

# catena-Poly[[tetrakis( $\mu$ -3,4,5-trimethoxybenzoato- $\kappa^2$ O:O')diruthenium(II,III)(Ru—Ru)]- $\mu$ -chlorido] with an unknown solvent

Patricia Delgado-Martínez,<sup>a</sup> Rodrigo González-Prieto,<sup>a\*</sup> Reyes Jiménez-Aparicio,<sup>a</sup> M. Rosario Torres<sup>b</sup> and José Luis Priego<sup>a\*</sup>

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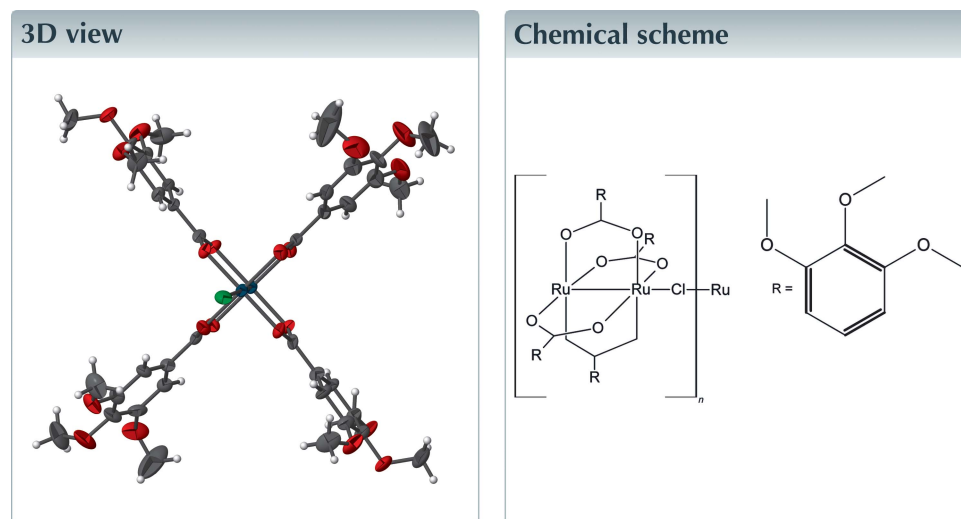
Keywords: crystal structure; diruthenium(II,III) complexes; metal–metal bond; carboxylates; 3,4,5-trimethoxybenzoate.

CCDC reference: 1816620

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

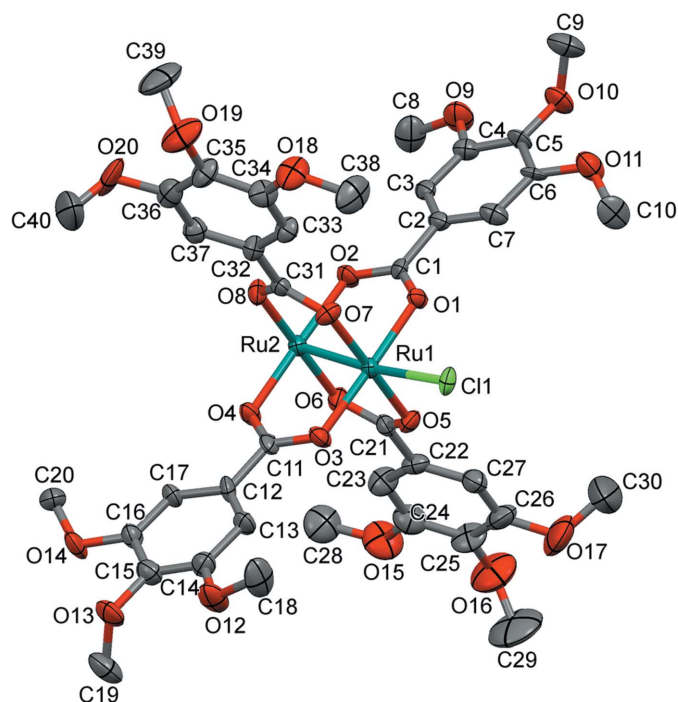
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$[\text{Ru}_2\text{Cl}\{\mu\text{-O}_2\text{CC}_6\text{H}_2\text{-3,4,5-(OMe)}_3\}_4]_n$  was prepared by the reaction of  $[\text{Ru}_2\text{Cl}(\mu\text{-O}_2\text{CCH}_3)_n]$  with 3,4,5-trimethoxybenzoic acid. The complex shows a paddlewheel structure with pairs of Ru atoms bridged by four carboxylate ligands. The axial positions are occupied by shared chloride ions giving zigzag chains. These chains are disposed parallel to each other to give a three-dimensional arrangement packed only by van der Waals forces. The final refinement shows high values of residual non-modelled electronic density. Therefore, the SQUEEZE utility [Spek (2015). *Acta Cryst.* **C71**, 9–18] was used to remove its contribution to the overall intensity data. The electron density modelled by SQUEEZE is consistent with around eight water molecules per unit cell.



## Structure description

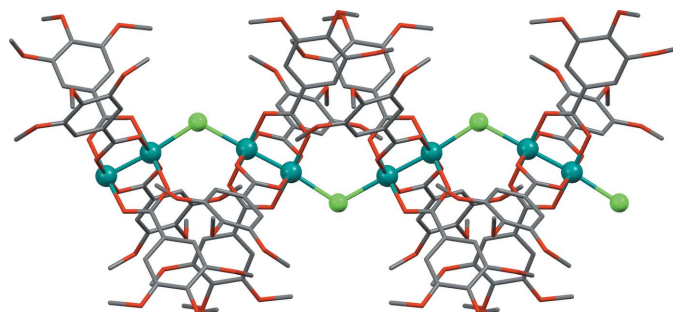
The asymmetric unit of the title compound  $[\text{Ru}_2\text{Cl}\{\mu\text{-O}_2\text{CC}_6\text{H}_2\text{-3,4,5-(OMe)}_3\}_4]_n$  contains a complete diruthenium unit (Fig. 1). The complex adopts a paddlewheel arrangement with two ruthenium atoms supported by four carboxylate bridging ligands. In this structure, each Ru atom shows a distorted octahedral environment, with the four equatorial positions occupied by the oxygen atoms of the carboxylate ligands, one axial position is occupied by one chloride ligand and the other one by the second Ru atom of the dimetallic unit. The cationic units  $[\text{Ru}_2(\mu\text{-O}_2\text{CR})_4]^+$  are bridged by chloride anions giving infinite zigzag chains  $(-\text{Ru}-\text{Ru}-\text{Cl}-)_n$  with an Ru1–Cl–Ru2 angle of 118.43 (7)° (Fig. 2). This angle has been related to the magnetic properties of this type of



**Figure 1**  
The structure of the dimeric unit of  $[\text{Ru}_2\text{Cl}\{\mu\text{-O}_2\text{CC}_6\text{H}_2\text{-3,4,5-(OMe)}_3\}_4]_n$  with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity.

compounds (Estiú *et al.*, 1999; Barral *et al.*, 2000). The magnetic moment at room temperature for this compound is  $4.49 \mu_B$ , which is consistent with the presence of three unpaired electrons per dimer unit and supports an electronic configuration of  $\sigma^2\pi^4\delta^2(\pi^*\delta^*)^3$  proposed by Norman *et al.* (1979). According to the Ru–Cl–Ru angle, a weak degree of antiferromagnetic coupling between the dimetallic units ( $zJ = -0.66 \text{ cm}^{-1}$ ) through the halide ligand is observed. The magnetic behaviour is also in accordance with a large zero-field splitting ( $D = 74.01 \text{ cm}^{-1}$ ) which is always observed in compounds containing  $\text{Ru}_2^{5+}$  units (Aquino, 2004; Cotton *et al.*, 2005; Barral *et al.*, 2000, and Delgado-Martínez *et al.*, 2014).

