (7)	0.0063 (7)	0.0016 (6)
C24	0.0250 (8)	0.0352 (9)	0.0349 (9)	−0.0015 (7)	0.0001 (7)	0.0003 (7)
C25	0.0267 (8)	0.0223 (7)	0.0282 (8)	0.0007 (6)	0.0063 (7)	−0.0004 (6)
C26	0.091 (2)	0.0409 (12)	0.0603 (15)	−0.0159 (13)	−0.0104 (14)	0.0066 (11)
C27	0.0656 (14)	0.0373 (11)	0.0438 (11)	0.0032 (10)	−0.0040 (10)	0.0086 (9)

Geometric parameters (Å, º)

Ru1—N5	2.0132 (14)	C9—C10	1.375 (3)
Ru1—N6	2.0304 (14)	C9—H7	0.9500
Ru1—Cl1	2.3576 (4)	C10—C11	1.389 (2)
Ru1—Cl2	2.3720 (4)	C10—H8	0.9500
Ru1—Cl3	2.3649 (4)	C11—H9	0.9500
Ru1—Cl4	2.3488 (4)	C12—C16	1.390 (2)
N1—C2	1.343 (2)	C13—C14	1.372 (3)
N1—C3	1.354 (2)	C13—H10	0.9500
N1—H1	0.87 (2)	C14—C15	1.381 (3)
N2—C8	1.338 (2)	C14—H11	0.9500
N2—C7	1.345 (2)	C15—C16	1.391 (2)
N3—C12	1.335 (2)	C15—H12	0.9500
N3—C13	1.343 (2)	C16—H13	0.9500
N4—C17	1.344 (2)	C17—C21	1.383 (2)
N4—C18	1.338 (2)	C18—C19	1.384 (3)
N5—C23	1.137 (2)	C18—H14	0.9500
N6—C25	1.139 (2)	C19—C20	1.373 (3)
N7—C27	1.130 (3)	C19—H15	0.9500
C1—C2	1.540 (2)	C20—C21	1.392 (3)
C1—C7	1.541 (2)	C20—H16	0.9500
C1—C12	1.551 (2)	C21—H17	0.9500
C1—C17	1.543 (2)	C22—C23	1.457 (2)
C2—C6	1.391 (2)	C22—H18	0.9800
C3—C4	1.371 (3)	C22—H19	0.9800
C3—H2	0.9500	C22—H20	0.9800
C4—C5	1.391 (3)	C24—C25	1.459 (2)

C4—H3	0.9500	C24—H21	0.9800
C5—C6	1.380 (3)	C24—H22	0.9800
C5—H4	0.9500	C24—H23	0.9800
C6—H5	0.9500	C26—C27	1.450 (3)
C7—C11	1.388 (2)	C26—H24	0.9800
C8—C9	1.384 (2)	C26—H25	0.9800
C8—H6	0.9500	C26—H26	0.9800

Cl1—Ru1—Cl2	88.500 (15)	C11—C10—H8	119.9
Cl1—Ru1—Cl3	179.093 (16)	C7—C11—C10	118.32 (15)
Cl1—Ru1—Cl4	90.883 (15)	C7—C11—H9	120.8
Cl2—Ru1—Cl3	91.067 (15)	C10—C11—H9	120.8
Cl2—Ru1—Cl4	179.116 (15)	N3—C12—C16	122.46 (15)
Cl3—Ru1—Cl4	89.542 (15)	N3—C12—C1	115.59 (14)
N5—Ru1—Cl1	90.76 (4)	C1—C12—C16	121.91 (14)
N5—Ru1—Cl2	89.25 (4)	N3—C13—C14	123.96 (18)
N5—Ru1—Cl3	88.44 (4)	N3—C13—H10	118.0
N5—Ru1—Cl4	90.13 (4)	C14—C13—H10	118.0
N6—Ru1—Cl1	88.87 (4)	C13—C14—C15	118.33 (17)
N6—Ru1—Cl2	89.48 (4)	C13—C14—H11	120.8
N6—Ru1—Cl3	91.92 (4)	C15—C14—H11	120.8
N6—Ru1—Cl4	91.14 (4)	C14—C15—C16	118.82 (18)
N5—Ru1—N6	178.68 (5)	C14—C15—H12	120.6
C2—N1—C3	123.85 (15)	C16—C15—H12	120.6
C2—N1—H1	114.1 (14)	C12—C16—C15	118.85 (17)
C3—N1—H1	122.0 (14)	C12—C16—H13	120.6
C7—N2—C8	118.95 (14)	C15—C16—H13	120.6
C12—N3—C13	117.57 (16)	N4—C17—C1	114.06 (13)
C17—N4—C18	117.67 (15)	N4—C17—C21	122.40 (15)
C23—N5—Ru1	177.78 (14)	C1—C17—C21	123.55 (15)
C25—N6—Ru1	175.99 (13)	N4—C18—C19	123.67 (18)
C2—C1—C7	113.18 (12)	N4—C18—H14	118.2
C2—C1—C12	108.21 (12)	C19—C18—H14	118.2
C2—C1—C17	106.74 (12)	C18—C19—C20	118.17 (17)
C7—C1—C12	108.28 (12)	C18—C19—H15	120.9
C7—C1—C17	109.44 (12)	C20—C19—H15	120.9
C12—C1—C17	111.01 (12)	C19—C20—C21	119.26 (17)
N1—C2—C1	120.01 (14)	C19—C20—H16	120.4
N1—C2—C6	117.51 (15)	C21—C20—H16	120.4
C1—C2—C6	122.45 (14)	C17—C21—C20	118.82 (17)
N1—C3—C4	119.61 (17)	C17—C21—H17	120.6
N1—C3—H2	120.2	C20—C21—H17	120.6
C4—C3—H2	120.2	C23—C22—H18	109.5
C3—C4—C5	118.54 (17)	C23—C22—H19	109.5
C3—C4—H3	120.7	C23—C22—H20	109.5
C5—C4—H3	120.7	H18—C22—H19	109.5
C4—C5—C6	120.30 (17)	H18—C22—H20	109.5
C4—C5—H4	119.8	H19—C22—H20	109.5

