metal-organic compounds

A tetragonal polymorph of tetra-μ_3-chlorido-tetrakis[(η^5-pentamethylcyclopentadienyl)ruthenium(II)]

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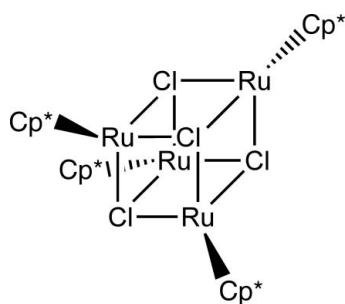Correspondence e-mail: p.jones@tu-bs.de

A new (third) polymorph of the title complex, [Ru$_4$(C$_{10}$H$_{15}$)$_4$Cl$_4$] or [Cp*Ru(μ_3-Cl)]$_4$ [Cp* = η^5-C$_5$(CH$_3$)$_5$], crystallizes in the tetragonal system, with imposed $\bar{4}$ symmetry. The complex contains a distorted cubic array of Ru and Cl atoms. The structure is an inversion twin.

Related literature

For related literature, see: Allen (2002); Fagan *et al.* (1990).

Experimental

Crystal data

[Ru$_4$(C$_{10}$H$_{15}$)$_4$Cl$_4$]	a = 12.0733 (8) Å
M_r = 1086.96	c = 14.9611 (15) Å
Tetragonal, $I\bar{4}$	V = 2180.8 (3) Å^3

Z = 2	T = 133 (2) K
Mo $K\alpha$ radiation	0.30 × 0.22 × 0.20 mm
μ = 1.63 mm^{-1}	

Data collection

Bruker SMART 1000 CCD diffractometer	13332 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1998) T_{min} = 0.530, T_{max} = 0.736	3314 independent reflections 3068 reflections with $I > 2\sigma(I)$ R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024	$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$wR(F^2)$ = 0.049	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
S = 1.07	Absolute structure: Flack (1983), 1573 Friedel pairs
3314 reflections	
115 parameters	Flack parameter: 0.43 (3)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ru—C1	2.115 (3)	Ru—C5	2.114 (2)
Ru—C2	2.118 (3)	Ru—Cl	2.5245 (6)
Ru—C3	2.122 (3)	Ru—Cl^i	2.5350 (6)
Ru—C4	2.124 (3)	Ru—Cl^{ii}	2.5427 (6)
Cl—Ru—Cl^i	82.715 (19)	Ru—Cl—Ru^{iii}	97.092 (19)
Cl—Ru—Cl^{ii}	81.533 (18)	Ru—Cl—Ru^{ii}	98.145 (18)
Cl^i—Ru—Cl^{ii}	82.354 (19)	Ru^{iii}—Cl—Ru^{ii}	96.627 (19)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2380).

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supplementary materials

A tetragonal polymorph of tetra-μ_3-chlorido-tetrakis[(η^5-pentamethylcyclopentadienyl)ruthenium(II)]

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Comment

Fagan *et al.* (1990) reported two polymorphs of the title complex (I) [Cp*Ru(μ_3-Cl)]$_4$. At 201 K the crystal is triclinic with space group $P\bar{1}$ (a = 11.281 (5), b = 11.354 (4), c = 18.846 (5) Å, α = 82.20 (2)°, β = 82.03 (3)°, γ = 65.45 (4) °; V = 2166.3 Å^3) whereas at room temperature it adopts a monoclinic cell (a = 19.040; b = 12.240; c = 18.850 Å; β = 99.38°; V = 4334.2 Å^3). Only the structure of the triclinic form was solved and refined; its Cambridge refcode (Allen, 2002) is JERTIJ.

