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## Structure Reports

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Di- $\mu_2$ -bromido-bis[bromido( $\eta^6$ -1,2,4,5-tetramethylbenzene)ruthenium(II)]

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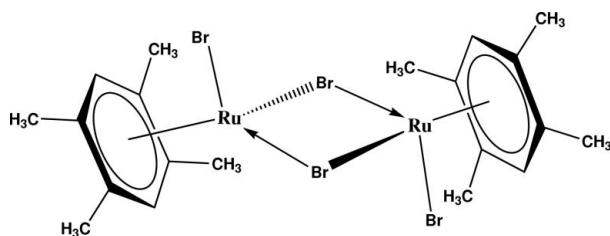
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.060; data-to-parameter ratio = 17.3.

The asymmetric unit of the title compound,  $[\text{Ru}_2\text{Br}_4(\text{C}_{10}\text{H}_{14})_2]$ , contains one half of the centrosymmetric molecule. Each Ru center is coordinated by tetramethylbenzene ring in a  $\eta^6$ -coordination mode, and one terminal and two bridging bromine atoms. The aromatic rings and the  $\text{Ru}_2\text{Br}_2$  four-membered ring form a dihedral angle of  $55.99$  ( $8$ )°. In the crystal structure, weak intermolecular  $\text{C}-\text{H}\cdots\text{Br}$  interactions link molecules into chains propagated in  $[001]$ .

## Related literature

For our work on the synthesis and catalytic applications of ruthenium-arene complexes, see: Cerón-Camacho *et al.* (2006); Díaz Camacho *et al.* (2008). For related structures, see: González-Torres *et al.* (2009) and references therein. For details of the synthesis, see: Bennett *et al.* (1982).



## Experimental

## Crystal data

 $[\text{Ru}_2\text{Br}_4(\text{C}_{10}\text{H}_{14})_2]$  $M_r = 790.20$ 

Triclinic,  $P\bar{1}$   
 $a = 7.8866$  (13) Å  
 $b = 8.2873$  (14) Å  
 $c = 9.8627$  (17) Å  
 $\alpha = 88.335$  (2)°  
 $\beta = 74.508$  (2)°  
 $\gamma = 69.648$  (2)°

$V = 580.96$  (17) Å<sup>3</sup>  
 $Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 8.18$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.35 \times 0.15 \times 0.12$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: face indexed-numerical (*SHELXTL*); Sheldrick, (2008)  
 $T_{\text{min}} = 0.139$ ,  $T_{\text{max}} = 0.478$

4786 measured reflections  
 2108 independent reflections  
 1878 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.063$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.060$   
 $S = 1.00$   
 2108 reflections

122 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.65$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{Br2}^i$	0.93	2.86	3.739 (4)	158

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2636).

## References

- Bennett, M. A., Huang, T. N., Matheson, T. W. & Smith, A. K. (1982). *Inorg. Synth.* **21**, 74–78.  
 Bruker (1999). *SMART* and *SAINT*. 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.  
 Díaz Camacho, F., Le Lagadec, R., Ryabov, A. D. & Alexandrova, L. (2008). *J. Polym. Sci.: Part A: Polym. Chem.* **46**, 4193–4204.  
 González-Torres, Y., Espinosa-Jalapa, N., Hernández-Ortega, S., Le Lagadec, R. & Morales-Morales, D. (2009). *Acta Cryst.* **E65**, m1369.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

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## Di- $\mu_2$ -bromido-bis[bromido( $\eta^6$ -1,2,4,5-tetramethylbenzene)ruthenium(II)]

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### Comment

In continuation of our studies of ruthenium arene complexes (Díaz Camacho *et al.* 2008; Cerón-Camacho *et al.* 2006; González-Torres, *et al.* 2009), we present here the title compound (I).

The asymmetric unit of (I) consists of a half molecule, which is completed with a symmetry operation of  $1 - x, 1 - y, 1 - z$  (Fig. 1). The bond lengths and angles in  $\eta^6$ -tetramethylbenzene fragment are in accordance with those observed in similar structures (González-Torres *et al.*, 2009 and references therein). Complex (I) exhibits a typical  $\eta^6$ -arene coordination of the tetramethylbenzene fragment to the ruthenium dinuclear structure bridged by two bromines and completing the coordination sphere two bromines one for each ruthenium atom arranged in a *trans* geometry. The  $\eta^6$ -arene fragment and the metal coordination center bridge (Br2—Ru—Br2 symmetry related) form a dihedral angle of 55.99 (8)°.