The Ru–Ru bond length is  $2.2930(8) \text{ \AA}$  (Table 1). This distance is very similar to those found in other analogous chloridotetracarboxylatodiruthenium complexes (Thompson



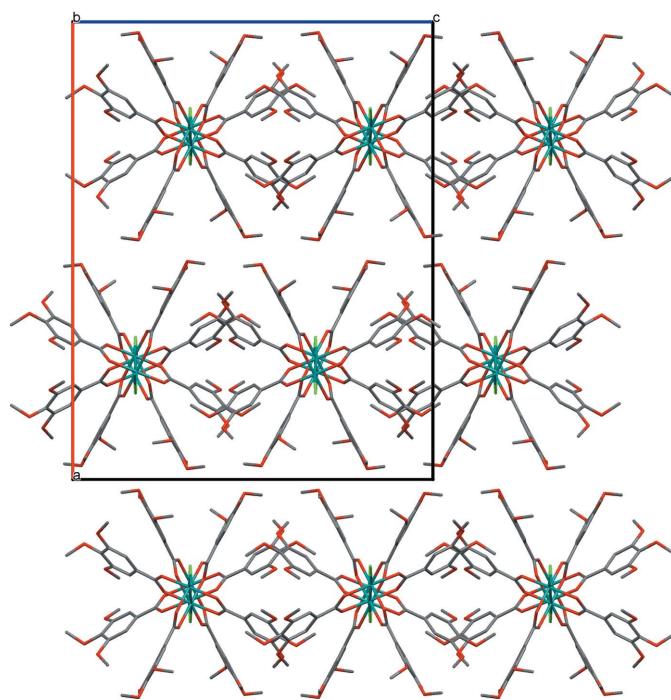
**Figure 2**  
Zigzag chain of  $[\text{Ru}_2\text{Cl}\{\mu\text{-O}_2\text{CC}_6\text{H}_2\text{-3,4,5-(OMe)}_3\}_4]_n$ . Hydrogen atoms have been omitted for clarity.

**Table 1**  
Selected bond lengths ( $\text{\AA}$ ).

Ru1–Ru2	2.2930 (8)		
Ru1–Cl1	2.584 (2)	Ru2–Cl1	2.561 (2)
Ru1–O1	2.015 (5)	Ru2–O2	2.041 (5)
Ru1–O3	2.029 (5)	Ru2–O4	1.996 (5)
Ru1–O5	2.035 (5)	Ru2–O6	2.014 (5)
Ru1–O7	2.009 (5)	Ru2–O8	2.026 (5)

*et al.*, 2015; Delgado *et al.*, 2012) and in other diruthenium complexes containing the  $\text{Ru}_2^{5+}$  unit (Aquino, 2004; Cotton *et al.*, 2005; Delgado-Martínez *et al.*, 2014). This distance is in accordance with the electronic configuration  $\sigma^2\pi^4\delta^2(\pi^*\delta^*)^3$ . The Ru–O and Ru–Cl distances are also similar to those in other  $[\text{Ru}_2\text{Cl}(\mu\text{-O}_2\text{CR})_4]_n$  complexes (Cotton *et al.*, 2005; Aquino, 2004).

In the packing of this compound, zigzag chains are disposed parallel to each other along the *b* axis, forming parallel layers (Fig. 3). The shortest Ru···Ru distance between adjacent chains in the same layer is  $12.144 \text{ \AA}$  (Ru2···Ru2). Every layer is displaced with respect to those above and below. The Ru2···Ru2 distances between different layers range from  $14.450$  to  $18.472 \text{ \AA}$ . As a consequence of this arrangement, every chain is surrounded by six other chains (Fig. 3). The presence of three bulky methoxy groups in the phenyl rings prevents the formation of  $\pi\text{-}\pi$  stacking interactions. Therefore, the packing of the chains in the solid state involves only van der Waals forces. Atoms O19, C29, O13 and C8 of each dimetallic unit are involved in the shortest distances between different chains. Hence, atoms O19 atom and C29 of each



**Figure 3**  
Crystal packing of zigzag chains of  $[\text{Ru}_2\text{Cl}\{\mu\text{-O}_2\text{CC}_6\text{H}_2\text{-3,4,5-(OMe)}_3\}_4]_n$  along *b* axis.

Table 2

Experimental details.

Crystal data	
Chemical formula	[Ru <sub>2</sub> Cl(C <sub>10</sub> H <sub>11</sub> O <sub>5</sub> ) <sub>4</sub> ]
<i>M<sub>r</sub></i>	1082.34
Crystal system, space group	Orthorhombic, <i>Pbcn</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	30.369 (4), 12.8816 (15), 23.898 (3)
<i>V</i> (Å <sup>3</sup> )	9348.9 (19)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
$\mu$ (mm <sup>-1</sup> )	0.78
Crystal size (mm)	0.57 × 0.16 × 0.06
Data collection	
Diffractionmeter	Bruker SMART CCD area detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2002)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.809, 1.000
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	67660, 8248, 3955
<i>R<sub>int</sub></i>	0.110
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.595
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.060, 0.146, 1.00
No. of reflections	8248
No. of parameters	568
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	1.13, -1.56

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006).

dimetallic unit are respectively connected (3.297 Å) with the C29 of another dimetallic unit belonging to the upper layer, and with atom O19 of another unit from the lower layer. Similarly, O13 and C8, are respectively connected with atoms C8 and O13 in two adjacent chains of the same layer (3.301 Å).

### Synthesis and crystallization

0.32 g of 3,4,5-trimethoxybenzoic acid (1.5 mmol) were added to a suspension of chloridotetra(acetato)diruthenium(II,III) (Mitchell *et al.*, 1973) in (0.12 g, 0.25 mmol) in 8 mL of EtOH placed in a 23 mL Teflon-lined autoclave and stirred for several minutes to become homogenized. The reactor was closed and heated under a three step program consisting of: 2 h heating ramp up to 130°C; 24 h isotherm; and 24 h cooling down to room temperature. The brown crystals obtained were filtered and washed with cold ethanol (2 × 10 mL). Yield: 81%.

### Refinement

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

Disordered solvent molecules were not modelled and the disordered density was taken into account using the SQUEEZE routine (Spek, 2015) in *PLATON* procedure. The final refinement show high values of residual non-modelled electronic density. Therefore, the SQUEEZE program was used to remove its contribution to the overall intensity data. An improvement was observed in all refinement parameters and the residuals when this procedure was applied. The electron density modelled by SQUEEZE is consistent with around eight water molecules per unit cell.

