

Tetra- μ -acetato- κ^8 O:O'-bis[(3-cyanopyridine- κ N¹)]ruthenium(II,III)](*Ru*—*Ru*) hexafluoridophosphate 1,2-dichloroethane monosolvate

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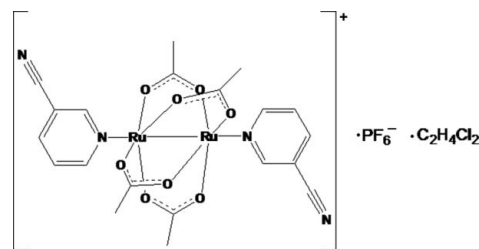
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Key indicators: single-crystal X-ray study; $T = 180$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; disorder in solvent or counterion; R factor = 0.028; wR factor = 0.078; data-to-parameter ratio = 14.0.

The title compound, $[\text{Ru}_2(\text{CH}_3\text{CO}_2)_4(\text{C}_6\text{H}_4\text{N}_2)_2]\text{PF}_6 \cdot \text{C}_2\text{H}_4\text{Cl}_2$, was obtained *via* a rapid substitution reaction in 2-propanol whereby 3-cyanopyridine replaces the axial water molecules in the diaquatetra- μ -acetato-diruthenium(II,III) hexafluoridophosphate starting material. The product rapidly precipitated and crystals were grown from 1,2-dichloroethane. The 1,2-dichloroethane molecule of solvation exhibits disorder with two different orientations [occupancy ratio 0.51 (6):0.49 (6)]. All three parts, the cation, the anion and the disordered solvent molecule lie on crystallographic inversion centers. The Ru—Ru bond length of 2.2702 (6) Å fits nicely into the range seen for similar complexes and correlates well with the reduction potential of the complex and donor strength of the axial ligand, 3-cyanopyridine, as postulated in a previous study [Vamvounis *et al.* (2000). *Inorg. Chim. Acta*, **305**, 87–98]. The 3-cyanopyridine ligands orient themselves in an *anti* configuration with respect to each other and the Ru—Ru—N angle [174.27 (7)°] is close to being linear.

Related literature

For related structures and physical measurements, see: Vamvounis *et al.* (2000).



Experimental

Crystal data

$[\text{Ru}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_6\text{H}_4\text{N}_2)_2]\text{PF}_6 \cdot \text{C}_2\text{H}_4\text{Cl}_2$
 $M_r = 890.46$
 Triclinic, $P\bar{1}$
 $a = 8.1743$ (6) Å
 $b = 10.3955$ (10) Å
 $c = 11.397$ (1) Å
 $\alpha = 105.860$ (6)°

$\beta = 108.929$ (5)°
 $\gamma = 104.099$ (5)°
 $V = 820.38$ (14) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 1.21$ mm⁻¹
 $T = 180$ K
 0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2010)
 $T_{\min} = 0.793$, $T_{\max} = 0.839$

6133 measured reflections
 3175 independent reflections
 2784 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.078$
 $S = 1.09$
 3175 reflections

226 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.85$ e Å⁻³
 $\Delta\rho_{\min} = -0.76$ e Å⁻³

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: NK2113).

References

- Bruker (2010). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Vamvounis, G., Caplan, J. F., Cameron, T. S., Robertson, K. N. & Aquino, M. A. S. (2000). *Inorg. Chim. Acta*, **305**, 87–98.

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Tetra- μ -acetato- $\kappa^8 O:O'$ -bis[(3-cyanopyridine- κN^1)]ruthenium(II,III)(*Ru-Ru*) hexafluoridophosphate 1,2-dichloroethane monosolvate

S. A. Minaker, R. Wang and M. A. S. Aquino

Comment

A number of years ago our lab synthesized and structurally characterized a series of diruthenium(II,III) tetraacetate complexes with different axial donor ligands of varying donor strengths (Vamvounis *et al.*, 2000). One reason to study these was to synthesize dimers with asymmetric bidentate axial donors that could act as bridges for mixed-metal metallopolymers and extended arrays (*i.e.* in the case of cyanopyridine adducts the pyridine end could be coordinated to a harder metal than the cyano end). The other reason was to correlate axial donor strength (as well as redox potential) with the Ru—Ru bond length. These ligands ranged from weak donors such as water and methanol to relatively strong donors such as dimethylformamide, dimethylsulfoxide and various pyridine derivatives. Unfortunately while we were able to structurally characterize the 4-cyanopyridine adduct in the earlier paper we were unable to obtain the 3-cyanopyridine adduct. This structure is now finally reported here.

