

cis,trans-Dicarbonyldichlorido(1,10-phenanthroline-5,6-dione- κ^2N,N')ruthenium(II)

Tsugiko Takase,^a Kasumi Takahashi^{b,c} and Dai Oyama^{b*}^aInstitute of Environmental Radioactivity, Fukushima University, 1 Kanayagawa, Fukushima 960-1296, Japan,^bDepartment of Industrial Systems Engineering, Cluster of Science and Engineering, Fukushima University, 1 Kanayagawa,Fukushima 960-1296, Japan, and ^cDepartment of Chemistry, Graduate School of Science, Tohoku University, 6-3

Aramaki, Aoba-ku, Sendai 980-8578, Japan. *Correspondence e-mail: daio@sss.fukushima-u.ac.jp

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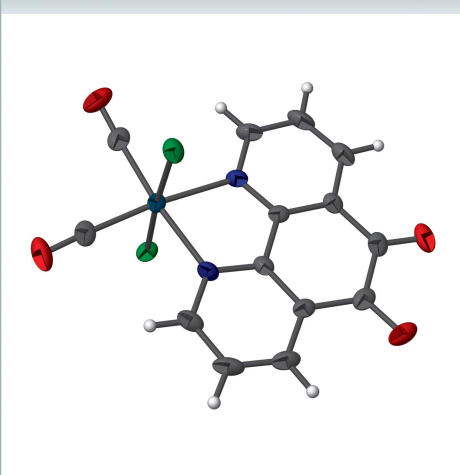
Keywords: crystal structure; ruthenium(II) complex; o-quinonoid framework; phenanthroline derivative.

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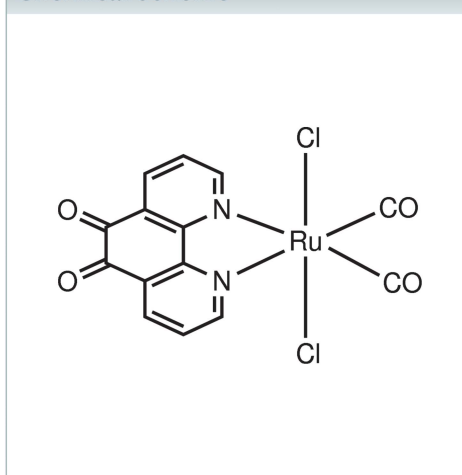
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[\text{RuCl}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_2)(\text{CO})_2]$, the Ru^{II} atom (site symmetry ..2) adopts a distorted octahedral coordination sphere defined by two carbonyl C atoms, two Cl^- anions and two N atoms from the chelating 1,10-phenanthroline-5,6-dione (phendione) ligand. The carbonyl ligands are *cis* to each other, while the Cl atoms are *trans*. In the phendione ligand, the $\text{C}=\text{O}$ [1.239 (5) Å] and the $\text{C}-\text{C}$ [1.537 (5) Å] bond lengths in the diketone moiety have typical values. In the crystal, $\text{C}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds lead to the formation of a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

Dicarbonylruthenium(II) complexes bearing bidentate polypyridyl co-ligands such as 2,2'-bipyridine and 1,10-phenanthroline can catalyse a variety of useful chemical reactions such as multi-electron reductions of CO_2 (Machan *et al.*, 2015). In addition, metal complexes with 1,10-phenanthroline-5,6-dione (phendione) are also of interest due to its dual chelating ability as either a diimine (N,N' -bidentate) or a dioxolene (O,O' -bidentate) (Calderazzo *et al.*, 1999; Fujihara *et al.*, 2003). We report here the synthesis and structural characterization of $[\text{Ru}(\text{CO})_2\text{Cl}_2(\text{phendione})]$.

The neutral complex crystallizes without disorder or solvent. The molecule has crystallographically imposed twofold symmetry with the Ru^{II} atom located on the twofold rotation axis. As shown in Fig. 1, the Ru^{II} atom has a distorted octahedral coordination environment, with two N atoms of the bidentate phendione ligand, two carbonyl carbon atoms and two chloride ions completing the first coordination sphere. Thus, the crystal structure indicates that the phendione ligand selectively coordinates to the Ru^{II} atom in the N,N' -bidentate mode. The title compound displays a *cis* orientation of the carbonyl

