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## Di- $\mu$ -nitrosyl-bis[( $\eta^5$ -pentamethylcyclopentadienyl)ruthenium(0)](*Ru—Ru*). Corrigendum

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The acknowledgement in the paper by Pearsal, Gembicky, Dominiak, Larsen & Coppens [*Acta Cryst.* (2007), **E63**, m2596] is extended and an omitted reference is added.

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In the paper by Pearsal *et al.* (2007), the complete acknowledgement should read:

"Support of the REU program CHE-0453206 by the National Science Foundation is gratefully acknowledged. The synthetic route to the title compound in this work (*via* 2-propanol oxidation) was first developed in the context of ALs PhD dissertation completed in 1996 under the supervision of Dr John L. Hubbard, whose contribution to this project is gratefully acknowledged."

A reference for the PhD dissertation [Larsen (*née* Svetlanova), 1996] is also added.

### References

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Pearsal, M., Gembicky, M., Dominiak, P., Larsen, A. & Coppens, P. (2007). *Acta Cryst.* **E63**, m2596.

## Di- $\mu$ -nitrosyl-bis[( $\eta^5$ -pentamethylcyclopentadienyl)ruthenium(0)]( $Ru-Ru$ )

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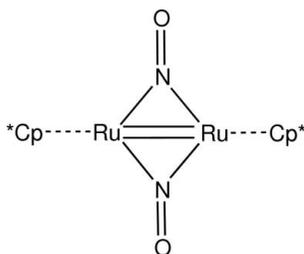
Received 4 September 2007; accepted 14 September 2007

Key indicators: single-crystal X-ray study;  $T = 90$  K; mean  $\sigma(C-C) = 0.010$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.139; data-to-parameter ratio = 20.6.

The title structure,  $[Ru_2(C_{10}H_{15})_2(NO)_2]$ , consists of the two Ru atoms doubly bridged *via* the N atoms of the two NO groups, with two pentamethylcyclopentadienyl ( $Cp^*$ ) rings protruding away from the bridged system on opposite sides. The asymmetric unit contains two independent dimer molecules with an average Ru–Ru distance of 2.538 (7) Å and an average Ru–N–Ru angle of 97.2 (3)°. The compound was obtained as the product of a facile reaction between  $Cp^*Ru(NO)(OSO_2CF_3)_2$  and excess neat 2-propanol. The crystals were grown from  $CH_2Cl_2$  solution at ambient temperature under a nitrogen atmosphere.

### Related literature

For related literature, see: Bergman & Chang (1987); Bernal *et al.* (1977); Bottomley (1983); Burns & Hubbard (1994); Hayton *et al.* (2002); Kubat-Martin *et al.* (1987).



### Experimental

#### Crystal data

$[Ru_2(C_{10}H_{15})_2(NO)_2]$   
 $M_r = 532.60$   
Triclinic,  $P\bar{1}$   
 $a = 10.7181$  (3) Å  
 $b = 10.7364$  (3) Å  
 $c = 17.9238$  (5) Å  
 $\alpha = 89.209$  (1)°  
 $\beta = 89.220$  (1)°

$\gamma = 85.373$  (1)°  
 $V = 2055.48$  (10) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 1.49$  mm<sup>-1</sup>  
 $T = 90$  (1) K  
 $0.3 \times 0.2 \times 0.13$  mm

#### Data collection

Bruker SMART APEXII  
diffractometer  
Absorption correction: multi-scan  
(SADABS; Bruker 2004)  
 $T_{min} = 0.705$ ,  $T_{max} = 0.824$

29941 measured reflections  
10102 independent reflections  
9591 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.040$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.139$   
 $S = 1.26$   
10102 reflections  
490 parameters

18 restraints  
H-atom parameters constrained  
 $\Delta\rho_{max} = 2.12$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -2.33$  e Å<sup>-3</sup>

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

Support of the REU program CHE-0453206 by the national Science Foundation is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2041).

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**supplementary materials**

*Acta Cryst.* (2007). E63, m2596 [ doi:10.1107/S1600536807045321 ]

## Di- $\mu$ -nitrosyl-bis[( $\eta^5$ -pentamethylcyclopentadienyl)ruthenium(0)](*Ru-Ru*)

M. Pearsal, M. Gembicky, P. Dominiak, A. Larsen and P. Coppens

### Comment

X-ray diffraction data on title compound were collected at 90 (1) K using a Bruker *SMART APEX2* CCD diffractometer installed at a rotating anode source (Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å), and equipped with an Oxford Cryosystems nitrogen gas-flow apparatus. The data were collected by the oscillation method with  $0.5^\circ$  frame-width ( $\omega$ -scan) and a 15 sec exposure per frame. Four sets of data (360 frames in each set) were collected, nominally covering complete reciprocal space. The data were integrated, scaled, sorted and averaged using the *APEX2* software package.

All crystals examined were twinned. The metric symmetry of the unit cell suggested a monoclinic C-centred cell. However the structure could be solved, with some difficulties, in the triclinic space group  $P\bar{1}$  only (Direct Methods, *SHELXTL* Version 6.14). The twin law (0 -1 0, -1 0 0, 0 0 -1) was used during refinement. The volume ratios of the twins refined to 0.298 (1): 0.702 (1).

All non-hydrogen atoms were refined anisotropically. Positions of hydrogen atoms were calculated from the geometry of surrounding carbon atoms. The  $\text{CH}_3$  H atoms were treated as part of idealized  $\text{CH}_3$  groups with  $U_{\text{iso}} = 1.5U_{\text{eq}}$ . For the carbon atoms C22, C31 and C35 isotropic restraints have been imposed to avoid non positive definite ADPs.

### Experimental

All synthetic procedures were carried out in the inert atmosphere of a glove box. The starting material -  $\text{Cp}^*\text{Ru}(\text{NO})\text{OTf}_2$  ( $\text{OTf} = \text{OSO}_2\text{CF}_3$ ) – was prepared according to synthetic methods reported by Burns & Hubbard (1994). 2-Propanol (10 ml) was added with a syringe to  $\text{Cp}^*\text{Ru}(\text{NO})\text{OTf}_2$  (125 mg, 0.22 mmol) with a syringe. A color change from green to red/brown was observed immediately upon addition of 2-propanol to  $\text{Cp}^*\text{Ru}(\text{NO})\text{OTf}_2$ . This color persisted throughout the reaction. The solution was stirred for ~2 h after which the deep red microcrystalline powder was collected by filtration. The product was washed with diethyl ether and dried, yielding 37 mg (.068 mmol, 62% yield). The structure was confirmed by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopy. Alternate routes entailing reductive elimination of  $\text{Cp}^*\text{Ru}(\text{NO})\text{Cl}_2$  or  $\text{Cp}^*\text{Ru}(\text{NO})\text{Ph}_2$  have been reported by Bergman & Chang (1987) and Hayton *et al.* (2002) Recrystallization was attempted in several solvents. The highest quality crystals (and ultimately, the crystal used for x-ray analysis) were obtained from  $\text{CH}_2\text{Cl}_2$  solutions.

### Refinement

Support of the REU program CHE-0453206 by the national Science Foundation is gratefully acknowledged.