### Funding information

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## full crystallographic data

*IUCrData* (2018). 3, x180079 [https://doi.org/10.1107/S2414314618000792]

**catena-Poly[[tetrakis( $\mu$ -3,4,5-trimethoxybenzoato- $\kappa^2$ O:O')diruthenium(II,III)(Ru—Ru)]- $\mu$ -chlorido] with an unknown solvent**

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*catena-Poly[[tetrakis( $\mu$ -3,4,5-trimethoxybenzoato- $\kappa^2$ O:O')diruthenium(II,III)(Ru—Ru)]- $\mu$ -chlorido]*

*Crystal data*

[Ru<sub>2</sub>Cl(C<sub>10</sub>H<sub>11</sub>O<sub>5</sub>)<sub>4</sub>]

$M_r = 1082.34$

Orthorhombic, *Pbcn*

$a = 30.369$  (4) Å

$b = 12.8816$  (15) Å

$c = 23.898$  (3) Å

$V = 9348.9$  (19) Å<sup>3</sup>

$Z = 8$

$F(000) = 4392$

$D_x = 1.538$  Mg m<sup>-3</sup>

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

Cell parameters from 5919 reflections

$\theta = 2.2$ – $28.8^\circ$

$\mu = 0.78$  mm<sup>-1</sup>

$T = 296$  K

Prismatic, brown

$0.57 \times 0.16 \times 0.06$  mm

*Data collection*

Bruker SMART CCD area detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2002)

$T_{\min} = 0.809$ ,  $T_{\max} = 1.000$

67660 measured reflections

8248 independent reflections

3955 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.110$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 1.3^\circ$

$h = -36 \rightarrow 33$

$k = -15 \rightarrow 15$

$l = -26 \rightarrow 28$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.146$

$S = 1.00$

8248 reflections

568 parameters

1 restraint

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

$w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$

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

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

$\Delta\rho_{\max} = 1.13$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -1.56$  e Å<sup>-3</sup>

*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.** The paper reports that unspecified disordered solvent molecules were not modelled and the disordered density was taken into account using the SQUEEZE/PLATON procedure.

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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.18915 (6)	0.25846 (13)	0.32602 (9)	0.0304 (4)
C1	0.2851 (3)	0.4519 (6)	0.4239 (3)	0.0283 (19)
C2	0.3048 (2)	0.4172 (6)	0.4780 (3)	0.0290 (18)
C3	0.3362 (2)	0.4745 (6)	0.5055 (3)	0.0299 (19)
H3	0.3445	0.5394	0.4922	0.036*
C4	0.3552 (3)	0.4344 (6)	0.5532 (3)	0.034 (2)
C5	0.3435 (3)	0.3388 (6)	0.5739 (3)	0.035 (2)
C6	0.3125 (3)	0.2799 (6)	0.5439 (3)	0.034 (2)
C7	0.2935 (2)	0.3188 (6)	0.4965 (3)	0.035 (2)
H7	0.2731	0.2794	0.4767	0.042*
C8	0.4091 (3)	0.5705 (7)	0.5582 (4)	0.058 (3)
H8A	0.4214	0.5506	0.5228	0.087*
H8B	0.4321	0.5948	0.5824	0.087*
H8C	0.3879	0.6250	0.5526	0.087*
C9	0.3380 (3)	0.2996 (8)	0.6705 (3)	0.064 (3)
H9A	0.3221	0.3637	0.6738	0.096*
H9B	0.3574	0.2920	0.7020	0.096*
H9C	0.3176	0.2427	0.6697	0.096*
C10	0.2865 (3)	0.1077 (6)	0.5256 (4)	0.046 (2)
H10A	0.2561	0.1242	0.5189	0.069*
H10B	0.2886	0.0394	0.5414	0.069*
H10C	0.3024	0.1100	0.4909	0.069*
C11	0.2195 (2)	0.5570 (5)	0.2290 (3)	0.0280 (19)
C12	0.1985 (2)	0.5946 (5)	0.1765 (3)	0.0314 (19)
C13	0.1691 (3)	0.5325 (6)	0.1475 (3)	0.035 (2)
H13	0.1626	0.4658	0.1599	0.042*
C14	0.1493 (3)	0.5723 (6)	0.0990 (3)	0.037 (2)
C15	0.1614 (3)	0.6701 (6)	0.0797 (3)	0.039 (2)
C16	0.1900 (2)	0.7339 (5)	0.1107 (3)	0.0305 (19)
C17	0.2089 (3)	0.6946 (6)	0.1584 (3)	0.031 (2)
H17	0.2286	0.7348	0.1787	0.038*
C18	0.0946 (3)	0.4377 (6)	0.0962 (4)	0.061 (3)
H18A	0.1147	0.3821	0.1041	0.092*
H18B	0.0715	0.4129	0.0722	0.092*

H18C	0.0821	0.4626	0.1305	0.092*
C19	0.1659 (3)	0.7038 (7)	-0.0174 (4)	0.062 (3)
H19A	0.1894	0.7534	-0.0146	0.094*
H19B	0.1477	0.7205	-0.0490	0.094*
H19C	0.1780	0.6355	-0.0221	0.094*
C20	0.2154 (3)	0.9047 (6)	0.1275 (3)	0.045 (2)
H20A	0.1963	0.9152	0.1590	0.068*
H20B	0.2198	0.9694	0.1084	0.068*
H20C	0.2433	0.8786	0.1403	0.068*
C21	0.3234 (2)	0.4248 (6)	0.2806 (3)	0.0269 (17)
C22	0.3634 (3)	0.3786 (6)	0.2550 (3)	0.032 (2)
C23	0.3957 (2)	0.4457 (7)	0.2339 (3)	0.042 (2)
H23	0.3924	0.5172	0.2369	0.051*
C24	0.4331 (3)	0.4035 (8)	0.2081 (4)	0.052 (3)
C25	0.4395 (3)	0.2964 (8)	0.2058 (4)	0.051 (3)
C26	0.4074 (3)	0.2308 (7)	0.2298 (4)	0.052 (3)
C27	0.3701 (3)	0.2723 (6)	0.2537 (3)	0.039 (2)
H27	0.3491	0.2283	0.2693	0.047*
C28	0.4613 (3)	0.5706 (7)	0.1853 (4)	0.067 (3)
H28A	0.4337	0.5893	0.1685	0.101*
H28B	0.4850	0.6012	0.1643	0.101*
H28C	0.4622	0.5955	0.2231	0.101*
C29	0.4717 (4)	0.1919 (11)	0.1365 (6)	0.139 (6)
H29A	0.4428	0.1617	0.1370	0.209*
H29B	0.4935	0.1380	0.1388	0.209*
H29C	0.4757	0.2302	0.1024	0.209*
C30	0.4201 (7)	0.0684 (10)	0.2756 (4)	0.210 (11)
H30A	0.4305	0.1129	0.3050	0.315*
H30B	0.4413	0.0143	0.2691	0.315*
H30C	0.3925	0.0382	0.2863	0.315*
C31	0.1826 (2)	0.5890 (5)	0.3726 (3)	0.0251 (17)
C32	0.1425 (2)	0.6304 (5)	0.3984 (3)	0.0291 (19)
C33	0.1124 (2)	0.5638 (6)	0.4209 (3)	0.0309 (19)
H33	0.1174	0.4926	0.4193	0.037*
C34	0.0751 (2)	0.5995 (6)	0.4457 (3)	0.037 (2)
C35	0.0677 (3)	0.7063 (6)	0.4503 (4)	0.040 (2)
C36	0.0969 (3)	0.7746 (7)	0.4256 (4)	0.042 (2)
C37	0.1348 (3)	0.7361 (6)	0.4004 (3)	0.034 (2)
H37	0.1550	0.7818	0.3847	0.040*
C38	0.0480 (3)	0.4276 (7)	0.4637 (4)	0.066 (3)
H38A	0.0510	0.4095	0.4249	0.099*
H38B	0.0225	0.3938	0.4789	0.099*
H38C	0.0737	0.4057	0.4838	0.099*
C39	0.0340 (3)	0.8084 (8)	0.5231 (4)	0.083 (4)
H39A	0.0610	0.7941	0.5425	0.125*
H39B	0.0096	0.7974	0.5478	0.125*
H39C	0.0340	0.8791	0.5105	0.125*
C40	0.0666 (6)	0.9225 (9)	0.3840 (5)	0.151 (7)

