



Received 20 January 2015

Accepted 16 March 2015

Edited by M. Weil, Vienna University of
Technology, Austria

Keywords: crystal structure; ruthenocene;
ruthenocenecarbonitrile; sandwich compound;
nitrile

CCDC reference: 1054219

Supporting information: this article has
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Crystal structure of ruthenocenecarbonitrile

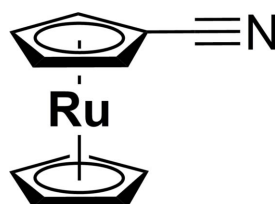
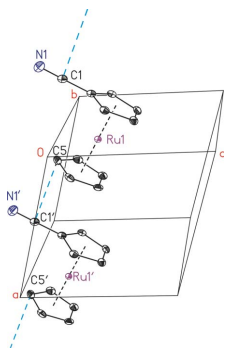
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The molecular structure of ruthenocenecarbonitrile, $[\text{Ru}(\eta^5\text{-C}_5\text{H}_4\text{C}\equiv\text{N})(\eta^5\text{-C}_5\text{H}_5)]$, exhibits point group symmetry m , with the mirror plane bisecting the molecule through the $\text{C}\equiv\text{N}$ substituent. The Ru^{II} atom is slightly shifted from the $\eta^5\text{-C}_5\text{H}_4$ centroid towards the $\text{C}\equiv\text{N}$ substituent. In the crystal, molecules are arranged in columns parallel to $[100]$. One-dimensional intermolecular $\pi\text{-}\pi$ interactions [3.363 (3) Å] between the $\text{C}\equiv\text{N}$ carbon atom and one carbon of the cyclopentadienyl ring of the overlaying molecule are present.

1. Chemical context

The nitrile group is isoelectronic with the acetylid function (Bonniard *et al.*, 2011), which has already been investigated in electron-transfer studies (see, for example, Lang *et al.*, 2006; Poppitz *et al.*, 2014; Speck *et al.*, 2012; Hildebrandt & Lang, 2013; Miesel *et al.*, 2013). Coordination of, for example, ferrocenecarbonitrile towards transition metals M will allow investigation of the electronic properties of $\text{-C}\equiv\text{N-M-}$ or $\text{-C}\equiv\text{N-M-N}\equiv\text{C-}$ bridging units. A synthesis for ferrocenecarbonitrile has already been described in 1957 (Graham *et al.*, 1957); however, only one example of an application in electrochemical studies has been described by Dowling *et al.* (1981). This prompted us to synthesize ferrocenecarbonitrile transition metal complexes to investigate the electronic properties of the $\text{-C}\equiv\text{N-M-N}\equiv\text{C-}$ bridging units (Strehler *et al.* 2013, 2014). In a continuation of this work, we present herein the synthesis and crystal structure of the related ruthenocenecarbonitrile, (I). The synthesis of this compound was realized by treatment of formyl-ruthenocene with hydroxylamine hydrochloride, zinc oxide and potassium iodide in acetonitrile, which is similar to a procedure already described for the synthesis of ferrocenecarbonitrile (Kivrak & Zora, 2007).



2. Structural commentary

The title compound contains one half-molecule in the asymmetric unit with a mirror plane bisecting the molecule through atoms C1, C2, C5, N1 and Ru1 (Fig. 1). The Ru1-centroid distance to the $\text{C}\equiv\text{N}$ -substituted cyclopentadienyl ring is

Table 1

Selected bond lengths (Å) and angles (°) for the clarification of the shift of the Ru1 atom towards the C≡N substituent in (I).

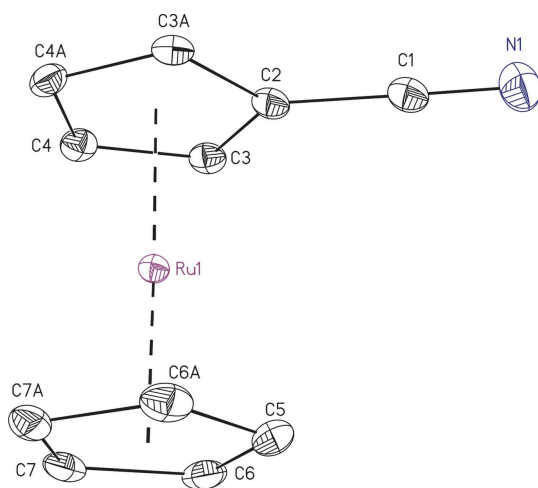
D is the centroid of the C₅H₄ or C₅H₅ ring.