The title compound (I) (Fig. 1) can be compared to the 4-cyanopyridine adduct reported previously (Vamvounis *et al.*, 2000). The Ru—Ru bond lengths are 2.2702 (6) Å and 2.2741 (7) Å respectively which fits well into correlation of Ru—Ru bond length with axial ligand donor strength as outlined in the earlier paper. (*i.e.* the 3-cyanopyridine being the slightly weaker donor as measured electrochemically manifests a shorter Ru—Ru bond length structurally in the complex because less electron density is being donated into the metal-metal antibonding HOMO). The 3-cyanopyridine ligands are situated *anti* with respect to each other and the pyridine planes essentially bifurcate the planes formed by the perpendicular carboxylate groups (O—C—O), *e.g.* the O1—Ru1—N1—C5 torsion angle is -48.5 °.

Experimental

The method of preparation of the title compound (I) was similar to the method used by (Vamvounis *et al.*, 2000) in preparing the earlier pyridine adducts of diruthenium(II,III) tetraacetate except that a 2.1:1 ligand to metal ratio was used instead of a 4:1 ratio. For example, [Ru₂(μ -O₂CCH₃)₄(H₂O)₂](PF₆) (0.100 g, 0.161 mmol) was dissolved in 10 ml of 2-propanol. A 2.1-fold excess of 3-cyanopyridine (0.037 g, 0.338 mmol) was added with stirring and a green precipitate formed immediately. The solution was stirred for another 5 minutes and the olive-green product collected *via* suction filtration, washed with 50 ml of 2-propanol and dried *in vacuo*. (Yield = 0.101 g, 79%). Crystals were grown by slow evaporation from 1,2-dichloroethane.

Refinement

The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically. All H atoms were placed in geometrically calculated positions, with C—H = 0.95 (aromatic), 0.99(CH₂) and 0.98 (methyl) Å, and refined as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ (methyl), and 1.2 $U_{\text{eq}}(\text{other C})$. In addition, the methyl groups were refined with AFIX 137, which allowed the rotation of the methyl groups whilst keeping the C—H distances and X—C—H angles fixed. The

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solvent molecule C₂H₄Cl₂ in the structure is disordered. It was split and refined into two parts with different orientations and with nearly equal occupancies.

Figures

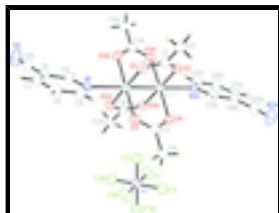


Fig. 1. The molecular structure of (I), with atom labels and 50% probability ellipsoids for the non-H atoms. Solvent molecule omitted for clarity. Symmetry operator A = $-x + 1, -y + 1, -z + 1$; B = $-x, -y + 1, -z$.

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Crystal data

[Ru₂(C₂H₃O₂)₄(C₆H₄N₂)₂]PF₆·C₂H₄Cl₂

$M_r = 890.46$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.1743\ (6)\ \text{\AA}$

$b = 10.3955\ (10)\ \text{\AA}$

$c = 11.397\ (1)\ \text{\AA}$

$\alpha = 105.860\ (6)^\circ$

$\beta = 108.929\ (5)^\circ$

$\gamma = 104.099\ (5)^\circ$

$V = 820.38\ (14)\ \text{\AA}^3$

$Z = 1$

$F(000) = 439$

$D_x = 1.802\ \text{Mg m}^{-3}$

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

Cell parameters from 4068 reflections

$\theta = 2.4\text{--}27.1^\circ$

$\mu = 1.21\ \text{mm}^{-1}$

$T = 180\ \text{K}$

Block, brown

$0.20 \times 0.20 \times 0.15\ \text{mm}$

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2010)