## Figures

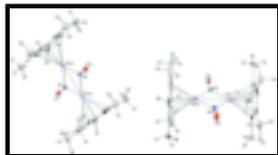


Fig. 1. Molecular structure of title compound, hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

## Di- $\mu$ -nitrosyl-bis[( $\eta^5$ -pentamethylcyclopentadienyl)ruthenium(0)](Ru—Ru)

### Crystal data

|  |   |
|--|---|
| $[\text{Ru}_2(\text{C}_{10}\text{H}_{15})_2(\text{NO})_2]$ | $Z = 4$                                 |
| $M_r = 532.60$   | $F_{000} = 1072$                        |
| Triclinic, $P\bar{1}$                                      | $D_x = 1.721 \text{ Mg m}^{-3}$         |
| Hall symbol: -P 1  | Mo $K\alpha$ radiation                  |
| $a = 10.7181 (3) \text{ \AA}$                              | $\lambda = 0.71073 \text{ \AA}$         |
| $b = 10.7364 (3) \text{ \AA}$                              | Cell parameters from 7139 reflections   |
| $c = 17.9238 (5) \text{ \AA}$                              | $\theta = 3\text{--}28^\circ$           |
| $\alpha = 89.209 (1)^\circ$                                | $\mu = 1.49 \text{ mm}^{-1}$            |
| $\beta = 89.220 (1)^\circ$                                 | $T = 90 (1) \text{ K}$                  |
| $\gamma = 85.373 (1)^\circ$                                | Parallelepiped, red                     |
| $V = 2055.48 (10) \text{ \AA}^3$                           | $0.3 \times 0.2 \times 0.13 \text{ mm}$ |

### Data collection

|   |  |
|---|--|
| Bruker SMART APEXII diffractometer                      | 10102 independent reflections          |
| Radiation source: rotating anode                        | 9591 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite                                 | $R_{\text{int}} = 0.040$               |
| Detector resolution: $8.33 \text{ pixels mm}^{-1}$      | $\theta_{\text{max}} = 28.3^\circ$     |
| $T = 90(1) \text{ K}$                                   | $\theta_{\text{min}} = 1.9^\circ$      |
| $\omega$ scans  | $h = -14 \rightarrow 14$               |
| Absorption correction: multi-scan (SADABS; Bruker 2004) | $k = -14 \rightarrow 14$               |
| $T_{\text{min}} = 0.705$ , $T_{\text{max}} = 0.824$     | $l = -23 \rightarrow 23$               |
| 29941 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 |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | H-atom parameters constrained                            |
| $wR(F^2) = 0.139$               | $w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 11.2766P]$       |
|                                 | where $P = (F_o^2 + 2F_c^2)/3$                           |

$S = 1.26$   $(\Delta/\sigma)_{\max} = 0.001$   
 10102 reflections  $\Delta\rho_{\max} = 2.12 \text{ e } \text{\AA}^{-3}$   
 490 parameters  $\Delta\rho_{\min} = -2.33 \text{ e } \text{\AA}^{-3}$   
 18 restraints Extinction correction: none  
 Primary atom site location: structure-invariant direct methods

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

|     | $x$         | $y$         | $z$         | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| Ru1 | 0.83429 (5) | 0.25167 (5) | 0.55223 (3) | 0.01071 (12)                     |
| Ru2 | 0.69033 (5) | 0.26716 (5) | 0.44039 (3) | 0.01077 (12)                     |
| Ru3 | 0.74543 (5) | 0.83347 (5) | 1.05050 (3) | 0.01092 (12)                     |
| Ru4 | 0.75823 (6) | 0.69028 (6) | 0.93893 (3) | 0.01274 (13)                     |
| N1  | 0.8686 (5)  | 0.2772 (5)  | 0.4483 (3)  | 0.0138 (10)                      |
| N2  | 0.6564 (5)  | 0.2350 (5)  | 0.5441 (3)  | 0.0120 (10)                      |
| N3  | 0.7691 (5)  | 0.8663 (5)  | 0.9461 (3)  | 0.0137 (10)                      |
| N4  | 0.7283 (6)  | 0.6576 (6)  | 1.0431 (3)  | 0.0165 (11)                      |
| O1  | 0.9603 (5)  | 0.2868 (5)  | 0.4067 (3)  | 0.0186 (10)                      |
| O2  | 0.5687 (5)  | 0.2106 (5)  | 0.5845 (3)  | 0.0178 (10)                      |
| O3  | 0.7819 (5)  | 0.9550 (5)  | 0.9043 (3)  | 0.0188 (10)                      |
| O4  | 0.7083 (6)  | 0.5701 (5)  | 1.0848 (3)  | 0.0248 (11)                      |
| C1  | 1.0123 (6)  | 0.3019 (6)  | 0.6016 (3)  | 0.0153 (12)                      |
| C2  | 0.9088 (6)  | 0.3454 (6)  | 0.6490 (3)  | 0.0133 (12)                      |
| C3  | 0.8506 (6)  | 0.2399 (7)  | 0.6759 (3)  | 0.0157 (13)                      |
| C4  | 0.9122 (7)  | 0.1307 (6)  | 0.6430 (3)  | 0.0157 (13)                      |
| C5  | 1.0147 (6)  | 0.1707 (7)  | 0.5976 (3)  | 0.0196 (14)                      |
| C6  | 1.1027 (7)  | 0.3803 (7)  | 0.5625 (4)  | 0.0229 (14)                      |
| H6A | 1.1861      | 0.3628      | 0.5839      | 0.034*                           |
| H6B | 1.0753      | 0.4689      | 0.5688      | 0.034*                           |
| H6C | 1.1060      | 0.3606      | 0.5093      | 0.034*                           |
| C7  | 0.8771 (8)  | 0.4764 (7)  | 0.6728 (4)  | 0.0242 (15)                      |
| H7A | 0.7871      | 0.4891      | 0.6836      | 0.036*                           |
| H7B | 0.8994      | 0.5339      | 0.6327      | 0.036*                           |
| H7C | 0.9240      | 0.4926      | 0.7177      | 0.036*                           |
| C8  | 0.7401 (7)  | 0.2394 (7)  | 0.7287 (4)  | 0.0229 (14)                      |

## supplementary materials

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|      |            |             |            |             |
|------|------------|-------------|------------|-------------|
| H8A  | 0.7593     | 0.1790      | 0.7692     | 0.034*      |
| H8B  | 0.6669     | 0.2159      | 0.7017     | 0.034*      |
| H8C  | 0.7223     | 0.3229      | 0.7495     | 0.034*      |
| C9   | 0.8799 (8) | -0.0006 (7) | 0.6564 (4) | 0.0271 (16) |
| H9A  | 0.7887     | -0.0033     | 0.6564     | 0.041*      |
| H9B  | 0.9125     | -0.0305     | 0.7048     | 0.041*      |
| H9C  | 0.9172     | -0.0542     | 0.6169     | 0.041*      |
| C10  | 1.1114 (7) | 0.0898 (7)  | 0.5546 (4) | 0.0245 (15) |
| H10A | 1.1234     | 0.1266      | 0.5050     | 0.037*      |
| H10B | 1.0828     | 0.0059      | 0.5496     | 0.037*      |
| H10C | 1.1908     | 0.0843      | 0.5814     | 0.037*      |
| C11  | 0.6615 (6) | 0.3406 (6)  | 0.3248 (3) | 0.0133 (12) |
| C12  | 0.5575 (6) | 0.3859 (7)  | 0.3712 (3) | 0.0165 (13) |
| C13  | 0.4952 (6) | 0.2823 (7)  | 0.3977 (3) | 0.0193 (14) |
| C14  | 0.5631 (6) | 0.1703 (7)  | 0.3703 (4) | 0.0177 (13) |
| C15  | 0.6642 (7) | 0.2080 (6)  | 0.3252 (3) | 0.0176 (13) |
| C16  | 0.7511 (7) | 0.4163 (7)  | 0.2847 (4) | 0.0208 (13) |
| H16A | 0.8368     | 0.3839      | 0.2962     | 0.031*      |
| H16B | 0.7379     | 0.5035      | 0.3004     | 0.031*      |
| H16C | 0.7379     | 0.4118      | 0.2308     | 0.031*      |
| C17  | 0.5142 (7) | 0.5198 (7)  | 0.3828 (4) | 0.0240 (15) |
| H17A | 0.4592     | 0.5493      | 0.3419     | 0.036*      |
| H17B | 0.5867     | 0.5697      | 0.3837     | 0.036*      |
| H17C | 0.4681     | 0.5283      | 0.4303     | 0.036*      |
| C18  | 0.3795 (7) | 0.2856 (8)  | 0.4461 (4) | 0.0272 (16) |
| H18A | 0.3560     | 0.3717      | 0.4612     | 0.041*      |
| H18B | 0.3960     | 0.2330      | 0.4905     | 0.041*      |
| H18C | 0.3110     | 0.2541      | 0.4180     | 0.041*      |
| C19  | 0.5247 (7) | 0.0418 (7)  | 0.3822 (4) | 0.0238 (14) |
| H19A | 0.4850     | 0.0355      | 0.4315     | 0.036*      |
| H19B | 0.5986     | -0.0180     | 0.3793     | 0.036*      |
| H19C | 0.4652     | 0.0231      | 0.3437     | 0.036*      |
| C20  | 0.7578 (7) | 0.1247 (7)  | 0.2829 (4) | 0.0227 (14) |
| H20A | 0.7445     | 0.1370      | 0.2292     | 0.034*      |
| H20B | 0.7477     | 0.0374      | 0.2965     | 0.034*      |
| H20C | 0.8425     | 0.1452      | 0.2951     | 0.034*      |
| C21  | 0.6700 (6) | 1.0141 (6)  | 1.0968 (3) | 0.0140 (12) |
| C22  | 0.6316 (6) | 0.9149 (7)  | 1.1443 (3) | 0.0164 (13) |
| C23  | 0.7421 (7) | 0.8505 (7)  | 1.1744 (3) | 0.0167 (13) |
| C24  | 0.8494 (7) | 0.9067 (7)  | 1.1437 (3) | 0.0179 (13) |
| C25  | 0.8036 (6) | 1.0098 (6)  | 1.0966 (3) | 0.0134 (12) |
| C26  | 0.5862 (7) | 1.1095 (7)  | 1.0562 (4) | 0.0230 (15) |
| H26A | 0.5833     | 1.1891      | 1.0826     | 0.035*      |
| H26B | 0.5017     | 1.0812      | 1.0541     | 0.035*      |
| H26C | 0.6187     | 1.1209      | 1.0054     | 0.035*      |
| C27  | 0.5004 (7) | 0.8876 (7)  | 1.1648 (4) | 0.0250 (15) |
| H27A | 0.4784     | 0.9221      | 1.2140     | 0.038*      |
| H27B | 0.4944     | 0.7970      | 1.1661     | 0.038*      |
| H27C | 0.4425     | 0.9260      | 1.1276     | 0.038*      |