C6—C5—H4	119.8	N5—C23—C22	179.9 (2)
C2—C6—C5	120.15 (16)	C25—C24—H21	109.5
C2—C6—H5	119.9	C25—C24—H22	109.5
C5—C6—H5	119.9	C25—C24—H23	109.5
N2—C7—C1	115.07 (13)	H21—C24—H22	109.5
N2—C7—C11	121.74 (14)	H21—C24—H23	109.5
C1—C7—C11	122.94 (14)	H22—C24—H23	109.5
N2—C8—C9	122.81 (16)	N6—C25—C24	179.5 (2)
N2—C8—H6	118.6	C27—C26—H24	109.5
C9—C8—H6	118.6	C27—C26—H25	109.5
C8—C9—C10	117.96 (16)	C27—C26—H26	109.5
C8—C9—H7	121.0	H24—C26—H25	109.5
C10—C9—H7	121.0	H24—C26—H26	109.5
C9—C10—C11	120.20 (16)	H25—C26—H26	109.5
C9—C10—H8	119.9	N7—C27—C26	178.7 (3)

C3—N1—C2—C6	1.8 (2)	N3—C12—C1—C7	−154.96 (14)
C3—N1—C2—C1	179.64 (15)	C16—C12—C1—C7	27.2 (2)
C13—N3—C12—C16	0.9 (3)	N3—C12—C1—C17	84.89 (17)
C13—N3—C12—C1	−176.98 (15)	C16—C12—C1—C17	−93.00 (18)
C18—N4—C17—C21	0.6 (2)	C2—N1—C3—C4	−0.6 (3)
C18—N4—C17—C1	−179.28 (15)	N1—C3—C4—C5	−0.6 (3)
C8—N2—C7—C11	−1.1 (2)	N3—C12—C16—C15	−1.1 (3)
C8—N2—C7—C1	−175.54 (15)	C1—C12—C16—C15	176.61 (16)
N1—C2—C1—C7	26.4 (2)	N2—C7—C11—C10	−0.2 (2)
C6—C2—C1—C7	−155.90 (14)	C1—C7—C11—C10	173.82 (14)
N1—C2—C1—C17	146.83 (14)	C7—N2—C8—C9	1.4 (3)
C6—C2—C1—C17	−35.45 (19)	C10—C9—C8—N2	−0.3 (3)
N1—C2—C1—C12	−93.63 (16)	N1—C2—C6—C5	−1.8 (2)
C6—C2—C1—C12	84.10 (18)	C1—C2—C6—C5	−179.56 (15)
N2—C7—C1—C2	−47.00 (18)	C8—C9—C10—C11	−1.0 (3)
C11—C7—C1—C2	138.63 (15)	C7—C11—C10—C9	1.2 (3)
N2—C7—C1—C17	−165.91 (13)	N4—C17—C21—C20	0.6 (3)
C11—C7—C1—C17	19.7 (2)	C1—C17—C21—C20	−179.60 (16)
N2—C7—C1—C12	72.96 (16)	C17—N4—C18—C19	−1.1 (3)
C11—C7—C1—C12	−101.41 (17)	C12—N3—C13—C14	0.3 (3)
N4—C17—C1—C2	−57.10 (17)	C15—C14—C13—N3	−1.2 (3)
C21—C17—C1—C2	123.06 (17)	C2—C6—C5—C4	0.7 (3)
N4—C17—C1—C7	65.73 (17)	C3—C4—C5—C6	0.5 (3)
C21—C17—C1—C7	−114.12 (17)	C17—C21—C20—C19	−1.2 (3)
N4—C17—C1—C12	−174.81 (14)	C13—C14—C15—C16	1.0 (3)
C21—C17—C1—C12	5.3 (2)	C12—C16—C15—C14	0.2 (3)
N3—C12—C1—C2	−31.93 (18)	C21—C20—C19—C18	0.6 (3)
C16—C12—C1—C2	150.18 (15)	N4—C18—C19—C20	0.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2	0.87 (2)	1.87 (2)	2.615 (2)	143.3 (19)
C22—H18···Cl1^{i}	0.98	2.69	3.5521 (19)	146
C22—H19···Cl4^{i}	0.98	2.78	3.5972 (19)	142
C24—H21···Cl1^{ii}	0.98	2.77	3.7393 (18)	172
C24—H22···Cl2^{iii}	0.98	2.77	3.6346 (18)	147
C24—H23···N4^{ii}	0.98	2.65	3.606 (2)	165
C6—H5···N7	0.95	2.45	3.248 (3)	142
C26—H26···Cl4^{iv}	0.98	2.84	3.749 (3)	154

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