H40A	0.0782	0.8978	0.3490	0.227*
H40B	0.0692	0.9967	0.3855	0.227*
H40C	0.0361	0.9034	0.3870	0.227*
O1	0.25943 (15)	0.3916 (3)	0.39925 (19)	0.0250 (12)
O2	0.29430 (16)	0.5435 (4)	0.4056 (2)	0.0304 (13)
O3	0.21139 (16)	0.4668 (4)	0.24674 (19)	0.0299 (12)
O4	0.24580 (16)	0.6197 (4)	0.25375 (19)	0.0283 (12)
O5	0.29024 (17)	0.3650 (3)	0.2874 (2)	0.0307 (13)
O6	0.32388 (16)	0.5200 (4)	0.2931 (2)	0.0318 (13)
O7	0.18248 (15)	0.4935 (4)	0.3587 (2)	0.0291 (13)
O8	0.21573 (16)	0.6462 (3)	0.3643 (2)	0.0299 (13)
O9	0.3877 (2)	0.4821 (4)	0.5834 (2)	0.0535 (17)
O10	0.36295 (18)	0.3004 (4)	0.6205 (2)	0.0468 (16)
O11	0.30471 (19)	0.1809 (4)	0.5634 (2)	0.0489 (16)
O12	0.1180 (2)	0.5214 (4)	0.0687 (2)	0.0524 (17)
O14	0.19586 (18)	0.8311 (4)	0.0900 (2)	0.0422 (15)
O13	0.14050 (18)	0.7068 (4)	0.0317 (2)	0.0453 (16)
O15	0.4659 (2)	0.4608 (6)	0.1850 (3)	0.073 (2)
O16	0.4764 (2)	0.2591 (6)	0.1823 (4)	0.097 (3)
O17	0.4146 (2)	0.1260 (5)	0.2271 (3)	0.084 (2)
O18	0.04302 (18)	0.5388 (4)	0.4688 (2)	0.0522 (17)
O19	0.03024 (18)	0.7414 (5)	0.4766 (3)	0.0655 (19)
O20	0.0890 (2)	0.8806 (5)	0.4259 (3)	0.065 (2)
Ru1	0.235314 (18)	0.42687 (4)	0.32304 (2)	0.02245 (17)
Ru2	0.270333 (18)	0.58420 (4)	0.32884 (2)	0.02336 (17)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0342 (10)	0.0132 (8)	0.0437 (11)	0.0025 (8)	-0.0027 (10)	-0.0003 (9)
C1	0.042 (5)	0.019 (4)	0.024 (5)	0.013 (4)	-0.001 (4)	-0.003 (3)
C2	0.036 (5)	0.033 (4)	0.018 (4)	0.011 (4)	-0.001 (4)	0.000 (4)
C3	0.038 (5)	0.031 (4)	0.021 (5)	0.016 (4)	0.001 (4)	-0.001 (4)
C4	0.042 (5)	0.036 (5)	0.024 (5)	0.001 (4)	0.000 (4)	-0.002 (4)
C5	0.050 (6)	0.038 (5)	0.017 (5)	0.006 (4)	-0.015 (4)	0.004 (4)
C6	0.056 (6)	0.039 (5)	0.007 (4)	0.004 (4)	0.001 (4)	-0.001 (4)
C7	0.034 (5)	0.046 (5)	0.024 (5)	-0.001 (4)	-0.003 (4)	0.003 (4)
C8	0.056 (6)	0.047 (6)	0.070 (7)	-0.007 (5)	-0.029 (5)	-0.003 (6)
C9	0.085 (8)	0.081 (7)	0.025 (6)	0.002 (6)	-0.001 (6)	0.003 (5)
C10	0.042 (5)	0.045 (5)	0.052 (6)	-0.033 (4)	-0.015 (5)	0.003 (5)
C11	0.038 (5)	0.023 (4)	0.023 (4)	0.002 (4)	0.010 (4)	0.009 (4)
C12	0.043 (5)	0.018 (4)	0.033 (5)	0.004 (3)	0.000 (4)	0.012 (4)
C13	0.049 (5)	0.030 (4)	0.025 (5)	0.005 (4)	-0.014 (4)	0.003 (4)
C14	0.044 (5)	0.033 (5)	0.034 (5)	0.006 (4)	-0.011 (4)	-0.003 (4)
C15	0.045 (6)	0.044 (5)	0.029 (5)	0.005 (5)	-0.005 (4)	0.005 (4)
C16	0.036 (5)	0.026 (4)	0.030 (5)	-0.003 (4)	-0.004 (4)	0.007 (4)
C17	0.043 (5)	0.027 (4)	0.024 (5)	0.006 (4)	-0.006 (4)	0.007 (4)
C18	0.071 (7)	0.039 (6)	0.074 (7)	-0.026 (5)	-0.028 (6)	0.006 (5)