In the crystal structure, the molecules are linked by weak C—H $\cdots$ Br interaction (Table 1) into chains along direction [001].

### Experimental

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

### Refinement

C-bound H atoms were placed in geometrically idealized positions (C—H 0.93-0.96 Å), and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2-1.5 U_{\text{eq}}(\text{C})$ .

### Figures

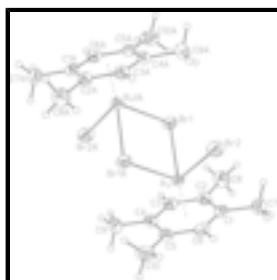


Fig. 1. Molecular structure of (I) showing the atomic numbering and 40% probability displacement ellipsoids [symmetry code: (A)  $1 - x, 1 - y, 1 - z$ ].

## Di- $\mu$ -bromido-bis[bromido( $\eta^6$ -1,2,4,5-tetramethylbenzene)ruthenium(II)]

### Crystal data

[Ru <sub>2</sub> Br <sub>4</sub> (C <sub>10</sub> H <sub>14</sub> ) <sub>2</sub> ]	$Z = 1$
$M_r = 790.20$	$F(000) = 376$
Triclinic, $P\bar{1}$	$D_x = 2.259 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.8866 (13) \text{ \AA}$	Cell parameters from 3668 reflections
$b = 8.2873 (14) \text{ \AA}$	$\theta = 2.6\text{--}25.4^\circ$
$c = 9.8627 (17) \text{ \AA}$	$\mu = 8.18 \text{ mm}^{-1}$
$\alpha = 88.335 (2)^\circ$	$T = 298 \text{ K}$
$\beta = 74.508 (2)^\circ$	Prism, red
$\gamma = 69.648 (2)^\circ$	$0.35 \times 0.15 \times 0.12 \text{ mm}$
$V = 580.96 (17) \text{ \AA}^3$	

### Data collection

Bruker SMART CCD area-detector diffractometer	2108 independent reflections
Radiation source: fine-focus sealed tube graphite	1878 reflections with $I > 2\sigma(I)$
Detector resolution: $0.83 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.063$
$\omega$ scans	$\theta_{\text{max}} = 25.4^\circ$ , $\theta_{\text{min}} = 2.2^\circ$
Absorption correction: face indexed-numerical ( <i>SHELXTL</i> ; Sheldrick, 2008)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.139$ , $T_{\text{max}} = 0.478$	$k = -9 \rightarrow 9$
4786 measured reflections	$l = -11 \rightarrow 11$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.024$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.060$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2]$
2108 reflections	where $P = (F_o^2 + 2F_c^2)/3$
122 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.52 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.65 \text{ e \AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ru	0.63750 (4)	0.49125 (3)	0.30491 (3)	0.02810 (10)
Br1	0.64758 (5)	0.29795 (4)	0.51434 (4)	0.04089 (12)
Br2	0.41130 (6)	0.36687 (6)	0.24801 (4)	0.05137 (14)
C1	0.8371 (5)	0.3925 (4)	0.0980 (4)	0.0367 (8)
C2	0.9352 (5)	0.3568 (4)	0.2017 (4)	0.0379 (8)
C3	0.9134 (5)	0.4943 (4)	0.2952 (4)	0.0377 (8)
H3	0.9789	0.4699	0.3634	0.045*
C4	0.7972 (5)	0.6654 (4)	0.2891 (4)	0.0407 (9)
C5	0.6944 (5)	0.7014 (4)	0.1860 (4)	0.0396 (9)
C6	0.7172 (5)	0.5650 (5)	0.0931 (4)	0.0389 (8)
H6	0.6507	0.5888	0.0255	0.047*
C7	0.8478 (6)	0.2543 (5)	-0.0040 (4)	0.0546 (11)
H7A	0.7734	0.3062	-0.0672	0.082*
H7B	0.8006	0.1717	0.0475	0.082*
H7C	0.9762	0.1974	-0.0572	0.082*
C8	1.0565 (6)	0.1754 (5)	0.2196 (5)	0.0557 (11)
H8A	1.1764	0.1450	0.1505	0.084*
H8B	0.9959	0.0967	0.2073	0.084*
H8C	1.0744	0.1692	0.3124	0.084*
C9	0.7843 (7)	0.8028 (5)	0.3909 (5)	0.0620 (12)
H9A	0.8514	0.7506	0.4584	0.093*
H9B	0.6547	0.8639	0.4392	0.093*
H9C	0.8385	0.8818	0.3405	0.093*
C10	0.5588 (7)	0.8778 (5)	0.1774 (5)	0.0629 (13)
H10A	0.4830	0.8707	0.1176	0.094*
H10B	0.6271	0.9520	0.1389	0.094*
H10C	0.4792	0.9236	0.2700	0.094*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ru	0.02570 (16)	0.02940 (16)	0.02784 (16)	-0.01036 (12)	-0.00439 (11)	0.00292 (10)