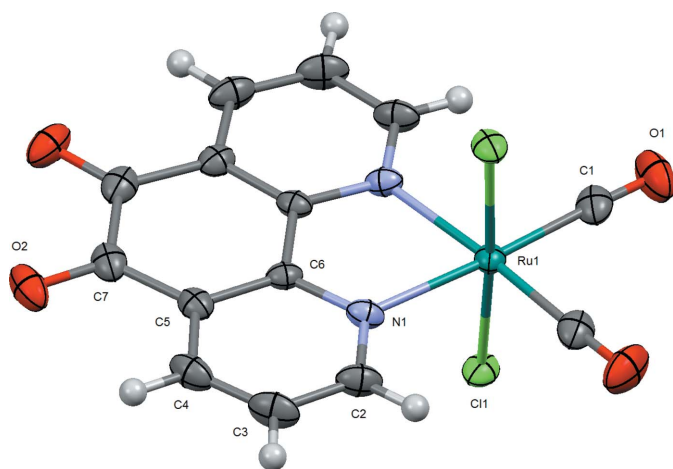


Figure 1
The molecular structure of the title compound, with atom labels and displacement ellipsoids for non-H atoms drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation ($y, x, -z + 1$).

ligands and a *trans* orientation of the chlorido ligands. The Ru–C–O bond angle of the complex [$176.1(3)^\circ$] is nearly linear, and the C≡O [1.128(4) Å], Ru–C [1.893(4) Å], Ru–Cl [2.3880(7) Å] and Ru–N [2.116(3) Å] distances are comparable to those in similar complexes (Ding *et al.*, 2016; Oyama *et al.*, 2009).

It is important to utilize the results of the structure determination in order to distinguish the carbon–oxygen bond as double or as single in quinone-based ligands. The C=O bond length of metal-free phendione is 1.210 Å (averaged) (Calderazzo *et al.*, 1999), while C=O bond lengths of metal complexes containing phendione as a ligand are in the range

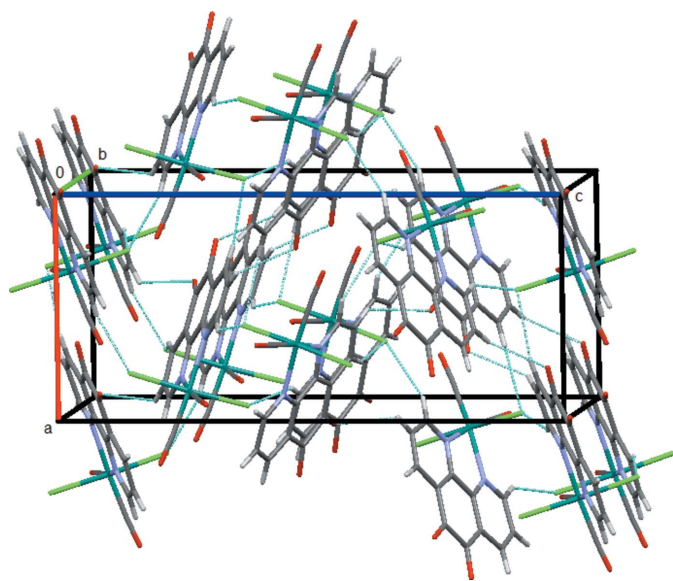


Figure 2
A view approximately along the *b* axis of the title compound, with hydrogen bonds shown as dashed lines (for numerical values see Table 1).

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H1···Cl1 ⁱ	0.95	2.66	3.478(4)	145
C3–H2···O2 ⁱⁱ	0.95	2.53	3.206(4)	128
C4–H3···Cl1 ⁱⁱⁱ	0.95	2.78	3.660(4)	155

Symmetry codes: (i) $y - \frac{1}{2}, -x + \frac{3}{2}, z + \frac{1}{4}$; (ii) $-x - \frac{1}{2}, y + \frac{5}{2}, -z + \frac{7}{4}$; (iii) $y, x + 1, -z + 1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	[RuCl ₂ (C ₁₂ H ₆ N ₂ O ₂)(CO) ₂]
<i>M_r</i>	438.19
Crystal system, space group	Tetragonal, <i>P</i> 4 ₃ 2 ₁ 2
Temperature (K)	93
<i>a</i> , <i>c</i> (Å)	8.8003(6), 19.772(2)
<i>V</i> (Å ³)	1531.3(3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.39
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Rigaku Saturn724
Absorption correction	Multi-scan (<i>REQAB</i> ; Rigaku, 1998)
<i>T_{min}</i> , <i>T_{max}</i>	0.812, 0.870
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	15312, 1728, 1653
<i>R_{int}</i>	0.039
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.646
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.025, 0.061, 1.08
No. of reflections	1728
No. of parameters	105
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.89, -0.26
Absolute structure	Flack (1983), 657 Friedel pairs
Absolute structure parameter	-0.02(5)