	C2	C3	C4	C5	C6	C7
Ru1—C	2.1650 (18)	2.1886 (13)	2.2013 (12)	2.1779 (18)	2.1847 (13)	2.1879 (12)
C—D—Ru1	88.90 (8)	89.63 (6)	90.93 (6)	89.75 (9)	89.95 (6)	90.16 (6)

slightly increased [1.8179 (1) Å] compared to the unsubstituted C₅H₅ unit [1.8157 (1) Å]. Both cyclopentadienyl rings adopt an ideally eclipsed conformation and are virtually oriented parallel towards each other, which is expressed by the bond angle at the Ru^{II} between the two centroids (= *D*), with $D(\text{C}_5\text{H}_4)\text{—Ru1—}D(\text{C}_5\text{H}_5) = 178.87 (1)^\circ$. However, the Ru^{II} atom is slightly shifted from the centre of the C₅ ring to the nitrile-bonded C2 atom, which can be explained best by the significantly different Ru—C bond lengths (Table 1) and also the Ru—D—C angles, which should ideally be 90° (Table 1). This is in accordance with the shift in the ferrocenedicarbonylnitrile structure (Altmannshofer *et al.*, 2008). The C≡N substituent itself is bent away from the metal atom in (I), with a maximum shift for N1 [0.047 (4) Å].

3. Supramolecular features

The packing of (I) consists of a layer-type structure parallel to (010) with the direction of the C≡N function aligned parallel to [10 $\bar{1}$], alternating between adjacent layers. A further order is observed by a columnar arrangement of slightly tilted molecules parallel to [100]. Weak intermolecular π – π interactions within the sum of the van der Waals radii ($\Sigma = 3.4$ Å; Bondi, 1964) are present between C5 and the C1' atom [3.363 (3) Å] of the overlying molecule in the same layer (Fig. 2).

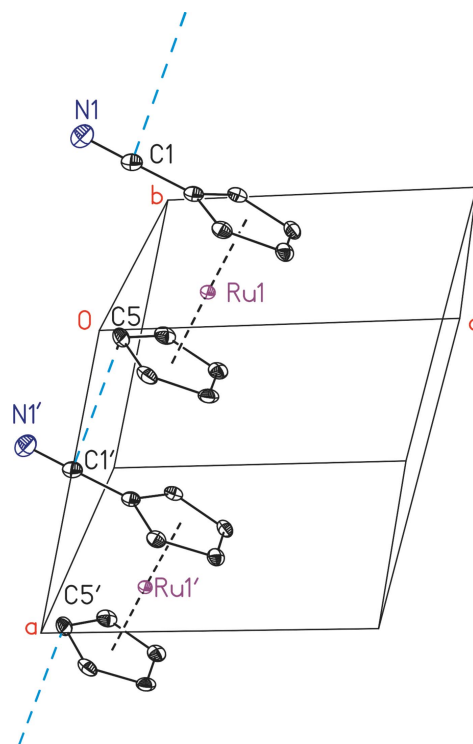
**Figure 1**

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry code: (A) $x, -y + \frac{1}{2}, z$.]

4. Database survey

The ruthenocene backbone is hardly described in the literature. Reported derivatives contain *sp* (ethynyl) (Sato *et al.*, 1997; Packheiser *et al.*, 2008; Jakob *et al.*, 2008, 2009a), *sp*² (Sato *et al.*, 1998, 2004; Jakob *et al.*, 2009b) and *sp*³ (Sokolov *et al.*, 2010; Barlow *et al.*, 2001) carbon substituents or a carboxylic acid moiety (Zhang & Coppens, 2001) and its respective Ru^{II} complex (Wyman *et al.*, 2005). They all exhibit similar Ru—D distances (1.795–1.823 Å) as compared to (I) [1.8179 (1)–1.8157 (1) Å] or unsubstituted ruthenocene (1.794–1.816 Å) (Ma & Coppens, 2003; Borissova *et al.*, 2008; Seiler & Dunitz, 1980).

Comparison of the C—C [1.431 (3) Å] and the C≡N distances [1.148 (3) Å] with the respective ferrocene carbonylnitrile derivatives (C≡N = 1.133–1.150; C—C = 1.428–1.433 Å; Altmannshofer *et al.*, 2008; Dayaker *et al.*, 2010; Bell *et al.*, 1996; Nemykin *et al.*, 2007; Erben *et al.*, 2007) reveals no significant influence of the central metal atom on the electronic properties of the substituent.