## supplementary materials

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Br1	0.0380 (2)	0.0341 (2)	0.0370 (2)	-0.00366 (16)	-0.00100 (16)	0.00683 (15)
Br2	0.0483 (3)	0.0736 (3)	0.0462 (2)	-0.0382 (2)	-0.0134 (2)	0.00497 (19)
C1	0.0333 (19)	0.0419 (19)	0.0313 (18)	-0.0173 (16)	0.0031 (15)	-0.0009 (15)
C2	0.0252 (17)	0.0367 (19)	0.045 (2)	-0.0104 (15)	0.0003 (15)	0.0011 (15)
C3	0.0300 (19)	0.045 (2)	0.042 (2)	-0.0177 (16)	-0.0095 (16)	0.0051 (16)
C4	0.045 (2)	0.0378 (19)	0.040 (2)	-0.0241 (17)	-0.0011 (17)	0.0014 (15)
C5	0.039 (2)	0.0362 (18)	0.040 (2)	-0.0169 (17)	-0.0010 (16)	0.0090 (15)
C6	0.041 (2)	0.049 (2)	0.0294 (17)	-0.0213 (18)	-0.0081 (16)	0.0099 (15)
C7	0.056 (3)	0.060 (3)	0.047 (2)	-0.029 (2)	0.001 (2)	-0.013 (2)
C8	0.038 (2)	0.046 (2)	0.069 (3)	-0.0035 (19)	-0.007 (2)	0.002 (2)
C9	0.084 (3)	0.057 (2)	0.056 (3)	-0.045 (3)	-0.008 (2)	-0.006 (2)
C10	0.066 (3)	0.043 (2)	0.065 (3)	-0.013 (2)	-0.006 (2)	0.021 (2)

### *Geometric parameters (Å, °)*

Ru—C6	2.150 (3)	C4—C5	1.427 (5)
Ru—C3	2.161 (4)	C4—C9	1.498 (5)
Ru—C5	2.180 (4)	C5—C6	1.408 (5)
Ru—C2	2.182 (3)	C5—C10	1.497 (5)
Ru—C1	2.191 (3)	C6—H6	0.9300
Ru—C4	2.200 (4)	C7—H7A	0.9600
Ru—Br2	2.5313 (6)	C7—H7B	0.9600
Ru—Br1 <sup>i</sup>	2.5676 (5)	C7—H7C	0.9600
Ru—Br1	2.5780 (5)	C8—H8A	0.9600
Br1—Ru <sup>i</sup>	2.5676 (5)	C8—H8B	0.9600
C1—C2	1.407 (5)	C8—H8C	0.9600
C1—C6	1.421 (5)	C9—H9A	0.9600
C1—C7	1.511 (5)	C9—H9B	0.9600
C2—C3	1.421 (5)	C9—H9C	0.9600
C2—C8	1.510 (5)	C10—H10A	0.9600
C3—C4	1.406 (5)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C6—Ru—C3	79.89 (15)	C4—C3—C2	122.8 (3)
C6—Ru—C5	37.93 (13)	C4—C3—Ru	72.7 (2)
C3—Ru—C5	68.14 (14)	C2—C3—Ru	71.7 (2)
C6—Ru—C2	68.16 (14)	C4—C3—H3	118.6
C3—Ru—C2	38.18 (13)	C2—C3—H3	118.6
C5—Ru—C2	81.73 (14)	Ru—C3—H3	129.7
C6—Ru—C1	38.21 (14)	C3—C4—C5	118.3 (3)
C3—Ru—C1	68.06 (13)	C3—C4—C9	119.3 (4)
C5—Ru—C1	69.31 (13)	C5—C4—C9	122.4 (3)
C2—Ru—C1	37.53 (14)	C3—C4—Ru	69.7 (2)
C6—Ru—C4	68.13 (14)	C5—C4—Ru	70.2 (2)
C3—Ru—C4	37.60 (13)	C9—C4—Ru	131.5 (3)
C5—Ru—C4	38.01 (14)	C6—C5—C4	118.6 (3)
C2—Ru—C4	69.00 (13)	C6—C5—C10	119.3 (4)
C1—Ru—C4	81.45 (13)	C4—C5—C10	122.0 (4)
C6—Ru—Br2	92.41 (11)	C6—C5—Ru	69.9 (2)