Here we report the structure of a new, tetragonal polymorph of (I), which crystallizes in space group $I\bar{4}$ (a = b = 12.0733 (8), c = 14.9611 (15) Å; V = 2180.8 (3) Å^3). It is noteworthy that the new form has a significantly larger cell volume then the triclinic form despite the lower temperature. The tetrameric complex possesses imposed $\bar{4}$ symmetry (Fig. 1) and consists, as does the triclinic form, of a distorted cubic array of four Ru and Cl atoms, with angles at ruthenium *ca* 82° and angles at chlorine *ca* 97°. Each Ru atom in the complex adopts an 18-electron configuration in a pseudooctahedral environment. The C$_5$Me$_5$ ligand coordinates in η^5 fashion to the Ru atom with a Cp* (centroid)—Ru distance of 1.727 Å, which is slightly longer than the average Cp*—Ru distance (1.720 Å) reported by Fagan *et al.* The C2—centroid vector eclipses the bond Ru···Cl (torsion angle 2.1°). The structure of the complex is closely similar to that of the triclinic form; a least-squares fit of the Ru$_4$Cl$_4$ core for one of the many possible atom permutations gave a r.m.s. deviation of 0.019 Å. In detail, the Ru—Cl bond lengths (av. 2.534 Å) are also slightly longer than in the triclinic form (av. 2.524 Å). The Ru···Ru distances are 3.8286 (4) to Ru[ii], 3.7920 (4) Å to Ru[i] and Ru[iii], *cf.* 3.776 (2)–3.821 Å (av. 3.797 Å) in the triclinic form. The thermal parameters of the Cp* rings are normal, but were high in the triclinic form; this and the above-mentioned bond lengthening effects (presumably attributable to reduced libration) may be a result of the lower measurement temperature of the current structure.

Experimental

The reaction between the title compound and four equivalents of the lithium salt of an imidazoline-2-imine in hexane afforded the new polymorph of the ruthenium starting complex as unreacted material, dark red-brown crystals of which were obtained by re-crystallization from hexane solution at −35 °C.

Refinement

Methyl hydrogen atoms were located in a difference synthesis; the methyl groups were idealized and refined as rigid groups allowed to rotate but not tip, with C—H 0.98 Å, H—C—H 109.5°. U(H) values were fixed at $1.2U_{eq}$(C). The structure was refined as a racemic twin, with components 0.57, 0.43 (3). The twinning (Flack) parameter is based on 1573 Friedel pairs.
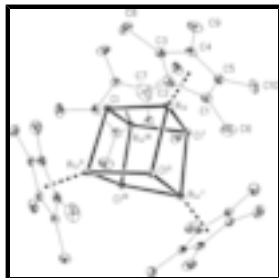
supplementary materials

Figures

Fig. 1. The molecule of the title compound in the crystal. Ellipsoids represent 30% probability levels. Symmetry operators are those of Table 1.

tetra-µ$_3$-chlorido-[tetrakis(η^5-pentamethylcyclopentadienyl)ruthenium(II)]

Crystal data

[Ru$_4$(C$_{10}$H$_{15}$)$_4$Cl$_4$]	$Z = 2$
$M_r = 1086.96$	$F_{000} = 1088$
Tetragonal, $I\overline{4}$	$D_x = 1.655$ Mg m^{-3}
$a = 12.0733$ (8) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 12.0733$ (8) Å	Cell parameters from 5126 reflections
$c = 14.9611$ (15) Å	$\theta = 2–30°$
$\alpha = 90°$	$\mu = 1.63$ mm^{-1}
$\beta = 90°$	$T = 133$ (2) K
$\gamma = 90°$	Tablet, dark red
$V = 2180.8$ (3) Å^3	$0.30 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART 1000 CCD diffractometer	3314 independent reflections
Radiation source: fine-focus sealed tube	3068 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
Detector resolution: 8.192 pixels mm^{-1}	$\theta_{max} = 30.5°$
$T = 133(2)$ K	$\theta_{min} = 2.2°$
ω and φ scans	$h = -16 \rightarrow 17$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -16 \rightarrow 17$
$T_{min} = 0.530$, $T_{max} = 0.736$	$l = -21 \rightarrow 21$
13332 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 1.4509P]$