**Figure 2**

Intermolecular π – π interactions (blue) between C5 and C1' in the crystal structure of (I). All H atoms have been omitted for clarity. [Symmetry code: (') $x - 1, y, z$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	[Ru(C ₅ H ₅)(C ₆ H ₄ N)]
<i>M_r</i>	256.26
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>m</i>
Temperature (K)	110
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.2023 (2), 8.6802 (2), 7.2922 (1)
β (°)	106.497 (2)
<i>V</i> (Å ³)	437.12 (2)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.74
Crystal size (mm)	0.38 × 0.30 × 0.30
Data collection	
Diffractometer	Oxford Gemini S CCD
Absorption correction	Multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2006)
<i>T</i> _{min} , <i>T</i> _{max}	0.849, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	27710, 900, 877
<i>R</i> _{int}	0.019
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.012, 0.032, 1.05
No. of reflections	900
No. of parameters	67
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.27, -0.39

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2006), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

5. Synthesis and crystallization

Formylruthenocene was prepared according to a published procedure (Mueller-Westerhoff *et al.*, 1993). Synthesis of ruthenocenecarbonitrile, (I): formylruthenocene (2.27 g, 8.8 mmol), hydroxylamine hydrochloride (0.96 g, 13.8 mmol), zinc oxide (0.86 g, 10.6 mmol) and potassium iodide (1.76 g, 10.6 mmol) were suspended in 120 ml of dry acetonitrile. The mixture was stirred for 4 h at precisely 368 K. After cooling the reaction mixture to ambient temperature, 18 ml of an aqueous Na₂S₂O₃ (5%) solution were added in a single portion, and stirring was continued for additional 20 min. Solid particles were removed by filtration and the filtrate was extracted with ethyl acetate (3 × 50 ml). The combined organic layers were dried over MgSO₄. All volatiles were removed under reduced pressure and the crude product was purified by flash chromatography on aluminum oxide using dichloromethane as eluent. Greenish crystals of (I) were obtained by slow evaporation of a saturated dichloromethane solution containing (I) at ambient temperature (yield: 820 mg, 3.3 mmol, 38% based on formylruthenocene). IR (KBr, cm⁻¹): ν = 2226 (*m*, C \equiv N), 2854 (*s*), 2925 (*s*), 3082 (*m*, C–H). ¹H NMR (500.3 MHz, CDCl₃, 298 K): δ 4.69 (*s*, 5H, C₅H₅), 4.70 (*pt*, 2H, *J*_{H,H} = 1.8 Hz), 4.70 (*pt*, 2H, *J*_{H,H} = 1.8 Hz). ¹³C{¹H} NMR (125.7 MHz, CDCl₃, 298 K): δ = 55.3 (C_i-C₅H₄), 72.4 (C₅H₄), 72.9 (C₅H₅), 73.5 (C₅H₄), 119.4 (CN). HRMS (ESI-TOF, *M*⁺): C₁₁H₉NRu: *m/z* = 256.9792 (calc. 256.9776).

6. Refinement

C-bonded H atoms were placed in calculated positions and constrained to ride on their parent atoms, with *U*_{iso}(H) = 1.2*U*_{eq}(C) and a C–H distance of 0.93 Å. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

MK is grateful to the Fonds der Chemischen Industrie for a Chemiefonds fellowship.

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supporting information

Acta Cryst. (2015). E71, 398-401 [doi:10.1107/S205698901500540X]

Crystal structure of ruthenocenecarbonitrile

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Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *pubCIF* (Westrip, 2010).

Ruthenocenecarbonitrile

Crystal data

[Ru(C₅H₅)(C₆H₄N)]

$M_r = 256.26$

Monoclinic, $P2_1/m$

$a = 7.2023$ (2) Å

$b = 8.6802$ (2) Å

$c = 7.2922$ (1) Å

$\beta = 106.497$ (2)°

$V = 437.12$ (2) Å³

$Z = 2$

$F(000) = 252$

$D_x = 1.947$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 26762 reflections

$\theta = 3.5$ – 28.7 °

$\mu = 1.74$ mm⁻¹

$T = 110$ K

Block, yellow green

$0.38 \times 0.30 \times 0.30$ mm

Data collection

Oxford Gemini S CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2006)

$T_{\min} = 0.849$, $T_{\max} = 1.000$

27710 measured reflections

900 independent reflections

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

$R_{\text{int}} = 0.019$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 3.5$ °