$T_{\min} = 0.793$, $T_{\max} = 0.839$

6133 measured reflections

3175 independent reflections

2784 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.028$$

$$wR(F^2) = 0.078$$

$$S = 1.09$$

3175 reflections

226 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 1.188P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.76 \text{ e } \text{\AA}^{-3}$$

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
P1	0.0000	0.5000	0.0000	0.0346 (3)	
Ru1	0.47865 (3)	0.38173 (3)	0.45928 (2)	0.02328 (10)	
O1	0.7543 (3)	0.4309 (2)	0.5531 (2)	0.0269 (5)	
O2	0.7964 (3)	0.6638 (2)	0.6343 (2)	0.0270 (5)	
O3	0.5095 (3)	0.3989 (2)	0.2954 (2)	0.0271 (5)	
O4	0.5481 (3)	0.6314 (2)	0.3736 (2)	0.0270 (5)	
N1	0.4058 (4)	0.1379 (3)	0.3754 (3)	0.0256 (6)	
N2	-0.0128 (5)	-0.2151 (4)	0.4373 (4)	0.0600 (10)	
C1	0.8583 (4)	0.5624 (4)	0.6211 (3)	0.0274 (7)	
C2	1.0631 (4)	0.6004 (4)	0.6875 (4)	0.0359 (8)	
H2A	1.1126	0.6717	0.7792	0.054*	
H2B	1.1218	0.6405	0.6364	0.054*	
H2C	1.0893	0.5140	0.6906	0.054*	
C3	0.5368 (4)	0.5203 (4)	0.2848 (3)	0.0272 (7)	
C4	0.5549 (5)	0.5324 (4)	0.1623 (4)	0.0373 (8)	
H4A	0.6669	0.6146	0.1884	0.056*	
H4B	0.4457	0.5463	0.1073	0.056*	
H4C	0.5640	0.4443	0.1104	0.056*	
C5	0.2756 (5)	0.0610 (4)	0.4029 (4)	0.0345 (8)	
H5A	0.2130	0.1083	0.4463	0.041*	
C6	0.2307 (4)	-0.0857 (4)	0.3693 (4)	0.0324 (7)	
C7	0.3223 (5)	-0.1549 (4)	0.3063 (4)	0.0347 (8)	
H7A	0.2967	-0.2547	0.2849	0.042*	
C8	0.4511 (5)	-0.0752 (4)	0.2759 (4)	0.0391 (8)	