|      |             |             |            |             |
|------|-------------|-------------|------------|-------------|
| C28  | 0.7445 (8)  | 0.7443 (7)  | 1.2286 (4) | 0.0246 (15) |
| H28A | 0.8299      | 0.7261      | 1.2470     | 0.037*      |
| H28B | 0.7173      | 0.6703      | 1.2040     | 0.037*      |
| H28C | 0.6880      | 0.7664      | 1.2707     | 0.037*      |
| C29  | 0.9852 (7)  | 0.8728 (7)  | 1.1631 (4) | 0.0227 (14) |
| H29A | 1.0022      | 0.9058      | 1.2123     | 0.034*      |
| H29B | 1.0395      | 0.9089      | 1.1256     | 0.034*      |
| H29C | 1.0017      | 0.7816      | 1.1639     | 0.034*      |
| C30  | 0.8801 (6)  | 1.0991 (7)  | 1.0552 (4) | 0.0196 (13) |
| H30A | 0.9692      | 1.0736      | 1.0616     | 0.029*      |
| H30B | 0.8614      | 1.1833      | 1.0749     | 0.029*      |
| H30C | 0.8598      | 1.0989      | 1.0021     | 0.029*      |
| C31  | 0.7173 (7)  | 0.6749 (7)  | 0.8191 (4) | 0.0205 (15) |
| C32  | 0.6613 (8)  | 0.5753 (9)  | 0.8593 (5) | 0.033 (2)   |
| C33  | 0.7600 (9)  | 0.4985 (8)  | 0.8929 (4) | 0.0311 (19) |
| C34  | 0.8759 (7)  | 0.5494 (7)  | 0.8756 (4) | 0.0207 (14) |
| C35  | 0.8486 (6)  | 0.6582 (6)  | 0.8296 (3) | 0.0141 (12) |
| C36  | 0.6512 (9)  | 0.7775 (10) | 0.7736 (4) | 0.042 (3)   |
| H36A | 0.6766      | 0.8584      | 0.7898     | 0.064*      |
| H36B | 0.5606      | 0.7753      | 0.7804     | 0.064*      |
| H36C | 0.6733      | 0.7659      | 0.7207     | 0.064*      |
| C37  | 0.5250 (11) | 0.5529 (14) | 0.8582 (7) | 0.073 (5)   |
| H37A | 0.5099      | 0.4958      | 0.8177     | 0.110*      |
| H37B | 0.4751      | 0.6324      | 0.8502     | 0.110*      |
| H37C | 0.5008      | 0.5157      | 0.9060     | 0.110*      |
| C38  | 0.7469 (14) | 0.3831 (9)  | 0.9393 (5) | 0.066 (4)   |
| H38A | 0.8107      | 0.3771      | 0.9782     | 0.100*      |
| H38B | 0.7580      | 0.3094      | 0.9075     | 0.100*      |
| H38C | 0.6635      | 0.3873      | 0.9626     | 0.100*      |
| C39  | 1.0063 (9)  | 0.4968 (9)  | 0.8946 (4) | 0.040 (2)   |
| H39A | 1.0023      | 0.4367      | 0.9361     | 0.060*      |
| H39B | 1.0563      | 0.5648      | 0.9091     | 0.060*      |
| H39C | 1.0451      | 0.4545      | 0.8510     | 0.060*      |
| C40  | 0.9426 (7)  | 0.7408 (7)  | 0.7966 (4) | 0.0248 (15) |
| H40A | 0.9467      | 0.7307      | 0.7423     | 0.037*      |
| H40B | 1.0251      | 0.7174      | 0.8178     | 0.037*      |
| H40C | 0.9172      | 0.8282      | 0.8082     | 0.037*      |

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

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$      | $U^{13}$      | $U^{23}$      |
|-----|------------|------------|------------|---------------|---------------|---------------|
| Ru1 | 0.0143 (3) | 0.0127 (2) | 0.0044 (2) | 0.00371 (17)  | -0.00232 (18) | -0.00081 (18) |
| Ru2 | 0.0137 (2) | 0.0132 (2) | 0.0047 (2) | 0.00386 (17)  | -0.00250 (18) | -0.00123 (18) |
| Ru3 | 0.0137 (2) | 0.0128 (3) | 0.0058 (2) | 0.00216 (17)  | -0.00055 (18) | -0.00242 (19) |
| Ru4 | 0.0167 (3) | 0.0142 (3) | 0.0073 (2) | -0.00047 (19) | 0.00158 (19)  | -0.0039 (2)   |
| N1  | 0.017 (3)  | 0.016 (3)  | 0.008 (2)  | 0.0050 (19)   | -0.002 (2)    | 0.000 (2)     |
| N2  | 0.013 (3)  | 0.012 (3)  | 0.011 (2)  | 0.0018 (18)   | -0.0028 (19)  | -0.0030 (19)  |
| N3  | 0.015 (3)  | 0.014 (3)  | 0.011 (2)  | 0.002 (2)     | -0.002 (2)    | -0.004 (2)    |