C3—Ru—Br2	154.25 (9)	C4—C5—Ru	71.7 (2)
C5—Ru—Br2	119.06 (11)	C10—C5—Ru	128.2 (3)
C2—Ru—Br2	116.19 (10)	C5—C6—C1	122.9 (3)
C1—Ru—Br2	90.67 (10)	C5—C6—Ru	72.2 (2)
C4—Ru—Br2	157.03 (10)	C1—C6—Ru	72.4 (2)
C6—Ru—Br1 <sup>i</sup>	119.11 (10)	C5—C6—H6	118.5
C3—Ru—Br1 <sup>i</sup>	118.25 (9)	C1—C6—H6	118.5
C5—Ru—Br1 <sup>i</sup>	92.02 (9)	Ru—C6—H6	129.5
C2—Ru—Br1 <sup>i</sup>	156.13 (10)	C1—C7—H7A	109.5
C1—Ru—Br1 <sup>i</sup>	157.12 (10)	C1—C7—H7B	109.5
C4—Ru—Br1 <sup>i</sup>	91.93 (9)	H7A—C7—H7B	109.5
Br2—Ru—Br1 <sup>i</sup>	87.02 (2)	C1—C7—H7C	109.5
C6—Ru—Br1	158.03 (10)	H7A—C7—H7C	109.5
C3—Ru—Br1	90.73 (10)	H7B—C7—H7C	109.5
C5—Ru—Br1	152.74 (10)	C2—C8—H8A	109.5
C2—Ru—Br1	92.20 (10)	C2—C8—H8B	109.5
C1—Ru—Br1	119.82 (10)	H8A—C8—H8B	109.5
C4—Ru—Br1	115.15 (10)	C2—C8—H8C	109.5
Br2—Ru—Br1	87.508 (18)	H8A—C8—H8C	109.5
Br1 <sup>i</sup> —Ru—Br1	82.838 (17)	H8B—C8—H8C	109.5
Ru <sup>i</sup> —Br1—Ru	97.162 (17)	C4—C9—H9A	109.5
C2—C1—C6	118.3 (3)	C4—C9—H9B	109.5
C2—C1—C7	122.8 (3)	H9A—C9—H9B	109.5
C6—C1—C7	118.8 (3)	C4—C9—H9C	109.5
C2—C1—Ru	70.89 (19)	H9A—C9—H9C	109.5
C6—C1—Ru	69.36 (18)	H9B—C9—H9C	109.5
C7—C1—Ru	129.3 (3)	C5—C10—H10A	109.5
C1—C2—C3	119.0 (3)	C5—C10—H10B	109.5
C1—C2—C8	121.6 (3)	H10A—C10—H10B	109.5
C3—C2—C8	119.3 (3)	C5—C10—H10C	109.5
C1—C2—Ru	71.58 (19)	H10A—C10—H10C	109.5
C3—C2—Ru	70.13 (19)	H10B—C10—H10C	109.5
C8—C2—Ru	128.1 (3)		
C6—Ru—Br1—Ru <sup>i</sup>	-177.6 (3)	Ru—C3—C4—C5	-52.5 (3)
C3—Ru—Br1—Ru <sup>i</sup>	118.39 (9)	C2—C3—C4—C9	-179.3 (4)
C5—Ru—Br1—Ru <sup>i</sup>	80.4 (2)	Ru—C3—C4—C9	127.1 (4)
C2—Ru—Br1—Ru <sup>i</sup>	156.56 (10)	C2—C3—C4—Ru	53.6 (3)
C1—Ru—Br1—Ru <sup>i</sup>	-176.65 (12)	C6—Ru—C4—C3	-102.2 (2)
C4—Ru—Br1—Ru <sup>i</sup>	88.77 (10)	C5—Ru—C4—C3	-132.1 (3)
Br2—Ru—Br1—Ru <sup>i</sup>	-87.31 (2)	C2—Ru—C4—C3	-28.2 (2)
Br1 <sup>i</sup> —Ru—Br1—Ru <sup>i</sup>	0.0	C1—Ru—C4—C3	-64.9 (2)
C6—Ru—C1—C2	131.8 (3)	Br2—Ru—C4—C3	-136.0 (2)
C3—Ru—C1—C2	29.9 (2)	Br1 <sup>i</sup> —Ru—C4—C3	137.1 (2)
C5—Ru—C1—C2	103.8 (2)	Br1—Ru—C4—C3	54.1 (2)
C4—Ru—C1—C2	66.5 (2)	C6—Ru—C4—C5	29.92 (19)