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C19	0.077 (7)	0.075 (7)	0.035 (6)	-0.005 (6)	-0.007 (6)	0.022 (5)
C20	0.071 (6)	0.036 (5)	0.028 (5)	0.009 (5)	0.000 (5)	-0.005 (4)
C21	0.031 (4)	0.026 (4)	0.024 (4)	0.004 (4)	0.001 (4)	0.007 (4)
C22	0.031 (5)	0.040 (5)	0.025 (5)	0.002 (4)	0.001 (4)	-0.009 (4)
C23	0.030 (5)	0.047 (5)	0.051 (6)	0.001 (4)	0.005 (4)	-0.005 (5)
C24	0.044 (6)	0.063 (7)	0.049 (6)	-0.008 (5)	0.005 (5)	0.003 (5)
C25	0.028 (5)	0.067 (7)	0.059 (7)	0.011 (5)	0.016 (5)	-0.011 (6)
C26	0.063 (7)	0.049 (6)	0.044 (6)	0.018 (5)	-0.003 (5)	-0.020 (5)
C27	0.046 (5)	0.043 (6)	0.029 (5)	0.009 (4)	0.003 (4)	0.004 (4)
C28	0.053 (6)	0.069 (7)	0.080 (8)	-0.017 (6)	0.015 (6)	0.003 (6)
C29	0.154 (14)	0.142 (13)	0.121 (13)	0.039 (11)	0.080 (11)	-0.044 (11)
C30	0.47 (3)	0.091 (11)	0.074 (11)	0.098 (16)	0.056 (16)	0.028 (9)
C31	0.035 (5)	0.023 (4)	0.018 (4)	0.000 (4)	-0.003 (4)	0.002 (3)
C32	0.029 (5)	0.024 (4)	0.034 (5)	0.002 (4)	-0.001 (4)	0.000 (4)
C33	0.023 (4)	0.032 (5)	0.038 (5)	0.005 (4)	0.001 (4)	-0.002 (4)
C34	0.029 (5)	0.041 (5)	0.041 (5)	-0.009 (4)	0.005 (4)	-0.001 (4)
C35	0.030 (5)	0.038 (5)	0.054 (6)	0.008 (4)	0.003 (4)	-0.009 (5)
C36	0.037 (5)	0.042 (6)	0.046 (6)	0.012 (4)	-0.019 (5)	-0.007 (4)
C37	0.033 (5)	0.033 (5)	0.035 (5)	0.000 (4)	-0.003 (4)	0.002 (4)
C38	0.066 (7)	0.044 (6)	0.089 (9)	-0.025 (5)	0.024 (6)	-0.009 (6)
C39	0.089 (9)	0.078 (8)	0.083 (9)	0.006 (7)	0.037 (7)	-0.040 (7)
C40	0.31 (2)	0.076 (9)	0.073 (10)	0.082 (12)	-0.025 (12)	0.013 (8)
O1	0.035 (3)	0.020 (3)	0.020 (3)	-0.007 (2)	-0.001 (2)	0.002 (2)
O2	0.040 (3)	0.029 (3)	0.023 (3)	-0.001 (3)	-0.011 (3)	0.004 (2)
O3	0.040 (3)	0.029 (3)	0.020 (3)	-0.006 (3)	-0.001 (2)	0.007 (2)
O4	0.035 (3)	0.026 (3)	0.023 (3)	-0.007 (2)	-0.009 (3)	0.005 (2)
O5	0.040 (3)	0.020 (3)	0.033 (3)	0.003 (3)	0.005 (3)	-0.007 (2)
O6	0.039 (3)	0.022 (3)	0.034 (3)	0.004 (3)	0.007 (3)	0.001 (3)
O7	0.026 (3)	0.028 (3)	0.033 (3)	-0.002 (2)	0.002 (2)	-0.010 (2)
O8	0.031 (3)	0.021 (3)	0.037 (3)	0.004 (2)	0.005 (3)	0.005 (2)
O9	0.068 (4)	0.047 (4)	0.045 (4)	-0.006 (3)	-0.025 (4)	0.000 (3)
O10	0.054 (4)	0.056 (4)	0.030 (4)	0.006 (3)	-0.015 (3)	0.009 (3)
O11	0.060 (4)	0.048 (4)	0.039 (4)	-0.008 (3)	-0.009 (3)	0.013 (3)
O12	0.074 (4)	0.047 (4)	0.036 (4)	-0.019 (3)	-0.026 (3)	0.005 (3)
O14	0.063 (4)	0.033 (3)	0.031 (3)	-0.011 (3)	-0.015 (3)	0.017 (3)
O13	0.056 (4)	0.053 (4)	0.028 (4)	0.004 (3)	-0.014 (3)	0.011 (3)
O15	0.045 (4)	0.094 (6)	0.081 (5)	-0.006 (4)	0.026 (4)	0.014 (5)
O16	0.072 (5)	0.110 (7)	0.110 (7)	0.030 (5)	0.037 (5)	-0.027 (6)
O17	0.100 (6)	0.049 (4)	0.104 (7)	0.033 (4)	-0.004 (5)	-0.023 (4)
O18	0.034 (3)	0.051 (4)	0.071 (5)	-0.005 (3)	0.022 (3)	-0.004 (4)
O19	0.034 (4)	0.078 (5)	0.085 (5)	0.012 (4)	0.006 (4)	-0.035 (4)
O20	0.075 (5)	0.029 (4)	0.091 (6)	0.020 (3)	-0.025 (4)	-0.030 (4)
Ru1	0.0298 (3)	0.0166 (3)	0.0210 (3)	0.0012 (3)	0.0000 (3)	0.0018 (3)
Ru2	0.0297 (4)	0.0187 (3)	0.0217 (4)	0.0012 (3)	0.0000 (3)	0.0025 (3)

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*Geometric parameters (Å, °)*

Ru1—Ru2	2.2930 (8)	C21—O6	1.263 (8)
Ru2—C11 <sup>i</sup>	2.5608 (18)	C22—C23	1.400 (10)
C11—Ru1	2.5838 (18)	C22—C27	1.384 (10)
C11—Ru2 <sup>ii</sup>	2.5607 (18)	C23—H23	0.9300
C1—C2	1.493 (10)	C23—C24	1.401 (11)
C1—O1	1.249 (8)	C24—C25	1.395 (12)
C1—O2	1.289 (8)	C24—O15	1.357 (10)
C2—C3	1.375 (10)	C25—C26	1.411 (12)
C2—C7	1.384 (10)	C25—O16	1.341 (10)
C3—H3	0.9300	C26—C27	1.378 (11)
C3—C4	1.378 (10)	C26—O17	1.369 (10)
C4—C5	1.374 (10)	C27—H27	0.9300
C4—O9	1.367 (9)	C28—H28A	0.9600
C5—C6	1.405 (10)	C28—H28B	0.9600
C5—O10	1.354 (8)	C28—H28C	0.9600
C6—C7	1.366 (10)	C28—O15	1.421 (11)
C6—O11	1.378 (9)	C29—H29A	0.9600
C7—H7	0.9300	C29—H29B	0.9600
C8—H8A	0.9600	C29—H29C	0.9600
C8—H8B	0.9600	C29—O16	1.402 (13)
C8—H8C	0.9600	C30—H30A	0.9600
C8—O9	1.444 (9)	C30—H30B	0.9600
C9—H9A	0.9600	C30—H30C	0.9600
C9—H9B	0.9600	C30—O17	1.386 (5)
C9—H9C	0.9600	C31—C32	1.465 (10)
C9—O10	1.416 (9)	C31—O7	1.275 (8)
C10—H10A	0.9600	C31—O8	1.263 (8)
C10—H10B	0.9600	C32—C33	1.366 (10)
C10—H10C	0.9600	C32—C37	1.382 (9)
C10—O11	1.417 (9)	C33—H33	0.9300
C11—C12	1.488 (10)	C33—C34	1.357 (10)
C11—O3	1.261 (8)	C34—C35	1.398 (11)
C11—O4	1.281 (8)	C34—O18	1.366 (9)
C12—C13	1.386 (10)	C35—C36	1.380 (11)
C12—C17	1.395 (9)	C35—O19	1.376 (9)
C13—H13	0.9300	C36—C37	1.391 (10)
C13—C14	1.402 (10)	C36—O20	1.387 (9)
C14—C15	1.392 (11)	C37—H37	0.9300
C14—O12	1.364 (9)	C38—H38A	0.9600
C15—C16	1.406 (10)	C38—H38B	0.9600
C15—O13	1.393 (9)	C38—H38C	0.9600
C16—C17	1.373 (9)	C38—O18	1.446 (9)
C16—O14	1.357 (8)	C39—H39A	0.9600
C17—H17	0.9300	C39—H39B	0.9600
C18—H18A	0.9600	C39—H39C	0.9600
C18—H18B	0.9600	C39—O19	1.411 (10)

