

Di- μ_2 -chlorido-bis[chlorido(η^6 -hexamethylbenzene)ruthenium(II)]

Yunuem González-Torres, Noel Espinosa-Jalapa, Simón Hernández-Ortega,* Ronan Le Lagadec and David Morales-Morales

Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, México 04510, Mexico

Correspondence e-mail: simonho@unam.mx

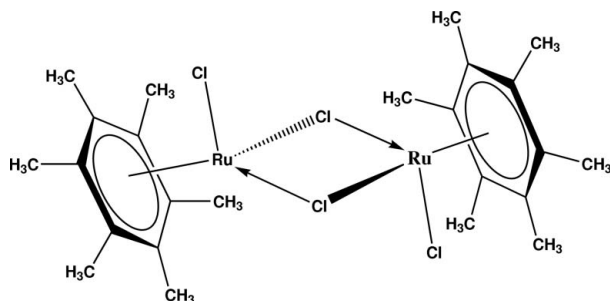
Received 29 September 2009; accepted 8 October 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.033; wR factor = 0.063; data-to-parameter ratio = 16.2.

Dimeric molecules of the title compound, $[\text{Ru}_2\text{Cl}_4(\text{C}_{12}\text{H}_{18})_2]$, are located on a crystallographic centre of inversion with one molecule in the asymmetric unit. The hexamethylbenzene rings are in an η^6 -coordination to the ruthenium centres, which are bridged by two chloride ligands. In addition, the ruthenium centres are bonded to another chloride ligand. The aromatic rings and the Ru_2Cl_2 four-membered ring enclose a dihedral angle of $55.85(6)^\circ$.

Related literature

For the properties and potential applications of half-sandwich ruthenium (II) complexes, see: Le Bozec *et al.* (1989); Leyva *et al.* (2007); Ryabov *et al.* (2001). For our work on the synthesis and catalytic applications of different ruthenium-arene complexes, see: Cerón-Camacho *et al.* (2006). For the synthesis, see: Bennett *et al.* (1982).



Experimental

Crystal data

$[\text{Ru}_2\text{Cl}_4(\text{C}_{12}\text{H}_{18})_2]$
 $M_r = 668.47$
 Monoclinic, $P2_1/n$
 $a = 8.9122(15)$ Å
 $b = 8.5192(15)$ Å
 $c = 16.642(3)$ Å
 $\beta = 97.084(3)^\circ$

$V = 1253.9(4)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.64$ mm⁻¹
 $T = 298$ K
 $0.23 \times 0.09 \times 0.05$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1999)
 $T_{\min} = 0.780$, $T_{\max} = 0.924$

10027 measured reflections
 2297 independent reflections
 1795 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.063$
 $S = 0.90$
 2297 reflections

142 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); 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.

The financial support of this research by CONACYT (F58692, 57556) and DGAPA-UNAM (IN227008, IN205209) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5080).

References

- Bennett, M. A., Huang, T. N., Matheson, T. W. & Smith, A. K. (1982). *Inorg. Synth.* **21**, 74–78.
 Bruker (1999). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Cerón-Camacho, R., Gómez-Benítez, V., Le Lagadec, R., Morales-Morales, D. & Toscano, R. A. (2006). *J. Mol. Catal. A*, **247**, 124–129.
 Le Bozec, H., Touchard, D. & Dixneuf, P. H. (1989). *Adv. Organomet. Chem.* **29**, 163–247.
 Leyva, L., Sirlin, C., Rubio, L., Franco, C., Le Lagadec, R., Bischoff, P., Gaidon, C., Loeffler, J.-P. & Pfeffer, M. (2007). *Eur. J. Inorg. Chem.* pp. 3055–3066.
 Ryabov, A. D., Sukharev, V. S., Alexandrova, L., Le Lagadec, R. & Pfeffer, M. (2001). *Inorg. Chem.* **40**, 6529–6532.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2009). E65, m1369 [doi:10.1107/S1600536809041154]

Di- μ_2 -chlorido-bis[chlorido(η^6 -hexamethylbenzene)ruthenium(II)]