## supplementary materials

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|     |            |            |           |              |              |              |
|-----|------------|------------|-----------|--------------|--------------|--------------|
| N4  | 0.018 (3)  | 0.018 (3)  | 0.014 (3) | -0.004 (2)   | 0.002 (2)    | -0.003 (2)   |
| O1  | 0.021 (2)  | 0.024 (3)  | 0.011 (2) | -0.0013 (19) | 0.0020 (18)  | -0.0005 (19) |
| O2  | 0.017 (2)  | 0.024 (3)  | 0.011 (2) | 0.0000 (18)  | 0.0014 (18)  | 0.0019 (19)  |
| O3  | 0.034 (3)  | 0.013 (2)  | 0.009 (2) | 0.0006 (19)  | -0.0011 (19) | 0.0024 (17)  |
| O4  | 0.041 (3)  | 0.019 (3)  | 0.016 (2) | -0.008 (2)   | 0.008 (2)    | 0.001 (2)    |
| C1  | 0.017 (3)  | 0.021 (3)  | 0.008 (3) | 0.000 (2)    | -0.005 (2)   | -0.005 (2)   |
| C2  | 0.017 (3)  | 0.015 (3)  | 0.007 (3) | 0.002 (2)    | -0.001 (2)   | -0.003 (2)   |
| C3  | 0.016 (3)  | 0.027 (4)  | 0.004 (3) | 0.000 (3)    | 0.000 (2)    | 0.002 (2)    |
| C4  | 0.024 (3)  | 0.014 (3)  | 0.010 (3) | -0.002 (2)   | -0.010 (2)   | 0.002 (2)    |
| C5  | 0.019 (3)  | 0.029 (4)  | 0.009 (3) | 0.012 (3)    | -0.005 (2)   | -0.002 (3)   |
| C6  | 0.023 (3)  | 0.033 (4)  | 0.012 (3) | 0.001 (3)    | 0.001 (2)    | -0.006 (3)   |
| C7  | 0.037 (4)  | 0.023 (3)  | 0.012 (3) | 0.005 (3)    | 0.001 (3)    | -0.010 (3)   |
| C8  | 0.025 (4)  | 0.034 (4)  | 0.009 (3) | -0.002 (3)   | 0.002 (3)    | 0.003 (3)    |
| C9  | 0.045 (5)  | 0.020 (3)  | 0.016 (3) | -0.004 (3)   | -0.008 (3)   | 0.005 (3)    |
| C10 | 0.027 (4)  | 0.027 (4)  | 0.018 (3) | 0.013 (3)    | -0.004 (3)   | -0.007 (3)   |
| C11 | 0.017 (3)  | 0.017 (3)  | 0.005 (2) | 0.003 (2)    | -0.001 (2)   | 0.000 (2)    |
| C12 | 0.017 (3)  | 0.023 (3)  | 0.008 (3) | 0.009 (2)    | -0.004 (2)   | -0.001 (2)   |
| C13 | 0.016 (3)  | 0.034 (4)  | 0.008 (3) | 0.004 (3)    | -0.004 (2)   | 0.001 (3)    |
| C14 | 0.019 (3)  | 0.025 (3)  | 0.009 (3) | -0.001 (2)   | -0.007 (2)   | 0.001 (2)    |
| C15 | 0.026 (3)  | 0.019 (3)  | 0.007 (3) | 0.007 (3)    | -0.007 (2)   | -0.007 (2)   |
| C16 | 0.027 (3)  | 0.024 (3)  | 0.011 (3) | 0.000 (3)    | -0.001 (2)   | 0.004 (3)    |
| C17 | 0.027 (4)  | 0.023 (3)  | 0.020 (3) | 0.011 (3)    | -0.006 (3)   | -0.004 (3)   |
| C18 | 0.022 (4)  | 0.044 (5)  | 0.015 (3) | 0.000 (3)    | -0.002 (3)   | 0.001 (3)    |
| C19 | 0.031 (4)  | 0.022 (3)  | 0.020 (3) | -0.009 (3)   | -0.004 (3)   | 0.004 (3)    |
| C20 | 0.030 (4)  | 0.026 (3)  | 0.010 (3) | 0.008 (3)    | -0.001 (3)   | -0.006 (3)   |
| C21 | 0.016 (3)  | 0.016 (3)  | 0.010 (3) | 0.003 (2)    | -0.001 (2)   | -0.006 (2)   |
| C22 | 0.019 (3)  | 0.024 (3)  | 0.006 (3) | 0.003 (2)    | 0.004 (2)    | -0.008 (2)   |
| C23 | 0.025 (3)  | 0.018 (3)  | 0.007 (3) | 0.000 (3)    | 0.000 (2)    | -0.007 (2)   |
| C24 | 0.028 (4)  | 0.018 (3)  | 0.008 (3) | 0.003 (3)    | -0.005 (2)   | -0.003 (2)   |
| C25 | 0.019 (3)  | 0.015 (3)  | 0.006 (2) | 0.001 (2)    | 0.000 (2)    | -0.002 (2)   |
| C26 | 0.020 (3)  | 0.024 (4)  | 0.023 (3) | 0.010 (3)    | -0.005 (3)   | -0.003 (3)   |
| C27 | 0.023 (3)  | 0.034 (4)  | 0.018 (3) | -0.003 (3)   | 0.009 (3)    | -0.006 (3)   |
| C28 | 0.041 (4)  | 0.021 (4)  | 0.012 (3) | -0.002 (3)   | -0.002 (3)   | -0.002 (3)   |
| C29 | 0.022 (3)  | 0.026 (4)  | 0.019 (3) | 0.006 (3)    | -0.006 (3)   | -0.001 (3)   |
| C30 | 0.025 (3)  | 0.018 (3)  | 0.016 (3) | -0.003 (2)   | 0.000 (2)    | -0.001 (2)   |
| C31 | 0.025 (3)  | 0.026 (4)  | 0.010 (3) | 0.004 (3)    | -0.004 (2)   | -0.013 (3)   |
| C32 | 0.027 (4)  | 0.047 (5)  | 0.026 (4) | -0.019 (4)   | 0.012 (3)    | -0.026 (4)   |
| C33 | 0.057 (6)  | 0.021 (4)  | 0.016 (3) | -0.011 (3)   | 0.016 (3)    | -0.010 (3)   |
| C34 | 0.034 (4)  | 0.020 (3)  | 0.006 (3) | 0.011 (3)    | -0.003 (2)   | -0.007 (2)   |
| C35 | 0.020 (3)  | 0.017 (3)  | 0.005 (2) | 0.002 (2)    | 0.004 (2)    | -0.006 (2)   |
| C36 | 0.045 (5)  | 0.058 (6)  | 0.019 (4) | 0.028 (4)    | -0.021 (3)   | -0.019 (4)   |
| C37 | 0.053 (7)  | 0.105 (11) | 0.069 (8) | -0.040 (7)   | 0.026 (6)    | -0.070 (8)   |
| C38 | 0.153 (13) | 0.023 (5)  | 0.026 (4) | -0.028 (6)   | 0.039 (6)    | -0.009 (4)   |
| C39 | 0.057 (6)  | 0.040 (5)  | 0.018 (3) | 0.033 (4)    | -0.011 (3)   | -0.010 (3)   |
| C40 | 0.035 (4)  | 0.029 (4)  | 0.011 (3) | -0.008 (3)   | 0.011 (3)    | -0.005 (3)   |

*Geometric parameters (Å, °)*

Ru1—N1

1.915 (5)

C14—C19

1.483 (10)