C18—H18C	0.9600	C40—H40A	0.9600
C18—O12	1.448 (9)	C40—H40B	0.9600
C19—H19A	0.9600	C40—H40C	0.9600
C19—H19B	0.9600	C40—O20	1.328 (12)
C19—H19C	0.9600	O1—Ru1	2.015 (5)
C19—O13	1.405 (9)	O2—Ru2	2.041 (5)
C20—H20A	0.9600	O3—Ru1	2.029 (5)
C20—H20B	0.9600	O4—Ru2	1.996 (5)
C20—H20C	0.9600	O5—Ru1	2.035 (5)
C20—O14	1.435 (8)	O6—Ru2	2.014 (5)
C21—C22	1.487 (10)	O7—Ru1	2.009 (5)
C21—O5	1.277 (8)	O8—Ru2	2.026 (5)
Ru2 <sup>ii</sup> —Cl1—Ru1	118.43 (7)	O15—C28—H28B	109.5
O1—C1—C2	118.1 (7)	O15—C28—H28C	109.5
O2—C1—C2	118.8 (7)	H29A—C29—H29B	109.5
O2—C1—O1	123.0 (7)	H29A—C29—H29C	109.5
C3—C2—C1	122.1 (7)	H29B—C29—H29C	109.5
C3—C2—C7	120.6 (7)	O16—C29—H29A	109.5
C7—C2—C1	116.9 (7)	O16—C29—H29B	109.5
C2—C3—H3	120.5	O16—C29—H29C	109.5
C2—C3—C4	119.0 (7)	H30A—C30—H30B	109.5
C4—C3—H3	120.5	H30A—C30—H30C	109.5
C5—C4—C3	121.7 (8)	H30B—C30—H30C	109.5
O9—C4—C3	124.7 (7)	O17—C30—H30A	109.5
O9—C4—C5	113.6 (7)	O17—C30—H30B	109.5
C4—C5—C6	118.3 (7)	O17—C30—H30C	109.5
O10—C5—C4	120.7 (7)	O7—C31—C32	117.3 (7)
O10—C5—C6	120.9 (7)	O8—C31—C32	121.0 (6)
C7—C6—C5	120.5 (7)	O8—C31—O7	121.6 (7)
O11—C6—C5	116.3 (7)	C33—C32—C31	119.6 (7)
O11—C6—C7	123.2 (7)	C33—C32—C37	119.4 (7)
C2—C7—H7	120.1	C37—C32—C31	121.0 (7)
C6—C7—C2	119.8 (8)	C32—C33—H33	119.4
C6—C7—H7	120.1	C32—C33—C34	121.2 (7)
H8A—C8—H8B	109.5	C34—C33—H33	119.4
H8A—C8—H8C	109.5	C33—C34—C35	120.1 (8)
H8B—C8—H8C	109.5	O18—C34—C33	125.3 (7)
O9—C8—H8A	109.5	O18—C34—C35	114.6 (7)
O9—C8—H8B	109.5	C36—C35—C34	119.4 (8)
O9—C8—H8C	109.5	C36—C35—O19	121.1 (8)
H9A—C9—H9B	109.5	O19—C35—C34	119.4 (8)
H9A—C9—H9C	109.5	C35—C36—C37	119.3 (8)
H9B—C9—H9C	109.5	C35—C36—O20	121.0 (8)
O10—C9—H9A	109.5	C37—C36—O20	119.7 (8)
O10—C9—H9B	109.5	C32—C37—H37	119.8
O10—C9—H9C	109.5	C36—C37—C32	120.4 (8)
H10A—C10—H10B	109.5	C36—C37—H37	119.8

H10A—C10—H10C	109.5	H38A—C38—H38B	109.5
H10B—C10—H10C	109.5	H38A—C38—H38C	109.5
O11—C10—H10A	109.5	H38B—C38—H38C	109.5
O11—C10—H10B	109.5	O18—C38—H38A	109.5
O11—C10—H10C	109.5	O18—C38—H38B	109.5
O3—C11—C12	120.0 (7)	O18—C38—H38C	109.5
O3—C11—O4	123.2 (7)	H39A—C39—H39B	109.5
O4—C11—C12	116.8 (6)	H39A—C39—H39C	109.5
C13—C12—C11	120.7 (6)	H39B—C39—H39C	109.5
C17—C12—C11	117.8 (7)	O19—C39—H39A	109.5
C17—C12—C13	121.5 (7)	O19—C39—H39B	109.5
C12—C13—H13	120.7	O19—C39—H39C	109.5
C12—C13—C14	118.7 (7)	H40A—C40—H40B	109.5
C14—C13—H13	120.7	H40A—C40—H40C	109.5
C15—C14—C13	119.4 (8)	H40B—C40—H40C	109.5
O12—C14—C13	124.2 (7)	O20—C40—H40A	109.5
O12—C14—C15	116.3 (7)	O20—C40—H40B	109.5
C14—C15—C16	121.2 (7)	O20—C40—H40C	109.5
C14—C15—O13	117.3 (7)	C1—O1—Ru1	120.9 (4)
O13—C15—C16	121.1 (7)	C1—O2—Ru2	117.6 (5)
C17—C16—C15	118.7 (7)	C11—O3—Ru1	117.7 (5)
O14—C16—C15	115.3 (7)	C11—O4—Ru2	120.2 (4)
O14—C16—C17	126.0 (7)	C21—O5—Ru1	117.6 (4)
C12—C17—C16	120.3 (8)	C21—O6—Ru2	119.3 (5)
C12—C17—H17	119.8	C31—O7—Ru1	121.4 (5)
C16—C17—H17	119.8	C31—O8—Ru2	119.2 (4)
H18A—C18—H18B	109.5	C4—O9—C8	117.3 (6)
H18A—C18—H18C	109.5	C5—O10—C9	117.6 (7)
H18B—C18—H18C	109.5	C6—O11—C10	117.9 (6)
O12—C18—H18A	109.5	C14—O12—C18	117.3 (6)
O12—C18—H18B	109.5	C16—O14—C20	115.8 (6)
O12—C18—H18C	109.5	C15—O13—C19	115.3 (6)
H19A—C19—H19B	109.5	C24—O15—C28	117.9 (8)
H19A—C19—H19C	109.5	C25—O16—C29	117.6 (9)
H19B—C19—H19C	109.5	C30—O17—C26	120.4 (9)
O13—C19—H19A	109.5	C34—O18—C38	117.3 (6)
O13—C19—H19B	109.5	C35—O19—C39	119.6 (7)
O13—C19—H19C	109.5	C40—O20—C36	119.0 (8)
H20A—C20—H20B	109.5	O1—Ru1—Cl1	89.03 (14)
H20A—C20—H20C	109.5	O1—Ru1—O3	178.32 (19)
H20B—C20—H20C	109.5	O1—Ru1—O5	89.54 (19)
O14—C20—H20A	109.5	O1—Ru1—O7	90.20 (19)
O14—C20—H20B	109.5	O1—Ru1—Ru2	88.62 (13)
O14—C20—H20C	109.5	O3—Ru1—Cl1	92.49 (14)
O5—C21—C22	117.2 (7)	O3—Ru1—Ru2	89.79 (13)
O5—C21—O6	124.4 (7)	O5—Ru1—Cl1	97.33 (14)
O6—C21—C22	118.4 (7)	O5—Ru1—O3	91.0 (2)
C23—C22—C21	118.3 (7)	O5—Ru1—Ru2	89.49 (14)