## supplementary materials

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Br2—Ru—C1—C2	-135.2 (2)	C3—Ru—C4—C5	132.1 (3)
Br1 <sup>i</sup> —Ru—C1—C2	140.9 (2)	C2—Ru—C4—C5	103.9 (2)
Br1—Ru—C1—C2	-47.7 (2)	C1—Ru—C4—C5	67.2 (2)
C3—Ru—C1—C6	-101.9 (2)	Br2—Ru—C4—C5	-3.9 (4)
C5—Ru—C1—C6	-27.9 (2)	Br1 <sup>i</sup> —Ru—C4—C5	-90.81 (19)
C2—Ru—C1—C6	-131.8 (3)	Br1—Ru—C4—C5	-173.80 (16)
C4—Ru—C1—C6	-65.3 (2)	C6—Ru—C4—C9	146.2 (4)
Br2—Ru—C1—C6	93.0 (2)	C3—Ru—C4—C9	-111.6 (5)
Br1 <sup>i</sup> —Ru—C1—C6	9.1 (4)	C5—Ru—C4—C9	116.3 (5)
Br1—Ru—C1—C6	-179.45 (18)	C2—Ru—C4—C9	-139.8 (4)
C6—Ru—C1—C7	-111.0 (4)	C1—Ru—C4—C9	-176.5 (4)
C3—Ru—C1—C7	147.2 (4)	Br2—Ru—C4—C9	112.4 (4)
C5—Ru—C1—C7	-138.9 (4)	Br1 <sup>i</sup> —Ru—C4—C9	25.5 (4)
C2—Ru—C1—C7	117.2 (4)	Br1—Ru—C4—C9	-57.5 (4)
C4—Ru—C1—C7	-176.3 (4)	C3—C4—C5—C6	-1.4 (5)
Br2—Ru—C1—C7	-17.9 (3)	C9—C4—C5—C6	179.0 (3)
Br1 <sup>i</sup> —Ru—C1—C7	-101.9 (4)	Ru—C4—C5—C6	-53.7 (3)
Br1—Ru—C1—C7	69.6 (4)	C3—C4—C5—C10	176.4 (4)
C6—C1—C2—C3	-1.2 (5)	C9—C4—C5—C10	-3.2 (6)
C7—C1—C2—C3	-178.6 (3)	Ru—C4—C5—C10	124.1 (4)
Ru—C1—C2—C3	-53.6 (3)	C3—C4—C5—Ru	52.3 (3)
C6—C1—C2—C8	176.3 (4)	C9—C4—C5—Ru	-127.3 (4)
C7—C1—C2—C8	-1.1 (6)	C3—Ru—C5—C6	102.0 (2)
Ru—C1—C2—C8	123.9 (4)	C2—Ru—C5—C6	64.8 (2)
C6—C1—C2—Ru	52.4 (3)	C1—Ru—C5—C6	28.1 (2)
C7—C1—C2—Ru	-125.0 (4)	C4—Ru—C5—C6	131.1 (3)
C6—Ru—C2—C1	-29.8 (2)	Br2—Ru—C5—C6	-50.6 (2)
C3—Ru—C2—C1	-131.6 (3)	Br1 <sup>i</sup> —Ru—C5—C6	-138.3 (2)
C5—Ru—C2—C1	-66.6 (2)	Br1—Ru—C5—C6	143.5 (2)
C4—Ru—C2—C1	-103.8 (2)	C6—Ru—C5—C4	-131.1 (3)
Br2—Ru—C2—C1	51.8 (2)	C3—Ru—C5—C4	-29.2 (2)
Br1 <sup>i</sup> —Ru—C2—C1	-142.7 (2)	C2—Ru—C5—C4	-66.3 (2)
Br1—Ru—C2—C1	140.1 (2)	C1—Ru—C5—C4	-103.0 (2)
C6—Ru—C2—C3	101.8 (2)	Br2—Ru—C5—C4	178.27 (16)
C5—Ru—C2—C3	64.9 (2)	Br1 <sup>i</sup> —Ru—C5—C4	90.55 (19)
C1—Ru—C2—C3	131.6 (3)	Br1—Ru—C5—C4	12.3 (3)
C4—Ru—C2—C3	27.8 (2)	C6—Ru—C5—C10	112.1 (5)
Br2—Ru—C2—C3	-176.69 (17)	C3—Ru—C5—C10	-146.0 (4)
Br1 <sup>i</sup> —Ru—C2—C3	-11.2 (4)	C2—Ru—C5—C10	176.9 (4)
Br1—Ru—C2—C3	-88.4 (2)	C1—Ru—C5—C10	140.2 (4)
C6—Ru—C2—C8	-146.0 (4)	C4—Ru—C5—C10	-116.8 (4)
C3—Ru—C2—C8	112.3 (4)	Br2—Ru—C5—C10	61.5 (4)
C5—Ru—C2—C8	177.2 (4)	Br1 <sup>i</sup> —Ru—C5—C10	-26.2 (4)
C1—Ru—C2—C8	-116.2 (4)	Br1—Ru—C5—C10	-104.5 (4)
C4—Ru—C2—C8	140.0 (4)	C4—C5—C6—C1	0.4 (5)
Br2—Ru—C2—C8	-64.4 (4)	C10—C5—C6—C1	-177.4 (4)
Br1 <sup>i</sup> —Ru—C2—C8	101.1 (4)	Ru—C5—C6—C1	-54.1 (3)