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

$wR(F^2) = 0.049$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.07$	$\Delta\rho_{max} = 0.84$ e Å^{-3}
3314 reflections	$\Delta\rho_{min} = -0.33$ e Å^{-3}
115 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1573 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.43 (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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ru	0.418223 (15)	0.864161 (15)	0.661262 (12)	0.01407 (5)
C1	0.4531 (2)	0.7131 (2)	0.59544 (18)	0.0208 (5)
C2	0.4159 (2)	0.7947 (2)	0.53127 (18)	0.0231 (5)
C3	0.3056 (2)	0.8280 (2)	0.55638 (18)	0.0223 (5)
C4	0.2743 (2)	0.7683 (2)	0.63523 (18)	0.0220 (5)
C5	0.3659 (2)	0.69705 (19)	0.6597 (2)	0.0205 (5)
C6	0.5628 (3)	0.6547 (3)	0.5945 (2)	0.0344 (7)
H6A	0.5772	0.6228	0.6535	0.041*
H6B	0.6214	0.7077	0.5795	0.041*
H6C	0.5613	0.5955	0.5496	0.041*
C7	0.4806 (3)	0.8323 (3)	0.4508 (2)	0.0405 (8)
H7A	0.4730	0.7775	0.4029	0.049*
H7B	0.5589	0.8400	0.4669	0.049*
H7C	0.4519	0.9039	0.4303	0.049*
C8	0.2339 (3)	0.9097 (3)	0.5071 (2)	0.0447 (9)
H8A	0.1893	0.8705	0.4624	0.054*
H8B	0.2809	0.9645	0.4771	0.054*
H8C	0.1849	0.9473	0.5495	0.054*
C9	0.1638 (2)	0.7708 (3)	0.6811 (2)	0.0391 (8)
H9A	0.1291	0.8433	0.6718	0.047*
H9B	0.1739	0.7579	0.7452	0.047*
H9C	0.1161	0.7128	0.6561	0.047*
C10	0.3684 (3)	0.6195 (2)	0.7381 (2)	0.0333 (7)
H10A	0.3344	0.5488	0.7212	0.040*

H10B	0.3270	0.6521	0.7879	0.040*
H10C	0.4453	0.6069	0.7564	0.040*
Cl	0.38208 (4)	1.06982 (5)	0.67020 (3)	0.01539 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru	0.01418 (10)	0.01413 (9)	0.01390 (7)	−0.00059 (7)	−0.00012 (8)	−0.00179 (8)
C1	0.0205 (13)	0.0188 (13)	0.0230 (13)	0.0005 (10)	0.0001 (10)	−0.0097 (10)
C2	0.0288 (14)	0.0238 (14)	0.0166 (11)	−0.0085 (11)	0.0025 (10)	−0.0060 (10)
C3	0.0248 (14)	0.0214 (13)	0.0208 (12)	−0.0013 (10)	−0.0061 (10)	−0.0066 (10)
C4	0.0173 (12)	0.0229 (13)	0.0258 (13)	−0.0043 (9)	0.0012 (9)	−0.0082 (10)
C5	0.0264 (12)	0.0163 (11)	0.0188 (11)	−0.0017 (8)	−0.0010 (11)	−0.0056 (11)
C6	0.0236 (15)	0.0338 (17)	0.0459 (19)	0.0055 (12)	−0.0031 (13)	−0.0193 (14)
C7	0.060 (2)	0.0366 (18)	0.0250 (16)	−0.0154 (16)	0.0137 (15)	−0.0080 (13)
C8	0.052 (2)	0.0400 (19)	0.0420 (19)	0.0067 (16)	−0.0282 (17)	−0.0007 (16)
C9	0.0246 (15)	0.0455 (19)	0.047 (2)	−0.0093 (13)	0.0071 (13)	−0.0194 (15)
C10	0.054 (2)	0.0184 (14)	0.0277 (15)	−0.0075 (12)	−0.0030 (14)	0.0014 (11)
Cl	0.0146 (2)	0.0162 (2)	0.0154 (2)	0.00040 (17)	0.0002 (2)	0.0005 (2)

Geometric parameters (Å, °)

Ru—C1	2.115 (3)	Cl—Ru^{iii}	2.5349 (6)
Ru—C2	2.118 (3)	Cl—Ru^{ii}	2.5428 (6)
Ru—C3	2.122 (3)	C6—H6A	0.9800
Ru—C4	2.124 (3)	C6—H6B	0.9800
Ru—C5	2.114 (2)	C6—H6C	0.9800
Ru—Cl	2.5245 (6)	C7—H7A	0.9800
Ru—Cl^i	2.5350 (6)	C7—H7B	0.9800
Ru—Cl^{ii}	2.5427 (6)	C7—H7C	0.9800
C1—C5	1.439 (4)	C8—H8A	0.9800
C1—C2	1.447 (4)	C8—H8B	0.9800
C1—C6	1.500 (4)	C8—H8C	0.9800
C2—C3	1.440 (4)	C9—H9A	0.9800
C2—C7	1.504 (4)	C9—H9B	0.9800
C3—C4	1.433 (4)	C9—H9C	0.9800
C3—C8	1.506 (4)	C10—H10A	0.9800
C4—C5	1.448 (4)	C10—H10B	0.9800
C4—C9	1.500 (4)	C10—H10C	0.9800
C5—C10	1.502 (4)		
C5—Ru—C1	39.77 (10)	C3—C4—C5	107.7 (2)
C5—Ru—C2	66.93 (11)	C3—C4—C9	127.0 (3)
C1—Ru—C2	39.99 (11)	C5—C4—C9	125.1 (3)
C5—Ru—C3	66.64 (10)	C3—C4—Ru	70.17 (15)
C1—Ru—C3	66.76 (11)	C5—C4—Ru	69.66 (14)
C2—Ru—C3	39.73 (11)	C9—C4—Ru	129.3 (2)
C5—Ru—C4	39.95 (10)	C1—C5—C4	108.1 (2)
C1—Ru—C4	66.90 (10)	C1—C5—C10	126.2 (3)