$h = -8 \rightarrow 8$

$k = -10 \rightarrow 10$

$l = -8 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.012$

$wR(F^2) = 0.032$

$S = 1.05$

900 reflections

67 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

$w = 1/[\sigma^2(F_o^2) + (0.0218P)^2 + 0.1909P]$

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

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

$\Delta\rho_{\max} = 0.27$ e Å⁻³

$\Delta\rho_{\min} = -0.39$ e Å⁻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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	−0.4152 (3)	0.2500	−0.0364 (3)	0.0162 (4)
C2	−0.3084 (3)	0.2500	0.1617 (3)	0.0142 (4)
C3	−0.24721 (18)	0.11497 (16)	0.27791 (19)	0.0142 (3)
H3C	−0.2679	0.0130	0.2382	0.017*
C4	−0.14854 (18)	0.16776 (15)	0.46603 (18)	0.0145 (3)
H4C	−0.0935	0.1053	0.5710	0.017*
C5	0.1429 (3)	0.2500	0.0334 (3)	0.0185 (4)
H5C	0.0744	0.2500	−0.0957	0.022*
C6	0.20428 (19)	0.11674 (17)	0.1491 (2)	0.0175 (3)
H6C	0.1832	0.0149	0.1089	0.021*
C7	0.30392 (17)	0.16746 (16)	0.33757 (19)	0.0158 (3)
H7C	0.3591	0.1045	0.4420	0.019*
N1	−0.5024 (2)	0.2500	−0.1949 (3)	0.0244 (4)
Ru1	0.00474 (2)	0.2500	0.26311 (2)	0.00953 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0120 (8)	0.0168 (9)	0.0198 (10)	0.000	0.0045 (7)	0.000
C2	0.0093 (8)	0.0168 (9)	0.0170 (9)	0.000	0.0044 (7)	0.000
C3	0.0111 (6)	0.0148 (7)	0.0182 (6)	−0.0022 (5)	0.0065 (5)	−0.0003 (5)
C4	0.0145 (6)	0.0163 (7)	0.0146 (6)	0.0003 (5)	0.0072 (5)	0.0029 (5)
C5	0.0155 (9)	0.0283 (11)	0.0145 (9)	0.000	0.0087 (7)	0.000
C6	0.0143 (6)	0.0190 (7)	0.0222 (7)	0.0005 (5)	0.0101 (5)	−0.0047 (6)
C7	0.0098 (6)	0.0191 (7)	0.0193 (6)	0.0033 (5)	0.0054 (5)	0.0029 (5)
N1	0.0222 (9)	0.0274 (10)	0.0208 (9)	0.000	0.0015 (7)	0.000
Ru1	0.00850 (10)	0.00992 (10)	0.01040 (10)	0.000	0.00305 (6)	0.000

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

C1—N1	1.148 (3)	C5—Ru1	2.1780 (18)
C1—C2	1.431 (3)	C5—H5C	0.9300
C2—C3 ⁱ	1.4401 (17)	C6—C7	1.4274 (19)
C2—C3	1.4401 (17)	C6—Ru1	2.1848 (13)
C2—Ru1	2.1649 (18)	C6—H6C	0.9300
C3—C4	1.4294 (18)	C7—C7 ⁱ	1.433 (3)