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H8A	0.5140	-0.1197	0.2307	0.047*	
C9	0.4882 (5)	0.0701 (4)	0.3115 (4)	0.0341 (8)	
H9A	0.5768	0.1239	0.2891	0.041*	
C10	0.0933 (5)	-0.1605 (4)	0.4058 (4)	0.0411 (9)	
F1	-0.0541 (3)	0.6132 (3)	0.0917 (2)	0.0518 (6)	
F2	0.1696 (3)	0.6283 (3)	0.0146 (2)	0.0474 (6)	
F3	0.1334 (3)	0.4879 (3)	0.1314 (2)	0.0485 (6)	
C11A	0.242 (4)	0.032 (3)	0.9565 (15)	0.163 (4)	0.51 (6)
C11A	0.056 (5)	0.077 (4)	1.010 (4)	0.108 (10)	0.51 (6)
H11A	0.1094	0.1457	1.1040	0.129*	0.51 (6)
H11B	-0.0193	0.1142	0.9496	0.129*	0.51 (6)
C11B	0.191 (4)	0.0453 (18)	0.914 (4)	0.152 (7)	0.49 (6)
C11B	0.013 (10)	-0.052 (7)	0.969 (5)	0.21 (3)	0.49 (6)
H11C	-0.1020	-0.1225	0.8912	0.246*	0.49 (6)
H11D	0.0663	-0.0995	1.0277	0.246*	0.49 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0257 (6)	0.0448 (8)	0.0286 (7)	0.0091 (6)	0.0114 (5)	0.0107 (6)
Ru1	0.02188 (14)	0.02672 (16)	0.02337 (15)	0.00927 (11)	0.01160 (11)	0.00975 (11)
O1	0.0250 (11)	0.0321 (13)	0.0288 (12)	0.0144 (10)	0.0142 (10)	0.0121 (10)
O2	0.0245 (11)	0.0280 (12)	0.0279 (12)	0.0087 (9)	0.0122 (9)	0.0093 (10)
O3	0.0275 (11)	0.0353 (13)	0.0221 (11)	0.0143 (10)	0.0128 (9)	0.0108 (10)
O4	0.0256 (11)	0.0331 (13)	0.0282 (12)	0.0126 (10)	0.0137 (10)	0.0157 (10)
N1	0.0284 (14)	0.0222 (13)	0.0245 (14)	0.0091 (11)	0.0094 (11)	0.0086 (11)
N2	0.056 (2)	0.047 (2)	0.086 (3)	0.0132 (18)	0.044 (2)	0.027 (2)
C1	0.0251 (16)	0.0387 (19)	0.0245 (16)	0.0123 (15)	0.0148 (13)	0.0150 (15)
C2	0.0217 (16)	0.044 (2)	0.039 (2)	0.0108 (15)	0.0114 (15)	0.0139 (17)
C3	0.0192 (15)	0.0380 (19)	0.0258 (16)	0.0125 (14)	0.0101 (13)	0.0117 (15)
C4	0.0389 (19)	0.055 (2)	0.0297 (19)	0.0225 (18)	0.0203 (16)	0.0222 (18)
C5	0.0313 (18)	0.0354 (19)	0.037 (2)	0.0124 (15)	0.0161 (16)	0.0123 (16)
C6	0.0256 (16)	0.0301 (18)	0.0351 (19)	0.0069 (14)	0.0086 (15)	0.0111 (15)
C7	0.0350 (19)	0.0246 (17)	0.0357 (19)	0.0116 (15)	0.0093 (15)	0.0049 (15)
C8	0.041 (2)	0.036 (2)	0.042 (2)	0.0174 (17)	0.0242 (18)	0.0055 (17)
C9	0.0359 (19)	0.0325 (19)	0.0364 (19)	0.0144 (15)	0.0200 (16)	0.0094 (16)
C10	0.035 (2)	0.033 (2)	0.052 (2)	0.0089 (16)	0.0180 (18)	0.0144 (18)
F1	0.0460 (13)	0.0548 (15)	0.0486 (14)	0.0190 (11)	0.0235 (11)	0.0064 (12)
F2	0.0361 (12)	0.0529 (14)	0.0419 (13)	0.0030 (10)	0.0152 (10)	0.0151 (11)
F3	0.0350 (12)	0.0666 (16)	0.0383 (13)	0.0138 (11)	0.0092 (10)	0.0239 (12)
C11A	0.185 (10)	0.204 (9)	0.091 (6)	0.089 (8)	0.039 (6)	0.050 (5)
C11A	0.15 (2)	0.068 (16)	0.075 (12)	0.049 (13)	0.014 (13)	0.018 (11)
C11B	0.132 (9)	0.179 (7)	0.158 (15)	0.066 (6)	0.068 (9)	0.067 (8)
C11B	0.20 (5)	0.18 (5)	0.11 (3)	0.06 (4)	0.00 (3)	-0.03 (2)