Y. González-Torres, N. Espinosa-Jalapa, S. Hernández-Ortega, R. Le Lagadec and D. Morales-Morales

Comment

For decades, arene ruthenium complexes have played an important role in organometallic chemistry as fundamental precursors for the synthesis of a plethora of species. This is particularly true for the synthesis of half sandwich ruthenium (II) complexes, species that have received considerable attention owing to their potential catalytic properties (Le Bozec *et al.*, 1989), interesting anti-tumor and anti-carcinogenic activity (Leyva *et al.*, 2007) and most recently for their potential applications in chemical and biological sensors (Ryabov, *et al.*, 2001). Thus, given our continuous interest in the synthesis and catalytic applications of different ruthenium arene complexes (Cerón-Camacho *et al.*, 2006) we determined the crystal structure of the title compound.

The asymmetric unit of the title compound consists of a half molecule, which is completed with a symmetry operation of $1 - x, 1 - y, 1 - z$. The complex exhibits a typical η^6 -arene coordination of the hexamethyl fragment to the ruthenium centres which are bridged by two chloro ligands. The coordination sphere of the Ru centres is completed by another chloro ligand. The aromatic rings and the Ru₂Cl₂ four-membered ring enclose a dihedral angle of 55.85 (6)°.

Experimental

The title compound was prepared according to the procedure reported by Bennett *et al.* (1982). The spectroscopic analysis agreed with that reported in the same reference.

Refinement

H atoms were placed in geometrically idealized positions with C-H = 0.96 Å and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ and refined using the riding model. The methyl groups were allowed to rotate but not to tip.

Figures

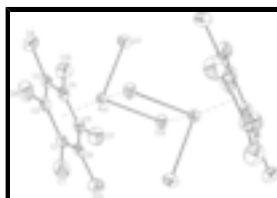


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms omitted.

Di- μ -chlorido-bis[chlorido(η^6 -hexamethylbenzene)ruthenium(II)]

Crystal data

[Ru ₂ Cl ₄ (C ₁₂ H ₁₈) ₂]	$F_{000} = 672$
$M_r = 668.47$	$D_x = 1.771 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2yn	Cell parameters from 4016 reflections
$a = 8.9122 (15) \text{ \AA}$	$\theta = 2.5\text{--}25.3^\circ$
$b = 8.5192 (15) \text{ \AA}$	$\mu = 1.64 \text{ mm}^{-1}$
$c = 16.642 (3) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 97.084 (3)^\circ$	Prism, red
$V = 1253.9 (4) \text{ \AA}^3$	$0.23 \times 0.09 \times 0.05 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2297 independent reflections
Radiation source: fine-focus sealed tube	1795 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.065$
Detector resolution: $0.83 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 25.4^\circ$
$T = 298 \text{ K}$	$\theta_{\text{min}} = 2.5^\circ$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$k = -10 \rightarrow 10$
$T_{\text{min}} = 0.780$, $T_{\text{max}} = 0.924$	$l = -20 \rightarrow 19$
10027 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2]$
$S = 0.90$	where $P = (F_o^2 + 2F_c^2)/3$
2297 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
142 parameters	$\Delta\rho_{\text{max}} = 0.48 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
	Extinction correction: none