C2—Ru—C4	66.75 (10)	C4—C5—C10	125.7 (3)
C3—Ru—C4	39.45 (11)	C1—C5—Ru	70.13 (14)
C5—Ru—Cl	152.55 (7)	C4—C5—Ru	70.39 (14)
C1—Ru—Cl	155.12 (8)	C10—C5—Ru	125.47 (19)
C2—Ru—Cl	115.82 (8)	Ru—Cl—Ru^{iii}	97.092 (19)
C3—Ru—Cl	97.53 (7)	Ru—Cl—Ru^{ii}	98.145 (18)
C4—Ru—Cl	113.84 (8)	Ru^{iii}—Cl—Ru^{ii}	96.627 (19)
C5—Ru—Cl^{i}	96.30 (8)	C1—C6—H6A	109.5
C1—Ru—Cl^{i}	121.70 (8)	C1—C6—H6B	109.5
C2—Ru—Cl^{i}	161.43 (8)	H6A—C6—H6B	109.5
C3—Ru—Cl^{i}	142.17 (8)	C1—C6—H6C	109.5
C4—Ru—Cl^{i}	105.99 (7)	H6A—C6—H6C	109.5
Cl—Ru—Cl^{i}	82.715 (19)	H6B—C6—H6C	109.5
C5—Ru—Cl^{ii}	125.67 (7)	C2—C7—H7A	109.5
C1—Ru—Cl^{ii}	96.09 (8)	C2—C7—H7B	109.5
C2—Ru—Cl^{ii}	100.65 (7)	H7A—C7—H7B	109.5
C3—Ru—Cl^{ii}	135.31 (8)	C2—C7—H7C	109.5
C4—Ru—Cl^{ii}	162.99 (7)	H7A—C7—H7C	109.5
Cl—Ru—Cl^{ii}	81.533 (18)	H7B—C7—H7C	109.5
Cl^{i}—Ru—Cl^{ii}	82.354 (19)	C3—C8—H8A	109.5
C5—C1—C2	107.9 (2)	C3—C8—H8B	109.5
C5—C1—C6	126.1 (3)	H8A—C8—H8B	109.5
C2—C1—C6	126.0 (3)	C3—C8—H8C	109.5
C5—C1—Ru	70.10 (13)	H8A—C8—H8C	109.5
C2—C1—Ru	70.12 (15)	H8B—C8—H8C	109.5
C6—C1—Ru	125.85 (19)	C4—C9—H9A	109.5
C3—C2—C1	107.6 (2)	C4—C9—H9B	109.5
C3—C2—C7	127.2 (3)	H9A—C9—H9B	109.5
C1—C2—C7	125.1 (3)	C4—C9—H9C	109.5
C3—C2—Ru	70.27 (15)	H9A—C9—H9C	109.5
C1—C2—Ru	69.89 (14)	H9B—C9—H9C	109.5
C7—C2—Ru	127.5 (2)	C5—C10—H10A	109.5
C4—C3—C2	108.6 (2)	C5—C10—H10B	109.5
C4—C3—C8	125.5 (3)	H10A—C10—H10B	109.5
C2—C3—C8	125.9 (3)	C5—C10—H10C	109.5
C4—C3—Ru	70.37 (15)	H10A—C10—H10C	109.5
C2—C3—Ru	70.00 (15)	H10B—C10—H10C	109.5
C8—C3—Ru	126.5 (2)		
C2—Ru—C1—C5	−118.6 (2)	Ru—C3—C4—C5	−59.79 (17)
C3—Ru—C1—C5	−80.87 (17)	C2—C3—C4—C9	−175.4 (3)
C4—Ru—C1—C5	−37.79 (16)	C8—C3—C4—C9	3.3 (4)
Cl—Ru—C1—C5	−134.95 (17)	Ru—C3—C4—C9	124.8 (3)
Cl^{i}—Ru—C1—C5	57.29 (17)	C2—C3—C4—Ru	59.79 (18)
Cl^{ii}—Ru—C1—C5	142.05 (14)	C8—C3—C4—Ru	−121.5 (3)
C5—Ru—C1—C2	118.6 (2)	C5—Ru—C4—C3	−118.6 (2)