|         |            |          |            |
|---------|------------|----------|------------|
| Ru1—N2  | 1.937 (5)  | C15—C20  | 1.495 (9)  |
| Ru1—C4  | 2.199 (6)  | C16—H16A | 0.9800     |
| Ru1—C2  | 2.208 (6)  | C16—H16B | 0.9800     |
| Ru1—C5  | 2.215 (6)  | C16—H16C | 0.9800     |
| Ru1—C1  | 2.223 (6)  | C17—H17A | 0.9800     |
| Ru1—C3  | 2.227 (6)  | C17—H17B | 0.9800     |
| Ru1—Ru2 | 2.5418 (7) | C17—H17C | 0.9800     |
| Ru2—N2  | 1.921 (5)  | C18—H18A | 0.9800     |
| Ru2—N1  | 1.929 (6)  | C18—H18B | 0.9800     |
| Ru2—C15 | 2.197 (6)  | C18—H18C | 0.9800     |
| Ru2—C14 | 2.199 (6)  | C19—H19A | 0.9800     |
| Ru2—C12 | 2.214 (6)  | C19—H19B | 0.9800     |
| Ru2—C11 | 2.224 (6)  | C19—H19C | 0.9800     |
| Ru2—C13 | 2.229 (7)  | C20—H20A | 0.9800     |
| Ru3—N3  | 1.917 (5)  | C20—H20B | 0.9800     |
| Ru3—N4  | 1.918 (6)  | C20—H20C | 0.9800     |
| Ru3—C21 | 2.208 (6)  | C21—C25  | 1.429 (9)  |
| Ru3—C24 | 2.208 (6)  | C21—C22  | 1.437 (10) |
| Ru3—C22 | 2.212 (6)  | C21—C26  | 1.494 (9)  |
| Ru3—C25 | 2.214 (6)  | C22—C23  | 1.430 (10) |
| Ru3—C23 | 2.230 (6)  | C22—C27  | 1.500 (9)  |
| Ru3—Ru4 | 2.5347 (7) | C23—C24  | 1.441 (10) |
| Ru4—N3  | 1.908 (6)  | C23—C28  | 1.488 (10) |
| Ru4—N4  | 1.923 (6)  | C24—C25  | 1.442 (9)  |
| Ru4—C35 | 2.194 (6)  | C24—C29  | 1.515 (9)  |
| Ru4—C34 | 2.206 (7)  | C25—C30  | 1.493 (9)  |
| Ru4—C31 | 2.210 (6)  | C26—H26A | 0.9800     |
| Ru4—C32 | 2.222 (7)  | C26—H26B | 0.9800     |
| Ru4—C33 | 2.227 (8)  | C26—H26C | 0.9800     |
| N1—O1   | 1.235 (7)  | C27—H27A | 0.9800     |
| N2—O2   | 1.222 (7)  | C27—H27B | 0.9800     |
| N3—O3   | 1.219 (7)  | C27—H27C | 0.9800     |
| N4—O4   | 1.224 (8)  | C28—H28A | 0.9800     |
| C1—C5   | 1.409 (10) | C28—H28B | 0.9800     |
| C1—C2   | 1.440 (9)  | C28—H28C | 0.9800     |
| C1—C6   | 1.495 (10) | C29—H29A | 0.9800     |
| C2—C3   | 1.412 (9)  | C29—H29B | 0.9800     |
| C2—C7   | 1.486 (9)  | C29—H29C | 0.9800     |
| C3—C4   | 1.428 (10) | C30—H30A | 0.9800     |
| C3—C8   | 1.506 (9)  | C30—H30B | 0.9800     |
| C4—C5   | 1.447 (10) | C30—H30C | 0.9800     |
| C4—C9   | 1.495 (9)  | C31—C35  | 1.419 (9)  |
| C5—C10  | 1.508 (9)  | C31—C32  | 1.447 (12) |
| C6—H6A  | 0.9800     | C31—C36  | 1.498 (11) |
| C6—H6B  | 0.9800     | C32—C33  | 1.423 (14) |
| C6—H6C  | 0.9800     | C32—C37  | 1.500 (13) |
| C7—H7A  | 0.9800     | C33—C34  | 1.425 (12) |
| C7—H7B  | 0.9800     | C33—C38  | 1.498 (12) |
| C7—H7C  | 0.9800     | C34—C35  | 1.435 (9)  |

## supplementary materials

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|            |             |               |            |
|------------|-------------|---------------|------------|
| C8—H8A     | 0.9800      | C34—C39       | 1.506 (11) |
| C8—H8B     | 0.9800      | C35—C40       | 1.505 (9)  |
| C8—H8C     | 0.9800      | C36—H36A      | 0.9800     |
| C9—H9A     | 0.9800      | C36—H36B      | 0.9800     |
| C9—H9B     | 0.9800      | C36—H36C      | 0.9800     |
| C9—H9C     | 0.9800      | C37—H37A      | 0.9800     |
| C10—H10A   | 0.9800      | C37—H37B      | 0.9800     |
| C10—H10B   | 0.9800      | C37—H37C      | 0.9800     |
| C10—H10C   | 0.9800      | C38—H38A      | 0.9800     |
| C11—C15    | 1.422 (9)   | C38—H38B      | 0.9800     |
| C11—C12    | 1.439 (9)   | C38—H38C      | 0.9800     |
| C11—C16    | 1.480 (9)   | C39—H39A      | 0.9800     |
| C12—C13    | 1.416 (10)  | C39—H39B      | 0.9800     |
| C12—C17    | 1.490 (9)   | C39—H39C      | 0.9800     |
| C13—C14    | 1.443 (10)  | C40—H40A      | 0.9800     |
| C13—C18    | 1.502 (10)  | C40—H40B      | 0.9800     |
| C14—C15    | 1.425 (10)  | C40—H40C      | 0.9800     |
| N1—Ru1—N2  | 97.3 (2)    | H10A—C10—H10C | 109.5      |
| N1—Ru1—C4  | 136.9 (3)   | H10B—C10—H10C | 109.5      |
| N2—Ru1—C4  | 110.0 (2)   | C15—C11—C12   | 107.2 (6)  |
| N1—Ru1—C2  | 128.8 (2)   | C15—C11—C16   | 125.7 (6)  |
| N2—Ru1—C2  | 120.6 (2)   | C12—C11—C16   | 127.0 (6)  |
| C4—Ru1—C2  | 63.1 (2)    | C15—C11—Ru2   | 70.2 (3)   |
| N1—Ru1—C5  | 104.3 (2)   | C12—C11—Ru2   | 70.7 (3)   |
| N2—Ru1—C5  | 146.3 (3)   | C16—C11—Ru2   | 123.6 (4)  |
| C4—Ru1—C5  | 38.3 (3)    | C13—C12—C11   | 108.5 (6)  |
| C2—Ru1—C5  | 62.9 (2)    | C13—C12—C17   | 125.5 (6)  |
| N1—Ru1—C1  | 100.8 (2)   | C11—C12—C17   | 125.7 (7)  |
| N2—Ru1—C1  | 158.4 (2)   | C13—C12—Ru2   | 72.0 (4)   |
| C4—Ru1—C1  | 63.0 (2)    | C11—C12—Ru2   | 71.4 (3)   |
| C2—Ru1—C1  | 37.9 (2)    | C17—C12—Ru2   | 127.5 (5)  |
| C5—Ru1—C1  | 37.0 (3)    | C12—C13—C14   | 107.9 (6)  |
| N1—Ru1—C3  | 163.2 (2)   | C12—C13—C18   | 127.0 (7)  |
| N2—Ru1—C3  | 99.1 (2)    | C14—C13—C18   | 125.1 (7)  |
| C4—Ru1—C3  | 37.7 (2)    | C12—C13—Ru2   | 70.8 (4)   |
| C2—Ru1—C3  | 37.1 (2)    | C14—C13—Ru2   | 69.8 (4)   |
| C5—Ru1—C3  | 62.8 (2)    | C18—C13—Ru2   | 124.6 (4)  |
| C1—Ru1—C3  | 62.4 (2)    | C15—C14—C13   | 107.3 (6)  |
| N1—Ru1—Ru2 | 48.86 (17)  | C15—C14—C19   | 127.6 (7)  |
| N2—Ru1—Ru2 | 48.52 (16)  | C13—C14—C19   | 124.9 (7)  |
| C4—Ru1—Ru2 | 145.59 (17) | C15—C14—Ru2   | 71.0 (4)   |
| C2—Ru1—Ru2 | 147.60 (18) | C13—C14—Ru2   | 72.1 (4)   |
| C5—Ru1—Ru2 | 146.00 (17) | C19—C14—Ru2   | 126.5 (5)  |
| C1—Ru1—Ru2 | 147.30 (17) | C11—C15—C14   | 109.0 (6)  |
| C3—Ru1—Ru2 | 147.23 (17) | C11—C15—C20   | 124.2 (7)  |
| N2—Ru2—N1  | 97.4 (2)    | C14—C15—C20   | 126.8 (7)  |
| N2—Ru2—C15 | 145.9 (3)   | C11—C15—Ru2   | 72.3 (3)   |
| N1—Ru2—C15 | 104.4 (2)   | C14—C15—Ru2   | 71.1 (4)   |
| N2—Ru2—C14 | 110.2 (2)   | C20—C15—Ru2   | 123.8 (4)  |