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR97* (Altomare *et al.*, 1999), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *CrystalStructure* (Rigaku, 2010), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

1.154–1.264 Å (Fujihara *et al.*, 2003, 2004; Larsson & Öhrström, 2004; Yokoyama *et al.*, 2006) and the C–O bond lengths of the corresponding diol ligand are 1.364–1.367 Å (Guan *et al.*, 2008; Larsson & Öhrström, 2004). The C=O bond length of the phendione ligand in the complex [1.239(5) Å] is nearly the same as that of metal-free phendione (Calderazzo *et al.*, 1999) or those of other Ru^{II}–phendione complexes (Fujihara *et al.*, 2003, 2004; Yokoyama *et al.*, 2006), indicating that the phendione ligand in the complex retains its double-bond character. Additionally, the C7–C7ⁱ [symmetry code: (i) $y, x, -z + 1$] distance in the diketone moiety of phendione represents a typical single bond [1.537(5) Å], compared with 1.534 Å in the metal-free compound (Calderazzo *et al.*, 1999).

In the crystal, (aryl)C–H···Cl and (aryl)C–H···O hydrogen-bonds (Table 1) lead to the formation of a three-dimensional supramolecular network (Fig. 2).

Synthesis and crystallization

The ligand 1,10-phenanthroline-5,6-dione (phendione) was prepared as described by Yamada *et al.* (1992). It proved to be analytically and spectroscopically pure (IR and ^1H NMR data). A methanol solution (5 ml) containing $[\text{Ru}(\text{CO})_2\text{Cl}_2]_n$ (50 mg) and phendione (70 mg) was refluxed for 1 h. The reaction mixture was allowed to stand at 277 K overnight. The light-brown-colored precipitate was collected by filtration and washed with diethyl ether, and then dried under vacuum (yield 56 mg, 38%). Crystals suitable for the X-ray diffraction experiment were grown by diffusion of diethyl ether into a DMF solution of the complex over a few days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). 2, x170288 [https://doi.org/10.1107/S2414314617002887]

***cis,trans*-Dicarbonyldichlorido(1,10-phenanthroline-5,6-dione- κ^2N,N')ruthenium(II)**

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cis,trans-Dicarbonyldichlorido(1,10-phenanthroline-5,6-dione- κ^2N,N')ruthenium(II)

Crystal data

[RuCl₂(C₁₂H₆N₂O₂)(CO)₂]

$M_r = 438.19$

Tetragonal, $P4_32_12$

Hall symbol: P 4nw 2abw

$a = 8.8003$ (6) Å

$c = 19.772$ (2) Å

$V = 1531.3$ (3) Å³

$Z = 4$

$F(000) = 856.00$

$D_x = 1.901$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 4550 reflections

$\theta = 3.1$ – 27.5°

$\mu = 1.39$ mm⁻¹

$T = 93$ K

Prism, brown

0.15 × 0.15 × 0.10 mm

Data collection

Rigaku Saturn724

diffractometer

Detector resolution: 7.111 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*REQAB*; Rigaku, 1998)

$T_{\min} = 0.812$, $T_{\max} = 0.870$

15312 measured reflections

1728 independent reflections

1653 reflections with $F^2 > 2.0\sigma(F^2)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.3^\circ$

$h = -10 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.061$

$S = 1.08$

1728 reflections

105 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.6276P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.89$ e Å⁻³

$\Delta\rho_{\min} = -0.26$ e Å⁻³

Absolute structure: Flack (1983), 657 Friedel

pairs

Absolute structure parameter: -0.02 (5)