supplementary materials

C3—Ru—C1—C2	37.76 (16)	C1—Ru—C4—C3	−80.99 (17)
C4—Ru—C1—C2	80.84 (17)	C2—Ru—C4—C3	−37.32 (15)
Cl—Ru—C1—C2	−16.3 (3)	Cl—Ru—C4—C3	71.86 (15)
Cl^i—Ru—C1—C2	175.93 (12)	Cl^i—Ru—C4—C3	160.85 (13)
Cl^{ii}—Ru—C1—C2	−99.32 (14)	Cl^{ii}—Ru—C4—C3	−81.5 (3)
C5—Ru—C1—C6	−120.8 (3)	C1—Ru—C4—C5	37.62 (16)
C2—Ru—C1—C6	120.6 (3)	C2—Ru—C4—C5	81.29 (17)
C3—Ru—C1—C6	158.4 (3)	C3—Ru—C4—C5	118.6 (2)
C4—Ru—C1—C6	−158.6 (3)	Cl—Ru—C4—C5	−169.53 (13)
Cl—Ru—C1—C6	104.3 (3)	Cl^i—Ru—C4—C5	−80.54 (15)
Cl^i—Ru—C1—C6	−63.5 (3)	Cl^{ii}—Ru—C4—C5	37.1 (4)
Cl^{ii}—Ru—C1—C6	21.3 (3)	C5—Ru—C4—C9	119.3 (4)
C5—C1—C2—C3	−0.3 (3)	C1—Ru—C4—C9	157.0 (3)
C6—C1—C2—C3	179.1 (2)	C2—Ru—C4—C9	−159.4 (3)
Ru—C1—C2—C3	−60.42 (18)	C3—Ru—C4—C9	−122.1 (3)
C5—C1—C2—C7	−177.5 (3)	Cl—Ru—C4—C9	−50.2 (3)
C6—C1—C2—C7	1.9 (4)	Cl^i—Ru—C4—C9	38.8 (3)
Ru—C1—C2—C7	122.3 (3)	Cl^{ii}—Ru—C4—C9	156.4 (2)
C5—C1—C2—Ru	60.17 (17)	C2—C1—C5—C4	0.3 (3)
C6—C1—C2—Ru	−120.5 (3)	C6—C1—C5—C4	−179.1 (2)
C5—Ru—C2—C3	80.69 (16)	Ru—C1—C5—C4	60.43 (17)
C1—Ru—C2—C3	118.3 (2)	C2—C1—C5—C10	179.8 (2)
C4—Ru—C2—C3	37.07 (16)	C6—C1—C5—C10	0.4 (4)
Cl—Ru—C2—C3	−69.24 (15)	Ru—C1—C5—C10	−120.0 (3)
Cl^i—Ru—C2—C3	107.4 (2)	C2—C1—C5—Ru	−60.18 (17)
Cl^{ii}—Ru—C2—C3	−154.91 (14)	C6—C1—C5—Ru	120.5 (3)
C5—Ru—C2—C1	−37.61 (15)	C3—C4—C5—C1	−0.2 (3)
C3—Ru—C2—C1	−118.3 (2)	C9—C4—C5—C1	175.4 (2)
C4—Ru—C2—C1	−81.24 (17)	Ru—C4—C5—C1	−60.27 (17)
Cl—Ru—C2—C1	172.45 (13)	C3—C4—C5—C10	−179.7 (2)
Cl^i—Ru—C2—C1	−10.9 (3)	C9—C4—C5—C10	−4.2 (4)
Cl^{ii}—Ru—C2—C1	86.78 (15)	Ru—C4—C5—C10	120.2 (3)
C5—Ru—C2—C7	−157.0 (3)	C3—C4—C5—Ru	60.12 (18)
C1—Ru—C2—C7	−119.4 (4)	C9—C4—C5—Ru	−124.4 (3)
C3—Ru—C2—C7	122.3 (3)	C2—Ru—C5—C1	37.81 (16)
C4—Ru—C2—C7	159.3 (3)	C3—Ru—C5—C1	81.21 (18)
Cl—Ru—C2—C7	53.0 (3)	C4—Ru—C5—C1	118.6 (2)
Cl^i—Ru—C2—C7	−130.4 (3)	Cl—Ru—C5—C1	139.76 (16)
Cl^{ii}—Ru—C2—C7	−32.6 (3)	Cl^i—Ru—C5—C1	−133.92 (15)
C1—C2—C3—C4	0.2 (3)	Cl^{ii}—Ru—C5—C1	−48.83 (18)
C7—C2—C3—C4	177.3 (3)	C1—Ru—C5—C4	−118.6 (2)
Ru—C2—C3—C4	−60.02 (18)	C2—Ru—C5—C4	−80.82 (17)
C1—C2—C3—C8	−178.6 (3)	C3—Ru—C5—C4	−37.42 (16)
C7—C2—C3—C8	−1.4 (5)	Cl—Ru—C5—C4	21.1 (3)
Ru—C2—C3—C8	121.3 (3)	Cl^i—Ru—C5—C4	107.45 (15)
C1—C2—C3—Ru	60.18 (18)	Cl^{ii}—Ru—C5—C4	−167.46 (12)