Br1—Ru—C2—C8	23.9 (3)	C4—C5—C6—Ru	54.6 (3)
C1—C2—C3—C4	0.2 (5)	C10—C5—C6—Ru	-123.3 (4)
C8—C2—C3—C4	-177.4 (4)	C2—C1—C6—C5	0.9 (5)
Ru—C2—C3—C4	-54.1 (3)	C7—C1—C6—C5	178.4 (3)
C1—C2—C3—Ru	54.3 (3)	Ru—C1—C6—C5	54.0 (3)
C8—C2—C3—Ru	-123.3 (3)	C2—C1—C6—Ru	-53.1 (3)
C6—Ru—C3—C4	67.1 (2)	C7—C1—C6—Ru	124.4 (3)
C5—Ru—C3—C4	29.5 (2)	C3—Ru—C6—C5	-67.3 (2)
C2—Ru—C3—C4	134.5 (3)	C2—Ru—C6—C5	-105.2 (2)
C1—Ru—C3—C4	105.1 (2)	C1—Ru—C6—C5	-134.5 (3)
Br2—Ru—C3—C4	141.4 (2)	C4—Ru—C6—C5	-30.0 (2)
Br1 <sup>i</sup> —Ru—C3—C4	-50.6 (2)	Br2—Ru—C6—C5	137.5 (2)
Br1—Ru—C3—C4	-132.8 (2)	Br1 <sup>i</sup> —Ru—C6—C5	49.5 (2)
C6—Ru—C3—C2	-67.4 (2)	Br1—Ru—C6—C5	-133.2 (2)
C5—Ru—C3—C2	-105.0 (2)	C3—Ru—C6—C1	67.2 (2)
C1—Ru—C3—C2	-29.4 (2)	C5—Ru—C6—C1	134.5 (3)
C4—Ru—C3—C2	-134.5 (3)	C2—Ru—C6—C1	29.3 (2)
Br2—Ru—C3—C2	6.9 (4)	C4—Ru—C6—C1	104.5 (2)
Br1 <sup>i</sup> —Ru—C3—C2	174.90 (17)	Br2—Ru—C6—C1	-88.0 (2)
Br1—Ru—C3—C2	92.6 (2)	Br1 <sup>i</sup> —Ru—C6—C1	-175.95 (18)
C2—C3—C4—C5	1.1 (5)	Br1—Ru—C6—C1	1.3 (4)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 <sup>iii</sup> —Br2 <sup>ii</sup>	0.93	2.86	3.739 (4)	158.

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