Special details

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 $F^2 > 2.0 \text{ sigma}(F^2)$ is used only for calculating R -factor (gt).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ru1	0.62055 (3)	0.62055 (3)	0.5000	0.02048 (10)
Cl1	0.54739 (9)	0.70536 (9)	0.38999 (3)	0.02686 (17)
O1	0.5929 (4)	0.3029 (3)	0.44361 (13)	0.0466 (7)
O2	1.0393 (4)	1.2397 (3)	0.52859 (11)	0.0386 (7)
N1	0.6585 (3)	0.8483 (3)	0.52981 (13)	0.0229 (6)
C1	0.6036 (4)	0.4194 (4)	0.46692 (15)	0.0311 (7)
C2	0.5590 (4)	0.9404 (4)	0.56163 (16)	0.0306 (8)
C3	0.5959 (5)	1.0865 (4)	0.58117 (16)	0.0360 (9)
C4	0.7374 (5)	1.1435 (4)	0.56831 (16)	0.0326 (8)
C5	0.8430 (4)	1.0512 (4)	0.53461 (14)	0.0239 (7)
C6	0.7996 (4)	0.9032 (4)	0.51691 (13)	0.0210 (6)
C7	0.9973 (4)	1.1078 (5)	0.51736 (14)	0.0293 (7)
H1	0.4598	0.9034	0.5709	0.0368*
H2	0.5226	1.1476	0.6037	0.0432*
H3	0.7638	1.2436	0.5819	0.0391*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02169 (12)	0.02169 (12)	0.01805 (14)	-0.00119 (14)	-0.00289 (9)	0.00289 (9)
Cl1	0.0252 (4)	0.0342 (5)	0.0211 (4)	-0.0016 (3)	-0.0024 (3)	0.0085 (3)
O1	0.072 (3)	0.0292 (14)	0.0389 (14)	-0.0112 (14)	-0.0159 (14)	-0.0037 (12)
O2	0.0642 (18)	0.0247 (13)	0.0270 (12)	-0.0067 (12)	-0.0128 (12)	0.0002 (10)
N1	0.0259 (14)	0.0229 (14)	0.0198 (11)	0.0057 (10)	0.0031 (10)	0.0028 (10)
C1	0.0369 (18)	0.0338 (18)	0.0226 (14)	-0.0064 (15)	-0.0094 (14)	0.0043 (13)
C2	0.0307 (18)	0.0354 (19)	0.0258 (15)	0.0123 (15)	0.0056 (14)	0.0015 (14)
C3	0.048 (3)	0.0335 (19)	0.0271 (16)	0.0165 (16)	0.0025 (15)	-0.0074 (13)
C4	0.049 (3)	0.0230 (17)	0.0260 (16)	0.0075 (15)	-0.0040 (15)	-0.0040 (13)
C5	0.0314 (18)	0.0228 (15)	0.0175 (13)	0.0008 (13)	-0.0047 (11)	0.0008 (12)
C6	0.0209 (14)	0.0255 (16)	0.0166 (12)	0.0045 (13)	-0.0011 (11)	0.0029 (11)
C7	0.0389 (19)	0.0285 (17)	0.0205 (14)	-0.0058 (15)	-0.0084 (13)	0.0033 (13)

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

Ru1—Cl1	2.3880 (7)	C2—C3	1.381 (5)
Ru1—Cl1 ⁱ	2.3880 (7)	C3—C4	1.366 (6)
Ru1—N1	2.116 (3)	C4—C5	1.403 (5)
Ru1—N1 ⁱ	2.116 (3)	C5—C6	1.401 (5)
Ru1—C1	1.893 (4)	C5—C7	1.486 (5)
Ru1—C1 ⁱ	1.893 (4)	C6—C6 ⁱ	1.452 (4)
O1—C1	1.128 (4)	C7—C7 ⁱ	1.537 (5)
O2—C7	1.239 (5)	C2—H1	0.950
N1—C2	1.349 (5)	C3—H2	0.950
N1—C6	1.356 (4)	C4—H3	0.950