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

P1—F1 ⁱ	1.598 (2)	C2—H2B	0.9800
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P1—F1	1.598 (2)	C2—H2C	0.9800
P1—F2	1.599 (2)	C3—C4	1.485 (4)
P1—F2 ⁱ	1.599 (2)	C4—H4A	0.9800
P1—F3	1.600 (2)	C4—H4B	0.9800
P1—F3 ⁱ	1.600 (2)	C4—H4C	0.9800
Ru1—O3	2.012 (2)	C5—C6	1.387 (5)
Ru1—O1	2.015 (2)	C5—H5A	0.9500
Ru1—O2 ⁱⁱ	2.016 (2)	C6—C7	1.387 (5)
Ru1—O4 ⁱⁱ	2.023 (2)	C6—C10	1.447 (5)
Ru1—Ru1 ⁱⁱ	2.2702 (6)	C7—C8	1.373 (5)
Ru1—N1	2.295 (3)	C7—H7A	0.9500
O1—C1	1.273 (4)	C8—C9	1.378 (5)
O2—C1	1.270 (4)	C8—H8A	0.9500
O2—Ru1 ⁱⁱ	2.016 (2)	C9—H9A	0.9500
O3—C3	1.273 (4)	C11A—C11A	1.93 (4)
O4—C3	1.272 (4)	C11A—C11A ⁱⁱⁱ	1.56 (7)
O4—Ru1 ⁱⁱ	2.023 (2)	C11A—H11A	0.9900
N1—C9	1.323 (4)	C11A—H11B	0.9900
N1—C5	1.345 (4)	C11B—C11B	1.93 (8)
N2—C10	1.130 (5)	C11B—C11B ⁱⁱⁱ	1.22 (11)
C1—C2	1.491 (4)	C11B—H11C	0.9900
C2—H2A	0.9800	C11B—H11D	0.9900
F1 ⁱ —P1—F1	180.00 (16)	H2A—C2—H2B	109.5
F1 ⁱ —P1—F2	89.90 (12)	C1—C2—H2C	109.5
F1—P1—F2	90.10 (12)	H2A—C2—H2C	109.5
F1 ⁱ —P1—F2 ⁱ	90.11 (12)	H2B—C2—H2C	109.5
F1—P1—F2 ⁱ	89.89 (12)	O4—C3—O3	123.1 (3)
F2—P1—F2 ⁱ	180.0	O4—C3—C4	118.5 (3)
F1 ⁱ —P1—F3	90.18 (13)	O3—C3—C4	118.5 (3)
F1—P1—F3	89.82 (13)	C3—C4—H4A	109.5
F2—P1—F3	89.81 (12)	C3—C4—H4B	109.5
F2 ⁱ —P1—F3	90.19 (12)	H4A—C4—H4B	109.5
F1 ⁱ —P1—F3 ⁱ	89.82 (13)	C3—C4—H4C	109.5
F1—P1—F3 ⁱ	90.18 (13)	H4A—C4—H4C	109.5
F2—P1—F3 ⁱ	90.19 (12)	H4B—C4—H4C	109.5
F2 ⁱ —P1—F3 ⁱ	89.81 (12)	N1—C5—C6	121.5 (3)
F3—P1—F3 ⁱ	180.0	N1—C5—H5A	119.3
O3—Ru1—O1	89.72 (9)	C6—C5—H5A	119.3
O3—Ru1—O2 ⁱⁱ	89.97 (9)	C7—C6—C5	119.4 (3)
O1—Ru1—O2 ⁱⁱ	178.99 (9)	C7—C6—C10	122.2 (3)
O3—Ru1—O4 ⁱⁱ	178.79 (9)	C5—C6—C10	118.4 (3)
O1—Ru1—O4 ⁱⁱ	89.53 (9)	C8—C7—C6	118.1 (3)
O2 ⁱⁱ —Ru1—O4 ⁱⁱ	90.77 (8)	C8—C7—H7A	120.9