C27—C22—C21	121.6 (7)	O7—Ru1—Cl1	85.04 (14)
C27—C22—C23	120.0 (8)	O7—Ru1—O3	89.2 (2)
C22—C23—H23	120.4	O7—Ru1—O5	177.61 (19)
C24—C23—C22	119.1 (8)	O7—Ru1—Ru2	88.13 (13)
C24—C23—H23	120.4	Ru2—Ru1—Cl1	172.77 (5)
C25—C24—C23	120.9 (9)	O2—Ru2—Cl1 <sup>i</sup>	94.43 (14)
O15—C24—C23	124.2 (9)	O2—Ru2—Ru1	89.60 (13)
O15—C24—C25	114.8 (9)	O4—Ru2—Cl1 <sup>i</sup>	87.41 (14)
C26—C25—C24	118.6 (8)	O4—Ru2—O2	178.16 (19)
O16—C25—C24	119.2 (9)	O4—Ru2—O6	90.8 (2)
O16—C25—C26	122.2 (9)	O4—Ru2—O8	88.9 (2)
C25—C26—C27	120.4 (8)	O4—Ru2—Ru1	88.57 (13)
C25—C26—O17	117.4 (8)	O6—Ru2—Cl1 <sup>i</sup>	87.77 (14)
O17—C26—C27	122.2 (9)	O6—Ru2—O2	89.3 (2)
C22—C27—H27	119.6	O6—Ru2—O8	178.8 (2)
C26—C27—C22	120.8 (8)	O6—Ru2—Ru1	89.18 (14)
C26—C27—H27	119.6	O8—Ru2—Cl1 <sup>i</sup>	93.37 (14)
H28A—C28—H28B	109.5	O8—Ru2—O2	91.0 (2)
H28A—C28—H28C	109.5	O8—Ru2—Ru1	89.66 (14)
H28B—C28—H28C	109.5	Ru1—Ru2—Cl1 <sup>i</sup>	174.92 (6)
O15—C28—H28A	109.5		
Cl1—Ru1—Ru2—Cl1 <sup>i</sup>	-146.0 (6)	C31—O7—Ru1—O1	88.6 (5)
Cl1—Ru1—Ru2—O2	71.6 (4)	C31—O7—Ru1—O3	-89.8 (5)
Cl1—Ru1—Ru2—O4	-108.3 (4)	C31—O7—Ru1—O5	5 (5)
Cl1—Ru1—Ru2—O6	160.9 (4)	C31—O7—Ru1—Ru2	0.0 (5)
Cl1—Ru1—Ru2—O8	-19.4 (4)	C31—O8—Ru2—Cl1 <sup>i</sup>	176.5 (5)
C1—C2—C3—C4	-175.4 (7)	C31—O8—Ru2—O2	-89.0 (5)
C1—C2—C7—C6	175.9 (7)	C31—O8—Ru2—O4	89.2 (5)
C1—O1—Ru1—Cl1	-177.2 (5)	C31—O8—Ru2—O6	14 (10)
C1—O1—Ru1—O3	-22 (7)	C31—O8—Ru2—Ru1	0.6 (5)
C1—O1—Ru1—O5	85.5 (5)	C32—C31—O7—Ru1	-179.9 (5)
C1—O1—Ru1—O7	-92.1 (5)	C32—C31—O8—Ru2	179.6 (5)
C1—O1—Ru1—Ru2	-4.0 (5)	C32—C33—C34—C35	-2.2 (13)
C1—O2—Ru2—Cl1 <sup>i</sup>	-174.3 (5)	C32—C33—C34—O18	179.5 (7)
C1—O2—Ru2—O4	7 (7)	C33—C32—C37—C36	0.8 (12)
C1—O2—Ru2—O6	-86.6 (5)	C33—C34—C35—C36	5.0 (13)
C1—O2—Ru2—O8	92.2 (5)	C33—C34—C35—O19	-178.6 (7)
C1—O2—Ru2—Ru1	2.6 (5)	C33—C34—O18—C38	-3.7 (12)
C2—C1—O1—Ru1	-174.9 (5)	C34—C35—C36—C37	-4.8 (13)
C2—C1—O2—Ru2	175.8 (5)	C34—C35—C36—O20	175.5 (8)
C2—C3—C4—C5	-0.1 (11)	C34—C35—O19—C39	122.6 (10)
C2—C3—C4—O9	178.0 (7)	C35—C34—O18—C38	177.9 (8)
C3—C2—C7—C6	2.7 (11)	C35—C36—C37—C32	2.0 (12)
C3—C4—C5—C6	2.4 (12)	C35—C36—O20—C40	-90.2 (13)
C3—C4—C5—O10	179.3 (7)	C36—C35—O19—C39	-61.1 (12)
C3—C4—O9—C8	-12.1 (11)	C37—C32—C33—C34	-0.7 (12)
C4—C5—C6—C7	-2.2 (12)	C37—C36—O20—C40	90.1 (13)