Ru1...O1 ⁱ	3.020 (3)	C7...Cl1 ^{ix}	3.331 (4)
Ru1...C2 ⁱ	3.115 (4)	C7...Cl1 ^{vi}	3.251 (3)
Ru1...C6 ⁱ	2.963 (3)	Ru1...H1	3.1883
O1...C1 ⁱ	3.531 (5)	Ru1...H1 ⁱ	3.1883
O2...O2 ⁱ	2.739 (4)	O1...H1 ⁱ	3.0752
O2...C4	2.897 (5)	O2...H3	2.6443
N1...C4	2.794 (5)	N1...H2	3.2400
C1...C2 ⁱ	3.258 (5)	C1...H1 ⁱ	2.7657
C2...C5	2.735 (5)	C2...H3	3.2444
C3...C6	2.726 (5)	C4...H1	3.2305
C5...C5 ⁱ	2.930 (5)	C5...H2	3.2454
C6...C7 ⁱ	2.916 (5)	C6...H1	3.1755
Cl1...O2 ⁱⁱ	3.433 (3)	C6...H3	3.2750
Cl1...C2 ⁱⁱⁱ	3.478 (4)	C7...H3	2.6986
Cl1...C7 ^{iv}	3.331 (4)	H1...H2	2.3113
Cl1...C7 ⁱⁱ	3.251 (3)	H2...H3	2.3241
O1...N1 ^{iv}	3.517 (4)	Cl1...H1 ⁱⁱⁱ	2.6578
O1...C2 ^{iv}	3.391 (5)	Cl1...H2 ⁱⁱⁱ	3.3550
O1...C3 ^v	3.320 (5)	Cl1...H3 ^{xi}	2.7786
O1...C3 ^{iv}	3.279 (5)	O1...H2 ^v	3.5019
O1...C4 ^v	3.109 (5)	O1...H3 ^v	3.1641
O1...C4 ^{iv}	3.286 (5)	O2...H1 ^{vii}	3.0084
O1...C5 ^{iv}	3.408 (4)	O2...H2 ^{viii}	2.5348
O1...C6 ^{iv}	3.494 (4)	O2...H3 ^{viii}	3.3956
O2...Cl1 ^{vi}	3.433 (3)	C1...H3 ^v	3.0904
O2...C2 ^{vii}	3.440 (5)	C4...H2 ^{viii}	3.4731
O2...C3 ^{viii}	3.206 (4)	C7...H2 ^{viii}	3.3448
N1...O1 ^{ix}	3.517 (4)	H1...Cl1 ^x	2.6578
C1...C4 ^v	3.362 (5)	H1...O2 ^{xi}	3.0084
C2...Cl1 ^x	3.478 (4)	H2...Cl1 ^x	3.3550
C2...O1 ^{ix}	3.391 (5)	H2...O1 ^{xii}	3.5019
C2...O2 ^{xi}	3.440 (5)	H2...O2 ^{xiii}	2.5348
C3...O1 ^{xii}	3.320 (5)	H2...C4 ^{xiii}	3.4731
C3...O1 ^{ix}	3.279 (5)	H2...C7 ^{xiii}	3.3448
C3...O2 ^{xiii}	3.206 (4)	H2...H3 ^{xiii}	2.7802
C4...O1 ^{xii}	3.109 (5)	H3...Cl1 ^{vii}	2.7786
C4...O1 ^{ix}	3.286 (5)	H3...O1 ^{xii}	3.1641
C4...C1 ^{xii}	3.362 (5)	H3...O2 ^{xiii}	3.3956
C5...O1 ^{ix}	3.408 (4)	H3...C1 ^{xii}	3.0904
C6...O1 ^{ix}	3.494 (4)	H3...H2 ^{viii}	2.7802
Cl1—Ru1—Cl1 ⁱ	176.52 (3)	N1—C2—C3	122.5 (4)
Cl1—Ru1—N1	90.01 (8)	C2—C3—C4	120.3 (4)
Cl1—Ru1—N1 ⁱ	87.27 (8)	C3—C4—C5	118.7 (3)
Cl1—Ru1—C1	87.50 (10)	C4—C5—C6	118.4 (3)
Cl1—Ru1—C1 ⁱ	95.00 (10)	C4—C5—C7	121.3 (3)
Cl1 ⁱ —Ru1—N1	87.27 (8)	C6—C5—C7	120.2 (3)
Cl1 ⁱ —Ru1—N1 ⁱ	90.01 (8)	N1—C6—C5	122.2 (3)