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ru1	0.37378 (4)	0.37262 (4)	0.55348 (2)	0.02300 (11)
C11	0.24729 (13)	0.30866 (15)	0.42186 (7)	0.0382 (3)
C12	0.61218 (11)	0.35592 (12)	0.49415 (6)	0.0297 (3)
C1	0.4006 (5)	0.4464 (5)	0.6809 (2)	0.0316 (11)
C2	0.2421 (5)	0.4425 (5)	0.6495 (2)	0.0293 (10)
C3	0.1792 (5)	0.3056 (5)	0.6121 (2)	0.0281 (10)
C4	0.2721 (5)	0.1702 (5)	0.6053 (3)	0.0312 (11)
C5	0.4287 (5)	0.1741 (5)	0.6343 (3)	0.0341 (11)
C6	0.4913 (5)	0.3142 (6)	0.6727 (2)	0.0325 (11)
C7	0.4686 (6)	0.5943 (6)	0.7198 (3)	0.0524 (15)
H7A	0.3892	0.6661	0.7287	0.063*
H7B	0.5335	0.6420	0.6849	0.063*
H7C	0.5263	0.5688	0.7707	0.063*
C8	0.1465 (5)	0.5866 (5)	0.6552 (3)	0.0458 (13)
H8A	0.1976	0.6762	0.6365	0.055*
H8B	0.1297	0.6027	0.7105	0.055*
H8C	0.0512	0.5729	0.6222	0.055*
C9	0.0143 (5)	0.2997 (6)	0.5765 (3)	0.0451 (13)
H9A	-0.0293	0.4025	0.5784	0.054*
H9B	-0.0391	0.2280	0.6073	0.054*
H9C	0.0068	0.2649	0.5213	0.054*
C10	0.2020 (6)	0.0244 (5)	0.5645 (3)	0.0504 (14)
H10A	0.2759	-0.0580	0.5677	0.060*
H10B	0.1680	0.0470	0.5087	0.060*
H10C	0.1177	-0.0082	0.5911	0.060*
C11	0.5297 (6)	0.0355 (6)	0.6247 (3)	0.0563 (15)
H11A	0.5450	-0.0223	0.6745	0.068*
H11B	0.6254	0.0718	0.6110	0.068*
H11C	0.4832	-0.0313	0.5823	0.068*
C12	0.6585 (5)	0.3210 (6)	0.7036 (3)	0.0537 (15)
H12A	0.6984	0.4212	0.6905	0.064*
H12B	0.7106	0.2392	0.6786	0.064*
H12C	0.6722	0.3069	0.7613	0.064*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02306 (18)	0.02546 (19)	0.02091 (18)	0.00141 (17)	0.00441 (13)	0.00103 (17)
C11	0.0363 (7)	0.0503 (8)	0.0268 (6)	-0.0021 (6)	-0.0011 (5)	-0.0047 (5)
C12	0.0296 (6)	0.0288 (6)	0.0324 (6)	0.0053 (5)	0.0104 (5)	0.0030 (5)
C1	0.036 (3)	0.042 (3)	0.018 (2)	-0.008 (2)	0.008 (2)	-0.002 (2)
C2	0.033 (3)	0.035 (3)	0.022 (2)	0.007 (2)	0.012 (2)	0.004 (2)
C3	0.027 (2)	0.036 (3)	0.023 (2)	0.000 (2)	0.0078 (19)	0.007 (2)
C4	0.038 (3)	0.029 (3)	0.028 (2)	-0.003 (2)	0.009 (2)	0.006 (2)
C5	0.040 (3)	0.034 (3)	0.030 (3)	0.004 (2)	0.011 (2)	0.010 (2)
C6	0.032 (3)	0.048 (3)	0.018 (2)	0.003 (2)	0.005 (2)	0.011 (2)
C7	0.055 (3)	0.064 (4)	0.040 (3)	-0.014 (3)	0.013 (3)	-0.017 (3)
C8	0.055 (3)	0.040 (3)	0.045 (3)	0.015 (3)	0.018 (3)	-0.006 (2)
C9	0.028 (3)	0.061 (3)	0.047 (3)	-0.005 (3)	0.004 (2)	0.004 (3)
C10	0.055 (3)	0.035 (3)	0.062 (4)	-0.005 (3)	0.010 (3)	-0.003 (3)
C11	0.061 (4)	0.048 (3)	0.061 (4)	0.018 (3)	0.012 (3)	0.010 (3)
C12	0.036 (3)	0.081 (4)	0.042 (3)	0.004 (3)	-0.003 (2)	0.014 (3)