|             |             |               |           |
|-------------|-------------|---------------|-----------|
| N1—Ru2—C14  | 137.1 (3)   | C11—C16—H16A  | 109.5     |
| C15—Ru2—C14 | 37.8 (3)    | C11—C16—H16B  | 109.5     |
| N2—Ru2—C12  | 121.4 (2)   | H16A—C16—H16B | 109.5     |
| N1—Ru2—C12  | 127.6 (3)   | C11—C16—H16C  | 109.5     |
| C15—Ru2—C12 | 62.9 (2)    | H16A—C16—H16C | 109.5     |
| C14—Ru2—C12 | 63.2 (3)    | H16B—C16—H16C | 109.5     |
| N2—Ru2—C11  | 159.2 (2)   | C12—C17—H17A  | 109.5     |
| N1—Ru2—C11  | 99.9 (2)    | C12—C17—H17B  | 109.5     |
| C15—Ru2—C11 | 37.5 (2)    | H17A—C17—H17B | 109.5     |
| C14—Ru2—C11 | 63.2 (2)    | C12—C17—H17C  | 109.5     |
| C12—Ru2—C11 | 37.8 (2)    | H17A—C17—H17C | 109.5     |
| N2—Ru2—C13  | 99.5 (2)    | H17B—C17—H17C | 109.5     |
| N1—Ru2—C13  | 162.6 (2)   | C13—C18—H18A  | 109.5     |
| C15—Ru2—C13 | 62.9 (3)    | C13—C18—H18B  | 109.5     |
| C14—Ru2—C13 | 38.0 (3)    | H18A—C18—H18B | 109.5     |
| C12—Ru2—C13 | 37.2 (3)    | C13—C18—H18C  | 109.5     |
| C11—Ru2—C13 | 62.7 (2)    | H18A—C18—H18C | 109.5     |
| N2—Ru2—Ru1  | 49.06 (16)  | H18B—C18—H18C | 109.5     |
| N1—Ru2—Ru1  | 48.36 (15)  | C14—C19—H19A  | 109.5     |
| C15—Ru2—Ru1 | 145.55 (17) | C14—C19—H19B  | 109.5     |
| C14—Ru2—Ru1 | 146.36 (18) | H19A—C19—H19B | 109.5     |
| C12—Ru2—Ru1 | 147.44 (18) | C14—C19—H19C  | 109.5     |
| C11—Ru2—Ru1 | 145.97 (17) | H19A—C19—H19C | 109.5     |
| C13—Ru2—Ru1 | 148.02 (17) | H19B—C19—H19C | 109.5     |
| N3—Ru3—N4   | 97.1 (2)    | C15—C20—H20A  | 109.5     |
| N3—Ru3—C21  | 104.8 (2)   | C15—C20—H20B  | 109.5     |
| N4—Ru3—C21  | 147.1 (2)   | H20A—C20—H20B | 109.5     |
| N3—Ru3—C24  | 127.1 (3)   | C15—C20—H20C  | 109.5     |
| N4—Ru3—C24  | 120.4 (3)   | H20A—C20—H20C | 109.5     |
| C21—Ru3—C24 | 63.5 (2)    | H20B—C20—H20C | 109.5     |
| N3—Ru3—C22  | 137.8 (3)   | C25—C21—C22   | 108.4 (6) |
| N4—Ru3—C22  | 111.1 (3)   | C25—C21—C26   | 124.9 (6) |
| C21—Ru3—C22 | 37.9 (2)    | C22—C21—C26   | 126.6 (6) |
| C24—Ru3—C22 | 63.6 (3)    | C25—C21—Ru3   | 71.4 (4)  |
| N3—Ru3—C25  | 99.8 (2)    | C22—C21—Ru3   | 71.2 (4)  |
| N4—Ru3—C25  | 158.4 (2)   | C26—C21—Ru3   | 125.0 (4) |
| C21—Ru3—C25 | 37.7 (2)    | C23—C22—C21   | 107.7 (6) |
| C24—Ru3—C25 | 38.1 (2)    | C23—C22—C27   | 124.8 (7) |
| C22—Ru3—C25 | 63.4 (2)    | C21—C22—C27   | 127.3 (6) |
| N3—Ru3—C23  | 162.8 (3)   | C23—C22—Ru3   | 71.9 (4)  |
| N4—Ru3—C23  | 99.3 (3)    | C21—C22—Ru3   | 70.9 (3)  |
| C21—Ru3—C23 | 62.9 (2)    | C27—C22—Ru3   | 126.3 (5) |
| C24—Ru3—C23 | 37.9 (3)    | C22—C23—C24   | 108.4 (6) |
| C22—Ru3—C23 | 37.6 (2)    | C22—C23—C28   | 125.4 (7) |
| C25—Ru3—C23 | 63.0 (2)    | C24—C23—C28   | 126.2 (6) |
| N3—Ru3—Ru4  | 48.36 (17)  | C22—C23—Ru3   | 70.6 (3)  |
| N4—Ru3—Ru4  | 48.78 (17)  | C24—C23—Ru3   | 70.3 (4)  |
| C21—Ru3—Ru4 | 146.67 (16) | C28—C23—Ru3   | 125.4 (5) |
| C24—Ru3—Ru4 | 145.42 (19) | C23—C24—C25   | 107.4 (6) |

## supplementary materials

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| C22—Ru3—Ru4 | 147.66 (18) | C23—C24—C29   | 126.6 (6)  |
| C25—Ru3—Ru4 | 145.37 (16) | C25—C24—C29   | 125.8 (7)  |
| C23—Ru3—Ru4 | 147.50 (18) | C23—C24—Ru3   | 71.9 (4)   |
| N3—Ru4—N4   | 97.2 (2)    | C25—C24—Ru3   | 71.2 (4)   |
| N3—Ru4—C35  | 99.6 (2)    | C29—C24—Ru3   | 126.9 (5)  |
| N4—Ru4—C35  | 155.4 (3)   | C21—C25—C24   | 108.0 (6)  |
| N3—Ru4—C34  | 130.1 (3)   | C21—C25—C30   | 125.1 (6)  |
| N4—Ru4—C34  | 117.9 (3)   | C24—C25—C30   | 126.9 (6)  |
| C35—Ru4—C34 | 38.1 (2)    | C21—C25—Ru3   | 70.9 (4)   |
| N3—Ru4—C31  | 100.5 (3)   | C24—C25—Ru3   | 70.8 (4)   |
| N4—Ru4—C31  | 153.2 (3)   | C30—C25—Ru3   | 124.7 (4)  |
| C35—Ru4—C31 | 37.6 (2)    | C21—C26—H26A  | 109.5      |
| C34—Ru4—C31 | 63.3 (2)    | C21—C26—H26B  | 109.5      |
| N3—Ru4—C32  | 132.2 (3)   | H26A—C26—H26B | 109.5      |
| N4—Ru4—C32  | 116.2 (3)   | C21—C26—H26C  | 109.5      |
| C35—Ru4—C32 | 63.2 (3)    | H26A—C26—H26C | 109.5      |
| C34—Ru4—C32 | 63.1 (3)    | H26B—C26—H26C | 109.5      |
| C31—Ru4—C32 | 38.1 (3)    | C22—C27—H27A  | 109.5      |
| N3—Ru4—C33  | 161.7 (3)   | C22—C27—H27B  | 109.5      |
| N4—Ru4—C33  | 101.0 (3)   | H27A—C27—H27B | 109.5      |
| C35—Ru4—C33 | 62.8 (3)    | C22—C27—H27C  | 109.5      |
| C34—Ru4—C33 | 37.5 (3)    | H27A—C27—H27C | 109.5      |
| C31—Ru4—C33 | 62.9 (3)    | H27B—C27—H27C | 109.5      |
| C32—Ru4—C33 | 37.3 (4)    | C23—C28—H28A  | 109.5      |
| N3—Ru4—Ru3  | 48.64 (16)  | C23—C28—H28B  | 109.5      |
| N4—Ru4—Ru3  | 48.63 (18)  | H28A—C28—H28B | 109.5      |
| C35—Ru4—Ru3 | 143.66 (18) | C23—C28—H28C  | 109.5      |
| C34—Ru4—Ru3 | 145.77 (19) | H28A—C28—H28C | 109.5      |
| C31—Ru4—Ru3 | 145.23 (19) | H28B—C28—H28C | 109.5      |
| C32—Ru4—Ru3 | 148.8 (2)   | C24—C29—H29A  | 109.5      |
| C33—Ru4—Ru3 | 149.5 (2)   | C24—C29—H29B  | 109.5      |
| O1—N1—Ru1   | 138.4 (5)   | H29A—C29—H29B | 109.5      |
| O1—N1—Ru2   | 138.7 (4)   | C24—C29—H29C  | 109.5      |
| Ru1—N1—Ru2  | 82.8 (2)    | H29A—C29—H29C | 109.5      |
| O2—N2—Ru2   | 139.1 (4)   | H29B—C29—H29C | 109.5      |
| O2—N2—Ru1   | 138.4 (4)   | C25—C30—H30A  | 109.5      |
| Ru2—N2—Ru1  | 82.4 (2)    | C25—C30—H30B  | 109.5      |
| O3—N3—Ru4   | 138.1 (4)   | H30A—C30—H30B | 109.5      |
| O3—N3—Ru3   | 138.9 (5)   | C25—C30—H30C  | 109.5      |
| Ru4—N3—Ru3  | 83.0 (2)    | H30A—C30—H30C | 109.5      |
| O4—N4—Ru3   | 137.9 (5)   | H30B—C30—H30C | 109.5      |
| O4—N4—Ru4   | 139.5 (5)   | C35—C31—C32   | 107.7 (7)  |
| Ru3—N4—Ru4  | 82.6 (2)    | C35—C31—C36   | 125.2 (8)  |
| C5—C1—C2    | 108.3 (6)   | C32—C31—C36   | 127.1 (8)  |
| C5—C1—C6    | 125.0 (6)   | C35—C31—Ru4   | 70.6 (3)   |
| C2—C1—C6    | 126.8 (6)   | C32—C31—Ru4   | 71.4 (4)   |
| C5—C1—Ru1   | 71.2 (4)    | C36—C31—Ru4   | 123.9 (5)  |
| C2—C1—Ru1   | 70.5 (4)    | C33—C32—C31   | 107.5 (7)  |
| C6—C1—Ru1   | 123.9 (4)   | C33—C32—C37   | 127.4 (10) |