C4—C5—C6—O11	174.3 (7)	O1—C1—C2—C3	174.3 (7)
C4—C5—O10—C9	106.1 (9)	O1—C1—C2—C7	1.2 (10)
C5—C4—O9—C8	166.2 (7)	O1—C1—O2—Ru2	-6.5 (9)
C5—C6—C7—C2	-0.3 (12)	O1—Ru1—Ru2—C11 <sup>i</sup>	142.9 (6)
C5—C6—O11—C10	-158.6 (7)	O1—Ru1—Ru2—O2	0.52 (19)
C6—C5—O10—C9	-77.1 (10)	O1—Ru1—Ru2—O4	-179.3 (2)
C7—C2—C3—C4	-2.5 (11)	O1—Ru1—Ru2—O6	89.80 (19)
C7—C6—O11—C10	17.9 (11)	O1—Ru1—Ru2—O8	-90.48 (19)
C11—C12—C13—C14	178.3 (7)	O2—C1—C2—C3	-7.8 (11)
C11—C12—C17—C16	-178.9 (7)	O2—C1—C2—C7	179.1 (7)
C11—O3—Ru1—C11	169.2 (5)	O2—C1—O1—Ru1	7.3 (10)
C11—O3—Ru1—O1	14 (7)	O3—C11—C12—C13	2.0 (11)
C11—O3—Ru1—O5	-93.4 (5)	O3—C11—C12—C17	-179.4 (7)
C11—O3—Ru1—O7	84.2 (5)	O3—C11—O4—Ru2	-8.1 (10)
C11—O3—Ru1—Ru2	-4.0 (5)	O3—Ru1—Ru2—C11 <sup>i</sup>	-37.6 (6)
C11—O4—Ru2—C11 <sup>i</sup>	-179.4 (5)	O3—Ru1—Ru2—O2	180.0 (2)
C11—O4—Ru2—O2	-1 (7)	O3—Ru1—Ru2—O4	0.1 (2)
C11—O4—Ru2—O6	92.8 (5)	O3—Ru1—Ru2—O6	-90.7 (2)
C11—O4—Ru2—O8	-86.0 (5)	O3—Ru1—Ru2—O8	89.00 (19)
C11—O4—Ru2—Ru1	3.7 (5)	O4—C11—C12—C13	-179.0 (7)
C12—C11—O3—Ru1	-173.0 (5)	O4—C11—C12—C17	-0.4 (10)
C12—C11—O4—Ru2	173.0 (5)	O4—C11—O3—Ru1	8.0 (9)
C12—C13—C14—C15	3.5 (12)	O5—C21—C22—C23	163.9 (7)
C12—C13—C14—O12	-176.1 (7)	O5—C21—C22—C27	-18.8 (11)
C13—C12—C17—C16	-0.3 (12)	O5—C21—O6—Ru2	2.2 (10)
C13—C14—C15—C16	-6.2 (12)	O5—Ru1—Ru2—C11 <sup>i</sup>	53.4 (6)
C13—C14—C15—O13	-179.4 (7)	O5—Ru1—Ru2—O2	-89.02 (19)
C13—C14—O12—C18	19.1 (12)	O5—Ru1—Ru2—O4	91.1 (2)
C14—C15—C16—C17	5.5 (12)	O5—Ru1—Ru2—O6	0.3 (2)
C14—C15—C16—O14	-173.9 (7)	O5—Ru1—Ru2—O8	180.0 (2)
C14—C15—O13—C19	-104.6 (9)	O6—C21—C22—C23	-14.8 (11)
C15—C14—O12—C18	-160.5 (8)	O6—C21—C22—C27	162.5 (7)
C15—C16—C17—C12	-2.2 (12)	O6—C21—O5—Ru1	-1.9 (9)
C15—C16—O14—C20	164.8 (7)	O7—C31—C32—C33	18.4 (11)
C16—C15—O13—C19	82.3 (10)	O7—C31—C32—C37	-161.6 (7)
C17—C12—C13—C14	-0.3 (12)	O7—C31—O8—Ru2	-0.8 (9)
C17—C16—O14—C20	-14.5 (11)	O7—Ru1—Ru2—C11 <sup>i</sup>	-126.8 (6)
C21—C22—C23—C24	-178.1 (7)	O7—Ru1—Ru2—O2	90.8 (2)
C21—C22—C27—C26	180.0 (7)	O7—Ru1—Ru2—O4	-89.1 (2)
C21—O5—Ru1—C11	-176.9 (5)	O7—Ru1—Ru2—O6	-180.0 (2)
C21—O5—Ru1—O1	-88.0 (5)	O7—Ru1—Ru2—O8	-0.2 (2)
C21—O5—Ru1—O3	90.4 (5)	O8—C31—C32—C33	-162.0 (7)
C21—O5—Ru1—O7	-4 (5)	O8—C31—C32—C37	18.1 (11)
C21—O5—Ru1—Ru2	0.6 (5)	O8—C31—O7—Ru1	0.5 (9)
C21—O6—Ru2—C11 <sup>i</sup>	-177.2 (5)	O9—C4—C5—C6	-175.9 (7)
C21—O6—Ru2—O2	88.3 (5)	O9—C4—C5—O10	1.0 (11)
C21—O6—Ru2—O4	-89.8 (5)	O10—C5—C6—C7	-179.1 (7)
C21—O6—Ru2—O8	-15 (10)	O10—C5—C6—O11	-2.5 (11)

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C21—O6—Ru2—Ru1	-1.3 (5)	O11—C6—C7—C2	-176.6 (7)
C22—C21—O5—Ru1	179.5 (5)	O12—C14—C15—C16	173.5 (7)
C22—C21—O6—Ru2	-179.2 (5)	O12—C14—C15—O13	0.3 (11)
C22—C23—C24—C25	-3.3 (14)	O14—C16—C17—C12	177.1 (7)
C22—C23—C24—O15	178.4 (8)	O13—C15—C16—C17	178.4 (7)
C23—C22—C27—C26	-2.7 (13)	O13—C15—C16—O14	-1.0 (11)
C23—C24—C25—C26	0.3 (15)	O15—C24—C25—C26	178.8 (8)
C23—C24—C25—O16	-178.0 (8)	O15—C24—C25—O16	0.5 (14)
C23—C24—O15—C28	-2.3 (14)	O16—C25—C26—C27	179.8 (9)
C24—C25—C26—C27	1.5 (14)	O16—C25—C26—O17	-1.7 (14)
C24—C25—C26—O17	-179.9 (9)	O17—C26—C27—C22	-178.8 (8)
C24—C25—O16—C29	-121.2 (12)	O18—C34—C35—C36	-176.5 (7)
C25—C24—O15—C28	179.3 (9)	O18—C34—C35—O19	-0.1 (12)
C25—C26—C27—C22	-0.4 (13)	O19—C35—C36—C37	178.8 (7)
C25—C26—O17—C30	116.6 (14)	O19—C35—C36—O20	-0.9 (13)
C26—C25—O16—C29	60.6 (15)	O20—C36—C37—C32	-178.3 (7)
C27—C22—C23—C24	4.5 (12)	Ru2 <sup>ii</sup> —Cl1—Ru1—O1	-63.82 (15)
C27—C26—O17—C30	-64.9 (16)	Ru2 <sup>ii</sup> —Cl1—Ru1—O3	116.89 (16)
C31—C32—C33—C34	179.3 (7)	Ru2 <sup>ii</sup> —Cl1—Ru1—O5	25.58 (17)
C31—C32—C37—C36	-179.2 (7)	Ru2 <sup>ii</sup> —Cl1—Ru1—O7	-154.10 (16)
C31—O7—Ru1—Cl1	177.6 (5)	Ru2 <sup>ii</sup> —Cl1—Ru1—Ru2	-134.9 (4)

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