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

Ru1—C3	2.168 (4)	C5—C11	1.505 (6)
Ru1—C4	2.175 (4)	C6—C12	1.516 (6)
Ru1—C5	2.179 (4)	C7—H7A	0.9600
Ru1—C2	2.179 (4)	C7—H7B	0.9600
Ru1—C6	2.184 (4)	C7—H7C	0.9600
Ru1—C1	2.196 (4)	C8—H8A	0.9600
Ru1—C11	2.3993 (12)	C8—H8B	0.9600
Ru1—C12 ⁱ	2.4528 (11)	C8—H8C	0.9600
Ru1—C12	2.4549 (11)	C9—H9A	0.9600
C12—Ru1 ⁱ	2.4528 (11)	C9—H9B	0.9600
C1—C6	1.403 (6)	C9—H9C	0.9600
C1—C2	1.445 (6)	C10—H10A	0.9600
C1—C7	1.509 (6)	C10—H10B	0.9600
C2—C3	1.406 (6)	C10—H10C	0.9600
C2—C8	1.504 (5)	C11—H11A	0.9600
C3—C4	1.432 (6)	C11—H11B	0.9600
C3—C9	1.516 (6)	C11—H11C	0.9600
C4—C5	1.420 (6)	C12—H12A	0.9600
C4—C10	1.513 (6)	C12—H12B	0.9600
C5—C6	1.435 (6)	C12—H12C	0.9600
C3—Ru1—C4	38.51 (15)	C5—C4—C3	120.5 (4)
C3—Ru1—C5	69.46 (16)	C5—C4—C10	120.4 (4)
C4—Ru1—C5	38.06 (15)	C3—C4—C10	119.1 (4)
C3—Ru1—C2	37.75 (15)	C5—C4—Ru1	71.1 (2)
C4—Ru1—C2	68.75 (16)	C3—C4—Ru1	70.5 (2)
C5—Ru1—C2	81.93 (16)	C10—C4—Ru1	129.9 (3)

C3—Ru1—C6	81.49 (16)	C4—C5—C6	118.9 (4)
C4—Ru1—C6	68.64 (16)	C4—C5—C11	121.4 (4)
C5—Ru1—C6	38.39 (16)	C6—C5—C11	119.7 (4)
C2—Ru1—C6	68.72 (16)	C4—C5—Ru1	70.8 (2)
C3—Ru1—C1	68.85 (16)	C6—C5—Ru1	71.0 (2)
C4—Ru1—C1	81.11 (16)	C11—C5—Ru1	129.4 (3)
C5—Ru1—C1	68.71 (17)	C1—C6—C5	120.9 (4)
C2—Ru1—C1	38.56 (16)	C1—C6—C12	119.4 (4)
C6—Ru1—C1	37.35 (16)	C5—C6—C12	119.7 (4)
C3—Ru1—C11	92.23 (12)	C1—C6—Ru1	71.8 (2)
C4—Ru1—C11	90.57 (12)	C5—C6—Ru1	70.6 (2)