|             |           |               |            |
|-------------|-----------|---------------|------------|
| C3—C2—C1    | 107.9 (6) | C31—C32—C37   | 124.9 (10) |
| C3—C2—C7    | 125.5 (6) | C33—C32—Ru4   | 71.6 (4)   |
| C1—C2—C7    | 126.2 (6) | C31—C32—Ru4   | 70.5 (4)   |
| C3—C2—Ru1   | 72.2 (4)  | C37—C32—Ru4   | 127.8 (6)  |
| C1—C2—Ru1   | 71.6 (3)  | C32—C33—C34   | 108.8 (7)  |
| C7—C2—Ru1   | 127.2 (5) | C32—C33—C38   | 126.6 (10) |
| C2—C3—C4    | 108.5 (6) | C34—C33—C38   | 124.6 (10) |
| C2—C3—C8    | 126.9 (6) | C32—C33—Ru4   | 71.1 (4)   |
| C4—C3—C8    | 124.5 (6) | C34—C33—Ru4   | 70.4 (4)   |
| C2—C3—Ru1   | 70.7 (3)  | C38—C33—Ru4   | 124.2 (5)  |
| C4—C3—Ru1   | 70.1 (3)  | C33—C34—C35   | 107.4 (7)  |
| C8—C3—Ru1   | 123.8 (4) | C33—C34—C39   | 128.4 (8)  |
| C3—C4—C5    | 107.3 (6) | C35—C34—C39   | 124.1 (8)  |
| C3—C4—C9    | 125.9 (7) | C33—C34—Ru4   | 72.1 (4)   |
| C5—C4—C9    | 126.8 (7) | C35—C34—Ru4   | 70.5 (4)   |
| C3—C4—Ru1   | 72.2 (3)  | C39—C34—Ru4   | 126.8 (5)  |
| C5—C4—Ru1   | 71.5 (3)  | C31—C35—C34   | 108.7 (6)  |
| C9—C4—Ru1   | 123.9 (4) | C31—C35—C40   | 125.2 (6)  |
| C1—C5—C4    | 107.9 (6) | C34—C35—C40   | 126.2 (7)  |
| C1—C5—C10   | 124.4 (7) | C31—C35—Ru4   | 71.8 (4)   |
| C4—C5—C10   | 127.7 (7) | C34—C35—Ru4   | 71.4 (4)   |
| C1—C5—Ru1   | 71.8 (4)  | C40—C35—Ru4   | 123.4 (4)  |
| C4—C5—Ru1   | 70.2 (4)  | C31—C36—H36A  | 109.5      |
| C10—C5—Ru1  | 125.0 (4) | C31—C36—H36B  | 109.5      |
| C1—C6—H6A   | 109.5     | H36A—C36—H36B | 109.5      |
| C1—C6—H6B   | 109.5     | C31—C36—H36C  | 109.5      |
| H6A—C6—H6B  | 109.5     | H36A—C36—H36C | 109.5      |
| C1—C6—H6C   | 109.5     | H36B—C36—H36C | 109.5      |
| H6A—C6—H6C  | 109.5     | C32—C37—H37A  | 109.5      |
| H6B—C6—H6C  | 109.5     | C32—C37—H37B  | 109.5      |
| C2—C7—H7A   | 109.5     | H37A—C37—H37B | 109.5      |
| C2—C7—H7B   | 109.5     | C32—C37—H37C  | 109.5      |
| H7A—C7—H7B  | 109.5     | H37A—C37—H37C | 109.5      |
| C2—C7—H7C   | 109.5     | H37B—C37—H37C | 109.5      |
| H7A—C7—H7C  | 109.5     | C33—C38—H38A  | 109.5      |
| H7B—C7—H7C  | 109.5     | C33—C38—H38B  | 109.5      |
| C3—C8—H8A   | 109.5     | H38A—C38—H38B | 109.5      |
| C3—C8—H8B   | 109.5     | C33—C38—H38C  | 109.5      |
| H8A—C8—H8B  | 109.5     | H38A—C38—H38C | 109.5      |
| C3—C8—H8C   | 109.5     | H38B—C38—H38C | 109.5      |
| H8A—C8—H8C  | 109.5     | C34—C39—H39A  | 109.5      |
| H8B—C8—H8C  | 109.5     | C34—C39—H39B  | 109.5      |
| C4—C9—H9A   | 109.5     | H39A—C39—H39B | 109.5      |
| C4—C9—H9B   | 109.5     | C34—C39—H39C  | 109.5      |
| H9A—C9—H9B  | 109.5     | H39A—C39—H39C | 109.5      |
| C4—C9—H9C   | 109.5     | H39B—C39—H39C | 109.5      |
| H9A—C9—H9C  | 109.5     | C35—C40—H40A  | 109.5      |
| H9B—C9—H9C  | 109.5     | C35—C40—H40B  | 109.5      |
| C5—C10—H10A | 109.5     | H40A—C40—H40B | 109.5      |