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O3—Ru1—Ru1 ⁱⁱ	90.35 (7)	C6—C7—H7A	120.9
O1—Ru1—Ru1 ⁱⁱ	90.07 (7)	C7—C8—C9	119.4 (3)
O2 ⁱⁱ —Ru1—Ru1 ⁱⁱ	88.97 (6)	C7—C8—H8A	120.3
O4 ⁱⁱ —Ru1—Ru1 ⁱⁱ	88.71 (7)	C9—C8—H8A	120.3
O3—Ru1—N1	92.05 (9)	N1—C9—C8	122.8 (3)
O1—Ru1—N1	95.14 (9)	N1—C9—H9A	118.6
O2 ⁱⁱ —Ru1—N1	85.83 (9)	C8—C9—H9A	118.6
O4 ⁱⁱ —Ru1—N1	88.95 (9)	N2—C10—C6	177.9 (4)
Ru1 ⁱⁱ —Ru1—N1	174.27 (7)	C11A ⁱⁱⁱ —C11A—C11A	97 (3)
C1—O1—Ru1	118.3 (2)	C11A ⁱⁱⁱ —C11A—H11A	112.3
C1—O2—Ru1 ⁱⁱ	119.4 (2)	C11A—C11A—H11A	112.3
C3—O3—Ru1	118.4 (2)	C11A ⁱⁱⁱ —C11A—H11B	112.3
C3—O4—Ru1 ⁱⁱ	119.5 (2)	C11A—C11A—H11B	112.3
C9—N1—C5	118.7 (3)	H11A—C11A—H11B	109.9
C9—N1—Ru1	125.8 (2)	C11B ⁱⁱⁱ —C11B—C11B	99 (9)
C5—N1—Ru1	115.4 (2)	C11B ⁱⁱⁱ —C11B—H11C	111.9
O2—C1—O1	123.2 (3)	C11B—C11B—H11C	111.9
O2—C1—C2	118.0 (3)	C11B ⁱⁱⁱ —C11B—H11D	111.9
O1—C1—C2	118.8 (3)	C11B—C11B—H11D	111.9
C1—C2—H2A	109.5	H11C—C11B—H11D	109.6
C1—C2—H2B	109.5		
O3—Ru1—O1—C1	90.1 (2)	Ru1 ⁱⁱ —O2—C1—C2	177.8 (2)
O4 ⁱⁱ —Ru1—O1—C1	-88.9 (2)	Ru1—O1—C1—O2	1.0 (4)
Ru1 ⁱⁱ —Ru1—O1—C1	-0.2 (2)	Ru1—O1—C1—C2	-178.2 (2)
N1—Ru1—O1—C1	-177.8 (2)	Ru1 ⁱⁱ —O4—C3—O3	-0.1 (4)
O1—Ru1—O3—C3	-91.2 (2)	Ru1 ⁱⁱ —O4—C3—C4	179.3 (2)
O2 ⁱⁱ —Ru1—O3—C3	87.8 (2)	Ru1—O3—C3—O4	1.0 (4)
Ru1 ⁱⁱ —Ru1—O3—C3	-1.2 (2)	Ru1—O3—C3—C4	-178.5 (2)
N1—Ru1—O3—C3	173.6 (2)	C9—N1—C5—C6	1.9 (5)
O3—Ru1—N1—C9	41.4 (3)	Ru1—N1—C5—C6	-173.9 (3)
O1—Ru1—N1—C9	-48.5 (3)	N1—C5—C6—C7	0.2 (5)
O2 ⁱⁱ —Ru1—N1—C9	131.3 (3)	N1—C5—C6—C10	178.1 (3)
O4 ⁱⁱ —Ru1—N1—C9	-137.9 (3)	C5—C6—C7—C8	-2.0 (5)
O3—Ru1—N1—C5	-143.1 (2)	C10—C6—C7—C8	-179.8 (4)
O1—Ru1—N1—C5	127.0 (2)	C6—C7—C8—C9	1.6 (5)
O2 ⁱⁱ —Ru1—N1—C5	-53.3 (2)	C5—N1—C9—C8	-2.3 (5)
O4 ⁱⁱ —Ru1—N1—C5	37.6 (2)	Ru1—N1—C9—C8	173.0 (3)
Ru1 ⁱⁱ —O2—C1—O1	-1.4 (4)	C7—C8—C9—N1	0.5 (6)

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

Fig. 1