C5—Ru1—C11	115.57 (13)	C12—C6—Ru1	129.8 (3)
C2—Ru1—C11	119.79 (12)	C1—C7—H7A	109.5
C6—Ru1—C11	153.69 (13)	C1—C7—H7B	109.5
C1—Ru1—C11	158.35 (12)	H7A—C7—H7B	109.5
C3—Ru1—C12 ⁱ	117.98 (12)	C1—C7—H7C	109.5
C4—Ru1—C12 ⁱ	156.34 (12)	H7A—C7—H7C	109.5
C5—Ru1—C12 ⁱ	156.20 (13)	H7B—C7—H7C	109.5
C2—Ru1—C12 ⁱ	91.89 (12)	C2—C8—H8A	109.5
C6—Ru1—C12 ⁱ	118.07 (13)	C2—C8—H8B	109.5
C1—Ru1—C12 ⁱ	92.19 (12)	H8A—C8—H8B	109.5
C11—Ru1—C12 ⁱ	87.48 (4)	C2—C8—H8C	109.5
C3—Ru1—C12	160.99 (12)	H8A—C8—H8C	109.5
C4—Ru1—C12	122.48 (12)	H8B—C8—H8C	109.5
C5—Ru1—C12	93.65 (12)	C3—C9—H9A	109.5
C2—Ru1—C12	151.86 (12)	C3—C9—H9B	109.5
C6—Ru1—C12	90.59 (12)	H9A—C9—H9B	109.5
C1—Ru1—C12	114.09 (12)	C3—C9—H9C	109.5
C11—Ru1—C12	87.26 (4)	H9A—C9—H9C	109.5
C12 ⁱ —Ru1—C12	81.00 (4)	H9B—C9—H9C	109.5
Ru1 ⁱ —C12—Ru1	99.00 (4)	C4—C10—H10A	109.5
C6—C1—C2	119.7 (4)	C4—C10—H10B	109.5
C6—C1—C7	120.4 (4)	H10A—C10—H10B	109.5
C2—C1—C7	119.8 (4)	C4—C10—H10C	109.5
C6—C1—Ru1	70.9 (2)	H10A—C10—H10C	109.5
C2—C1—Ru1	70.1 (2)	H10B—C10—H10C	109.5
C7—C1—Ru1	130.1 (3)	C5—C11—H11A	109.5
C3—C2—C1	119.8 (4)	C5—C11—H11B	109.5
C3—C2—C8	120.5 (4)	H11A—C11—H11B	109.5
C1—C2—C8	119.7 (4)	C5—C11—H11C	109.5
C3—C2—Ru1	70.7 (2)	H11A—C11—H11C	109.5
C1—C2—Ru1	71.3 (2)	H11B—C11—H11C	109.5
C8—C2—Ru1	129.0 (3)	C6—C12—H12A	109.5
C2—C3—C4	120.0 (4)	C6—C12—H12B	109.5
C2—C3—C9	121.0 (4)	H12A—C12—H12B	109.5
C4—C3—C9	119.0 (4)	C6—C12—H12C	109.5
C2—C3—Ru1	71.6 (2)	H12A—C12—H12C	109.5