C7—C2—C3—Ru	−122.6 (3)	C1—Ru—C5—C10	121.0 (3)
C5—Ru—C3—C4	37.88 (15)	C2—Ru—C5—C10	158.8 (3)
C1—Ru—C3—C4	81.36 (17)	C3—Ru—C5—C10	−157.8 (3)
C2—Ru—C3—C4	119.4 (2)	C4—Ru—C5—C10	−120.4 (3)
Cl—Ru—C3—C4	−118.75 (14)	Cl—Ru—C5—C10	−99.3 (3)
Cl^i—Ru—C3—C4	−30.9 (2)	Cl^i—Ru—C5—C10	−13.0 (2)
Cl^{ii}—Ru—C3—C4	155.70 (12)	Cl^{ii}—Ru—C5—C10	72.1 (3)
C5—Ru—C3—C2	−81.48 (16)	C5—Ru—Cl—Ru^{iii}	81.26 (18)
C1—Ru—C3—C2	−38.00 (16)	C1—Ru—Cl—Ru^{iii}	−177.91 (18)
C4—Ru—C3—C2	−119.4 (2)	C2—Ru—Cl—Ru^{iii}	170.52 (8)
Cl—Ru—C3—C2	121.89 (14)	C3—Ru—Cl—Ru^{iii}	133.45 (8)
Cl^i—Ru—C3—C2	−150.30 (13)	C4—Ru—Cl—Ru^{iii}	95.92 (8)
Cl^{ii}—Ru—C3—C2	36.34 (19)	Cl^i—Ru—Cl—Ru^{iii}	−8.388 (18)
C5—Ru—C3—C8	158.1 (3)	Cl^{ii}—Ru—Cl—Ru^{iii}	−91.693 (16)
C1—Ru—C3—C8	−158.4 (3)	C5—Ru—Cl—Ru^{ii}	179.04 (17)
C2—Ru—C3—C8	−120.4 (4)	C1—Ru—Cl—Ru^{ii}	−80.13 (18)
C4—Ru—C3—C8	120.2 (3)	C2—Ru—Cl—Ru^{ii}	−91.70 (8)
Cl—Ru—C3—C8	1.5 (3)	C3—Ru—Cl—Ru^{ii}	−128.78 (8)
Cl^i—Ru—C3—C8	89.3 (3)	C4—Ru—Cl—Ru^{ii}	−166.30 (8)
Cl^{ii}—Ru—C3—C8	−84.1 (3)	Cl^i—Ru—Cl—Ru^{ii}	89.387 (18)
C2—C3—C4—C5	0.0 (3)	Cl^{ii}—Ru—Cl—Ru^{ii}	6.08 (2)
C8—C3—C4—C5	178.7 (3)		

Symmetry codes: (i) −y+3/2, x+1/2, −z+3/2; (ii) −x+1, −y+2, z; (iii) y−1/2, −x+3/2, −z+3/2.

Fig. 1