C3—Ru1	2.1885 (13)	C7—Ru1	2.1878 (12)
C3—H3C	0.9300	C7—H7C	0.9300
C4—C4 ⁱ	1.428 (3)	Ru1—C6 ⁱ	2.1848 (13)
C4—Ru1	2.2013 (12)	Ru1—C7 ⁱ	2.1878 (12)
C4—H4C	0.9300	Ru1—C3 ⁱ	2.1885 (13)
C5—C6 ⁱ	1.4262 (18)	Ru1—C4 ⁱ	2.2013 (12)
C5—C6	1.4262 (18)		
N1—C1—C2	179.4 (2)	C5—Ru1—C6	38.16 (5)
C1—C2—C3 ⁱ	125.52 (8)	C6 ⁱ —Ru1—C6	63.94 (8)
C1—C2—C3	125.52 (8)	C2—Ru1—C7 ⁱ	160.38 (4)
C3 ⁱ —C2—C3	108.96 (16)	C5—Ru1—C7 ⁱ	63.77 (6)
C1—C2—Ru1	123.64 (13)	C6 ⁱ —Ru1—C7 ⁱ	38.11 (5)
C3 ⁱ —C2—Ru1	71.57 (8)	C6—Ru1—C7 ⁱ	63.89 (5)
C3—C2—Ru1	71.57 (8)	C2—Ru1—C7	160.38 (4)
C4—C3—C2	106.82 (12)	C5—Ru1—C7	63.77 (6)
C4—C3—Ru1	71.48 (7)	C6 ⁱ —Ru1—C7	63.89 (5)
C2—C3—Ru1	69.80 (9)	C6—Ru1—C7	38.11 (5)
C4—C3—H3C	126.6	C7 ⁱ —Ru1—C7	38.23 (7)
C2—C3—H3C	126.6	C2—Ru1—C3 ⁱ	38.63 (4)
Ru1—C3—H3C	123.8	C5—Ru1—C3 ⁱ	127.17 (5)
C4 ⁱ —C4—C3	108.70 (8)	C6 ⁱ —Ru1—C3 ⁱ	112.30 (6)
C4 ⁱ —C4—Ru1	71.08 (3)	C6—Ru1—C3 ⁱ	161.19 (5)
C3—C4—Ru1	70.51 (7)	C7 ⁱ —Ru1—C3 ⁱ	125.76 (5)
C4 ⁱ —C4—H4C	125.7	C7—Ru1—C3 ⁱ	159.25 (5)
C3—C4—H4C	125.7	C2—Ru1—C3	38.63 (4)
Ru1—C4—H4C	124.4	C5—Ru1—C3	127.17 (5)
C6 ⁱ —C5—C6	108.40 (17)	C6 ⁱ —Ru1—C3	161.18 (5)
C6 ⁱ —C5—Ru1	71.18 (9)	C6—Ru1—C3	112.30 (6)
C6—C5—Ru1	71.18 (9)	C7 ⁱ —Ru1—C3	159.25 (5)
C6 ⁱ —C5—H5C	125.8	C7—Ru1—C3	125.76 (5)
C6—C5—H5C	125.8	C3 ⁱ —Ru1—C3	64.76 (7)
Ru1—C5—H5C	123.5	C2—Ru1—C4 ⁱ	63.69 (6)
C5—C6—C7	107.83 (13)	C5—Ru1—C4 ⁱ	160.55 (4)
C5—C6—Ru1	70.66 (9)	C6 ⁱ —Ru1—C4 ⁱ	126.43 (5)
C7—C6—Ru1	71.06 (7)	C6—Ru1—C4 ⁱ	159.58 (5)
C5—C6—H6C	126.1	C7 ⁱ —Ru1—C4 ⁱ	111.94 (5)
C7—C6—H6C	126.1	C7—Ru1—C4 ⁱ	125.87 (5)
Ru1—C6—H6C	123.8	C3 ⁱ —Ru1—C4 ⁱ	38.01 (5)
C6—C7—C7 ⁱ	107.97 (8)	C3—Ru1—C4 ⁱ	63.86 (5)
C6—C7—Ru1	70.83 (7)	C2—Ru1—C4	63.69 (6)
C7 ⁱ —C7—Ru1	70.88 (4)	C5—Ru1—C4	160.55 (4)
C6—C7—H7C	126.0	C6 ⁱ —Ru1—C4	159.58 (5)
C7 ⁱ —C7—H7C	126.0	C6—Ru1—C4	126.42 (5)
Ru1—C7—H7C	123.9	C7 ⁱ —Ru1—C4	125.87 (5)
C2—Ru1—C5	113.36 (7)	C7—Ru1—C4	111.94 (5)
C2—Ru1—C6 ⁱ	127.17 (5)	C3 ⁱ —Ru1—C4	63.86 (5)
C5—Ru1—C6 ⁱ	38.16 (5)	C3—Ru1—C4	38.01 (5)

C2—Ru1—C6	127.17 (5)	C4 ⁱ —Ru1—C4	37.84 (7)
C1—C2—C3—C4	-179.04 (16)	C2—C3—C4—Ru1	-61.20 (10)
C3 ⁱ —C2—C3—C4	0.13 (19)	C6 ⁱ —C5—C6—C7	0.1 (2)
Ru1—C2—C3—C4	62.30 (9)	Ru1—C5—C6—C7	-61.69 (9)
C1—C2—C3—Ru1	118.66 (18)	C6 ⁱ —C5—C6—Ru1	61.79 (12)
C3 ⁱ —C2—C3—Ru1	-62.17 (12)	C5—C6—C7—C7 ⁱ	-0.06 (12)
C2—C3—C4—C4 ⁱ	-0.08 (12)	Ru1—C6—C7—C7 ⁱ	-61.50 (4)
Ru1—C3—C4—C4 ⁱ	61.12 (4)	C5—C6—C7—Ru1	61.44 (10)

Symmetry code: (i) $x, -y+1/2, z$.