supplementary materials

C4—C3—Ru1	71.0 (2)	H12B—C12—H12C	109.5
C9—C3—Ru1	128.6 (3)		
C3—Ru1—C12—Ru1 ⁱ	176.8 (4)	C9—C3—C4—C10	-1.3 (6)
C4—Ru1—C12—Ru1 ⁱ	176.81 (14)	Ru1—C3—C4—C10	-125.6 (4)
C5—Ru1—C12—Ru1 ⁱ	-156.66 (13)	C2—C3—C4—Ru1	-54.2 (3)
C2—Ru1—C12—Ru1 ⁱ	-77.0 (2)	C9—C3—C4—Ru1	124.3 (4)
C6—Ru1—C12—Ru1 ⁱ	-118.35 (13)	C3—Ru1—C4—C5	-133.7 (4)
C1—Ru1—C12—Ru1 ⁱ	-88.37 (14)	C2—Ru1—C4—C5	-104.6 (3)
C11—Ru1—C12—Ru1 ⁱ	87.88 (4)	C6—Ru1—C4—C5	-30.0 (3)
C12 ⁱ —Ru1—C12—Ru1 ⁱ	0.0	C1—Ru1—C4—C5	-66.6 (3)
C3—Ru1—C1—C6	104.2 (3)	C11—Ru1—C4—C5	133.4 (2)
C4—Ru1—C1—C6	66.3 (3)	C12 ⁱ —Ru1—C4—C5	-141.6 (3)
C5—Ru1—C1—C6	28.9 (3)	C12—Ru1—C4—C5	46.3 (3)
C2—Ru1—C1—C6	133.2 (4)	C5—Ru1—C4—C3	133.7 (4)
C11—Ru1—C1—C6	134.7 (3)	C2—Ru1—C4—C3	29.1 (2)
C12 ⁱ —Ru1—C1—C6	-136.6 (2)	C6—Ru1—C4—C3	103.7 (3)
C12—Ru1—C1—C6	-55.4 (3)	C1—Ru1—C4—C3	67.1 (3)
C3—Ru1—C1—C2	-29.0 (2)	C11—Ru1—C4—C3	-92.9 (2)
C4—Ru1—C1—C2	-66.9 (3)	C12 ⁱ —Ru1—C4—C3	-7.8 (5)
C5—Ru1—C1—C2	-104.3 (3)	C12—Ru1—C4—C3	-180.0 (2)
C6—Ru1—C1—C2	-133.2 (4)	C3—Ru1—C4—C10	112.1 (5)
C11—Ru1—C1—C2	1.6 (5)	C5—Ru1—C4—C10	-114.2 (5)
C12 ⁱ —Ru1—C1—C2	90.3 (2)	C2—Ru1—C4—C10	141.1 (5)
C12—Ru1—C1—C2	171.4 (2)	C6—Ru1—C4—C10	-144.3 (5)
C3—Ru1—C1—C7	-141.7 (5)	C1—Ru1—C4—C10	179.1 (4)
C4—Ru1—C1—C7	-179.6 (5)	C11—Ru1—C4—C10	19.2 (4)
C5—Ru1—C1—C7	143.0 (5)	C12 ⁱ —Ru1—C4—C10	104.2 (4)
C2—Ru1—C1—C7	-112.7 (5)	C12—Ru1—C4—C10	-67.9 (4)
C6—Ru1—C1—C7	114.1 (5)	C3—C4—C5—C6	1.9 (6)
C11—Ru1—C1—C7	-111.1 (4)	C10—C4—C5—C6	-180.0 (4)
C12 ⁱ —Ru1—C1—C7	-22.4 (4)	Ru1—C4—C5—C6	54.2 (4)
C12—Ru1—C1—C7	58.7 (5)	C3—C4—C5—C11	-177.4 (4)
C6—C1—C2—C3	0.9 (6)	C10—C4—C5—C11	0.7 (6)
C7—C1—C2—C3	179.0 (4)	Ru1—C4—C5—C11	-125.1 (4)
Ru1—C1—C2—C3	53.4 (3)	C3—C4—C5—Ru1	-52.3 (3)
C6—C1—C2—C8	-177.4 (4)	C10—C4—C5—Ru1	125.9 (4)
C7—C1—C2—C8	0.7 (6)	C3—Ru1—C5—C4	28.7 (3)
Ru1—C1—C2—C8	-124.9 (4)	C2—Ru1—C5—C4	65.6 (3)
C6—C1—C2—Ru1	-52.5 (3)	C6—Ru1—C5—C4	131.3 (4)
C7—C1—C2—Ru1	125.6 (4)	C1—Ru1—C5—C4	103.2 (3)
C4—Ru1—C2—C3	-29.6 (2)	C11—Ru1—C5—C4	-53.6 (3)
C5—Ru1—C2—C3	-66.7 (3)	C12 ⁱ —Ru1—C5—C4	141.8 (3)
C6—Ru1—C2—C3	-104.1 (3)	C12—Ru1—C5—C4	-142.3 (2)
C1—Ru1—C2—C3	-132.4 (4)	C3—Ru1—C5—C6	-102.6 (3)
C11—Ru1—C2—C3	48.2 (3)	C4—Ru1—C5—C6	-131.3 (4)