Cl1 ⁱ —Ru1—C1	95.00 (10)	N1—C6—C6 ⁱ	116.0 (3)
Cl1 ⁱ —Ru1—C1 ⁱ	87.50 (10)	C5—C6—C6 ⁱ	121.8 (3)
N1—Ru1—N1 ⁱ	77.18 (10)	O2—C7—C5	123.1 (3)
N1—Ru1—C1	174.02 (13)	O2—C7—C7 ⁱ	119.0 (3)
N1—Ru1—C1 ⁱ	97.26 (13)	C5—C7—C7 ⁱ	117.9 (3)
N1 ⁱ —Ru1—C1	97.26 (13)	N1—C2—H1	118.764
N1 ⁱ —Ru1—C1 ⁱ	174.02 (13)	C3—C2—H1	118.772
C1—Ru1—C1 ⁱ	88.38 (15)	C2—C3—H2	119.871
Ru1—N1—C2	126.6 (3)	C4—C3—H2	119.866
Ru1—N1—C6	115.43 (19)	C3—C4—H3	120.672
C2—N1—C6	117.9 (3)	C5—C4—H3	120.668
Ru1—C1—O1	176.1 (3)		
Cl1—Ru1—N1—C2	94.41 (19)	C6—N1—C2—C3	−0.0 (5)
Cl1—Ru1—N1—C6	−87.72 (16)	N1—C2—C3—C4	0.3 (5)
Cl1—Ru1—N1 ⁱ —C2 ⁱ	−87.76 (19)	C2—C3—C4—C5	0.5 (5)
Cl1—Ru1—N1 ⁱ —C6 ⁱ	90.11 (16)	C3—C4—C5—C6	−1.4 (5)
Cl1 ⁱ —Ru1—N1—C2	−87.76 (19)	C3—C4—C5—C7	178.2 (3)
Cl1 ⁱ —Ru1—N1—C6	90.11 (16)	C4—C5—C6—N1	1.6 (4)
Cl1 ⁱ —Ru1—N1 ⁱ —C2 ⁱ	94.41 (19)	C4—C5—C6—C6 ⁱ	−178.8 (3)
Cl1 ⁱ —Ru1—N1 ⁱ —C6 ⁱ	−87.72 (16)	C4—C5—C7—O2	−3.4 (5)
N1—Ru1—N1 ⁱ —C2 ⁱ	−178.4 (3)	C4—C5—C7—C7 ⁱ	177.9 (3)
N1—Ru1—N1 ⁱ —C6 ⁱ	−0.53 (16)	C6—C5—C7—O2	176.2 (3)
N1 ⁱ —Ru1—N1—C2	−178.4 (3)	C6—C5—C7—C7 ⁱ	−2.5 (4)
N1 ⁱ —Ru1—N1—C6	−0.53 (16)	C7—C5—C6—N1	−178.0 (3)
C1 ⁱ —Ru1—N1—C2	−0.6 (3)	C7—C5—C6—C6 ⁱ	1.6 (4)
C1 ⁱ —Ru1—N1—C6	177.23 (18)	N1—C6—C6 ⁱ —N1 ⁱ	−1.9 (4)
C1—Ru1—N1 ⁱ —C2 ⁱ	−0.6 (3)	N1—C6—C6 ⁱ —C5 ⁱ	178.5 (3)
C1—Ru1—N1 ⁱ —C6 ⁱ	177.23 (18)	C5—C6—C6 ⁱ —N1 ⁱ	178.5 (3)
Ru1—N1—C2—C3	177.77 (18)	C5—C6—C6 ⁱ —C5 ⁱ	−1.1 (4)
Ru1—N1—C6—C5	−178.98 (16)	O2—C7—C7 ⁱ —O2 ⁱ	5.5 (4)
Ru1—N1—C6—C6 ⁱ	1.4 (3)	O2—C7—C7 ⁱ —C5 ⁱ	−175.8 (3)
C2—N1—C6—C5	−0.9 (4)	C5—C7—C7 ⁱ —O2 ⁱ	−175.8 (3)
C2—N1—C6—C6 ⁱ	179.5 (3)	C5—C7—C7 ⁱ —C5 ⁱ	2.9 (4)

Symmetry codes: (i) $y, x, -z+1$; (ii) $-x+3/2, y-1/2, -z+3/4$; (iii) $-y+3/2, x+1/2, z-1/4$; (iv) $-y+3/2, x-1/2, z-1/4$; (v) $x, y-1, z$; (vi) $-x+3/2, y+1/2, -z+3/4$; (vii) $y, x+1, -z+1$; (viii) $x+1/2, -y+5/2, -z+5/4$; (ix) $y+1/2, -x+3/2, z+1/4$; (x) $y-1/2, -x+3/2, z+1/4$; (xi) $y-1, x, -z+1$; (xii) $x, y+1, z$; (xiii) $x-1/2, -y+5/2, -z+5/4$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H1 \cdots Cl1 ^x	0.95	2.66	3.478 (4)	145
C3—H2 \cdots O2 ^{xiv}	0.95	2.53	3.206 (4)	128
C4—H3 \cdots Cl1 ^{vii}	0.95	2.78	3.660 (4)	155

Symmetry codes: (vii) $y, x+1, -z+1$; (x) $y-1/2, -x+3/2, z+1/4$; (xiv) $-x-1/2, y+5/2, -z+7/4$.