Cl2 ⁱ —Ru1—C2—C3	136.4 (2)	C2—Ru1—C5—C6	-65.7 (3)
Cl2—Ru1—C2—C3	-149.3 (2)	C1—Ru1—C5—C6	-28.1 (2)
C3—Ru1—C2—C1	132.4 (4)	Cl1—Ru1—C5—C6	175.0 (2)
C4—Ru1—C2—C1	102.8 (3)	Cl2 ⁱ —Ru1—C5—C6	10.5 (5)
C5—Ru1—C2—C1	65.8 (3)	Cl2—Ru1—C5—C6	86.3 (2)
C6—Ru1—C2—C1	28.4 (3)	C3—Ru1—C5—C11	144.1 (5)
Cl1—Ru1—C2—C1	-179.3 (2)	C4—Ru1—C5—C11	115.4 (5)
Cl2 ⁱ —Ru1—C2—C1	-91.2 (2)	C2—Ru1—C5—C11	-179.0 (5)
Cl2—Ru1—C2—C1	-16.8 (4)	C6—Ru1—C5—C11	-113.2 (5)
C3—Ru1—C2—C8	-114.0 (5)	C1—Ru1—C5—C11	-141.4 (5)
C4—Ru1—C2—C8	-143.7 (5)	Cl1—Ru1—C5—C11	61.8 (5)
C5—Ru1—C2—C8	179.3 (4)	Cl2 ⁱ —Ru1—C5—C11	-102.8 (5)
C6—Ru1—C2—C8	141.9 (5)	Cl2—Ru1—C5—C11	-26.9 (4)
C1—Ru1—C2—C8	113.5 (5)	C2—C1—C6—C5	-0.6 (6)
Cl1—Ru1—C2—C8	-65.8 (4)	C7—C1—C6—C5	-178.7 (4)
Cl2 ⁱ —Ru1—C2—C8	22.4 (4)	Ru1—C1—C6—C5	-52.8 (4)
Cl2—Ru1—C2—C8	96.7 (4)	C2—C1—C6—C12	178.2 (4)
C1—C2—C3—C4	0.2 (6)	C7—C1—C6—C12	0.1 (6)
C8—C2—C3—C4	178.5 (4)	Ru1—C1—C6—C12	126.1 (4)
Ru1—C2—C3—C4	53.9 (3)	C2—C1—C6—Ru1	52.2 (3)
C1—C2—C3—C9	-178.3 (4)	C7—C1—C6—Ru1	-125.9 (4)
C8—C2—C3—C9	0.0 (6)	C4—C5—C6—C1	-0.8 (6)
Ru1—C2—C3—C9	-124.5 (4)	Cl1—C5—C6—C1	178.5 (4)
C1—C2—C3—Ru1	-53.7 (3)	Ru1—C5—C6—C1	53.3 (4)
C8—C2—C3—Ru1	124.6 (4)	C4—C5—C6—C12	-179.6 (4)
C4—Ru1—C3—C2	132.3 (4)	Cl1—C5—C6—C12	-0.3 (6)
C5—Ru1—C3—C2	103.8 (3)	Ru1—C5—C6—C12	-125.5 (4)
C6—Ru1—C3—C2	66.0 (3)	C4—C5—C6—Ru1	-54.1 (4)
C1—Ru1—C3—C2	29.6 (2)	Cl1—C5—C6—Ru1	125.2 (4)
Cl1—Ru1—C3—C2	-139.6 (2)	C3—Ru1—C6—C1	-66.1 (3)
Cl2 ⁱ —Ru1—C3—C2	-51.3 (3)	C4—Ru1—C6—C1	-103.8 (3)
Cl2—Ru1—C3—C2	132.3 (3)	C5—Ru1—C6—C1	-133.6 (4)
C5—Ru1—C3—C4	-28.4 (2)	C2—Ru1—C6—C1	-29.2 (2)
C2—Ru1—C3—C4	-132.3 (4)	Cl1—Ru1—C6—C1	-143.8 (3)
C6—Ru1—C3—C4	-66.2 (3)	Cl2 ⁱ —Ru1—C6—C1	51.1 (3)
C1—Ru1—C3—C4	-102.7 (3)	Cl2—Ru1—C6—C1	131.2 (2)
Cl1—Ru1—C3—C4	88.1 (2)	C3—Ru1—C6—C5	67.5 (3)
Cl2 ⁱ —Ru1—C3—C4	176.4 (2)	C4—Ru1—C6—C5	29.8 (2)
Cl2—Ru1—C3—C4	0.0 (5)	C2—Ru1—C6—C5	104.4 (3)
C4—Ru1—C3—C9	-112.4 (5)	C1—Ru1—C6—C5	133.6 (4)
C5—Ru1—C3—C9	-140.8 (4)	Cl1—Ru1—C6—C5	-10.1 (4)
C2—Ru1—C3—C9	115.4 (5)	Cl2 ⁱ —Ru1—C6—C5	-175.2 (2)
C6—Ru1—C3—C9	-178.6 (4)	Cl2—Ru1—C6—C5	-95.1 (2)
C1—Ru1—C3—C9	144.9 (5)	C3—Ru1—C6—C12	-179.5 (5)
Cl1—Ru1—C3—C9	-24.3 (4)	C4—Ru1—C6—C12	142.7 (5)
Cl2 ⁱ —Ru1—C3—C9	64.1 (4)	C5—Ru1—C6—C12	113.0 (6)
Cl2—Ru1—C3—C9	-112.3 (4)	C2—Ru1—C6—C12	-142.6 (5)

supplementary materials

C2—C3—C4—C5	-1.7 (6)	C1—Ru1—C6—C12	-113.4 (6)
C9—C3—C4—C5	176.9 (4)	C11—Ru1—C6—C12	102.8 (5)
Ru1—C3—C4—C5	52.5 (4)	C12 ⁱ —Ru1—C6—C12	-62.3 (5)
C2—C3—C4—C10	-179.8 (4)	C12—Ru1—C6—C12	17.8 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Fig. 1