## supplementary materials

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| C5—C10—H10B    | 109.5      | C35—C40—H40C    | 109.5      |
| H10A—C10—H10B  | 109.5      | H40A—C40—H40C   | 109.5      |
| C5—C10—H10C    | 109.5      | H40B—C40—H40C   | 109.5      |
| N1—Ru1—Ru2—N2  | 177.2 (3)  | C14—Ru2—C12—C11 | -80.1 (4)  |
| C4—Ru1—Ru2—N2  | 61.1 (4)   | C13—Ru2—C12—C11 | -117.5 (6) |
| C2—Ru1—Ru2—N2  | -82.7 (4)  | Ru1—Ru2—C12—C11 | 119.6 (4)  |
| C5—Ru1—Ru2—N2  | 132.4 (4)  | N2—Ru2—C12—C17  | 60.4 (7)   |
| C1—Ru1—Ru2—N2  | -157.1 (4) | N1—Ru2—C12—C17  | -71.0 (7)  |
| C3—Ru1—Ru2—N2  | -10.2 (4)  | C15—Ru2—C12—C17 | -158.6 (7) |
| N2—Ru1—Ru2—N1  | -177.2 (3) | C14—Ru2—C12—C17 | 158.8 (7)  |
| C4—Ru1—Ru2—N1  | -116.1 (4) | C11—Ru2—C12—C17 | -121.2 (8) |
| C2—Ru1—Ru2—N1  | 100.1 (4)  | C13—Ru2—C12—C17 | 121.4 (8)  |
| C5—Ru1—Ru2—N1  | -44.8 (4)  | Ru1—Ru2—C12—C17 | -1.6 (9)   |
| C1—Ru1—Ru2—N1  | 25.8 (4)   | C11—C12—C13—C14 | 2.2 (7)    |
| C3—Ru1—Ru2—N1  | 172.6 (4)  | C17—C12—C13—C14 | 176.1 (6)  |
| N1—Ru1—Ru2—C15 | 44.9 (4)   | Ru2—C12—C13—C14 | -60.3 (4)  |
| N2—Ru1—Ru2—C15 | -132.3 (4) | C11—C12—C13—C18 | -178.1 (6) |
| C4—Ru1—Ru2—C15 | -71.2 (5)  | C17—C12—C13—C18 | -4.2 (11)  |
| C2—Ru1—Ru2—C15 | 145.0 (5)  | Ru2—C12—C13—C18 | 119.4 (7)  |
| C5—Ru1—Ru2—C15 | 0.1 (5)    | C11—C12—C13—Ru2 | 62.5 (4)   |
| C1—Ru1—Ru2—C15 | 70.6 (5)   | C17—C12—C13—Ru2 | -123.6 (6) |
| C3—Ru1—Ru2—C15 | -142.5 (5) | N2—Ru2—C13—C12  | 130.8 (4)  |
| N1—Ru1—Ru2—C14 | 115.7 (4)  | N1—Ru2—C13—C12  | -34.3 (10) |
| N2—Ru1—Ru2—C14 | -61.5 (4)  | C15—Ru2—C13—C12 | -80.1 (4)  |
| C4—Ru1—Ru2—C14 | -0.5 (5)   | C14—Ru2—C13—C12 | -118.3 (5) |
| C2—Ru1—Ru2—C14 | -144.3 (5) | C11—Ru2—C13—C12 | -37.8 (4)  |
| C5—Ru1—Ru2—C14 | 70.9 (5)   | Ru1—Ru2—C13—C12 | 121.4 (4)  |
| C1—Ru1—Ru2—C14 | 141.4 (5)  | N2—Ru2—C13—C14  | -110.8 (4) |
| C3—Ru1—Ru2—C14 | -71.8 (5)  | N1—Ru2—C13—C14  | 84.0 (10)  |
| N1—Ru1—Ru2—C12 | -97.2 (4)  | C15—Ru2—C13—C14 | 38.2 (4)   |
| N2—Ru1—Ru2—C12 | 85.6 (4)   | C12—Ru2—C13—C14 | 118.3 (5)  |
| C4—Ru1—Ru2—C12 | 146.7 (5)  | C11—Ru2—C13—C14 | 80.6 (4)   |
| C2—Ru1—Ru2—C12 | 2.9 (5)    | Ru1—Ru2—C13—C14 | -120.2 (4) |
| C5—Ru1—Ru2—C12 | -142.0 (5) | N2—Ru2—C13—C18  | 8.5 (7)    |
| C1—Ru1—Ru2—C12 | -71.5 (5)  | N1—Ru2—C13—C18  | -156.6 (7) |
| C3—Ru1—Ru2—C12 | 75.4 (5)   | C15—Ru2—C13—C18 | 157.6 (8)  |
| N1—Ru1—Ru2—C11 | -24.8 (4)  | C14—Ru2—C13—C18 | 119.4 (8)  |
| N2—Ru1—Ru2—C11 | 158.0 (4)  | C12—Ru2—C13—C18 | -122.3 (8) |
| C4—Ru1—Ru2—C11 | -140.9 (5) | C11—Ru2—C13—C18 | -160.1 (8) |
| C2—Ru1—Ru2—C11 | 75.3 (4)   | Ru1—Ru2—C13—C18 | -0.8 (9)   |
| C5—Ru1—Ru2—C11 | -69.6 (5)  | C12—C13—C14—C15 | -1.8 (7)   |
| C1—Ru1—Ru2—C11 | 0.9 (4)    | C18—C13—C14—C15 | 178.5 (6)  |
| C3—Ru1—Ru2—C11 | 147.8 (5)  | Ru2—C13—C14—C15 | -62.7 (4)  |
| N1—Ru1—Ru2—C13 | -170.5 (4) | C12—C13—C14—C19 | -176.7 (6) |
| N2—Ru1—Ru2—C13 | 12.3 (4)   | C18—C13—C14—C19 | 3.6 (10)   |
| C4—Ru1—Ru2—C13 | 73.4 (5)   | Ru2—C13—C14—C19 | 122.4 (6)  |
| C2—Ru1—Ru2—C13 | -70.4 (5)  | C12—C13—C14—Ru2 | 60.9 (4)   |
| C5—Ru1—Ru2—C13 | 144.7 (5)  | C18—C13—C14—Ru2 | -118.8 (6) |
| C1—Ru1—Ru2—C13 | -144.8 (5) | N2—Ru2—C14—C15  | -164.5 (4) |

|                 |            |                 |            |
|-----------------|------------|-----------------|------------|
| C3—Ru1—Ru2—C13  | 2.1 (5)    | N1—Ru2—C14—C15  | -37.8 (5)  |
| N4—Ru3—Ru4—N3   | 177.4 (3)  | C12—Ru2—C14—C15 | 79.6 (4)   |
| C21—Ru3—Ru4—N3  | 43.1 (4)   | C11—Ru2—C14—C15 | 37.0 (4)   |
| C24—Ru3—Ru4—N3  | -97.6 (4)  | C13—Ru2—C14—C15 | 116.2 (6)  |
| C22—Ru3—Ru4—N3  | 116.7 (4)  | Ru1—Ru2—C14—C15 | -119.5 (4) |
| C25—Ru3—Ru4—N3  | -27.6 (4)  | N2—Ru2—C14—C13  | 79.3 (4)   |
| C23—Ru3—Ru4—N3  | -169.5 (4) | N1—Ru2—C14—C13  | -154.0 (4) |
| N3—Ru3—Ru4—N4   | -177.4 (3) | C15—Ru2—C14—C13 | -116.2 (6) |
| C21—Ru3—Ru4—N4  | -134.3 (4) | C12—Ru2—C14—C13 | -36.6 (4)  |
| C24—Ru3—Ru4—N4  | 85.0 (4)   | C11—Ru2—C14—C13 | -79.2 (4)  |
| C22—Ru3—Ru4—N4  | -60.6 (4)  | Ru1—Ru2—C14—C13 | 124.3 (4)  |
| C25—Ru3—Ru4—N4  | 155.1 (4)  | N2—Ru2—C14—C19  | -41.4 (7)  |
| C23—Ru3—Ru4—N4  | 13.2 (4)   | N1—Ru2—C14—C19  | 85.4 (7)   |
| N3—Ru3—Ru4—C35  | 34.7 (4)   | C15—Ru2—C14—C19 | 123.2 (8)  |
| N4—Ru3—Ru4—C35  | -147.9 (4) | C12—Ru2—C14—C19 | -157.2 (7) |
| C21—Ru3—Ru4—C35 | 77.8 (4)   | C11—Ru2—C14—C19 | 160.2 (7)  |
| C24—Ru3—Ru4—C35 | -62.9 (4)  | C13—Ru2—C14—C19 | -120.6 (8) |
| C22—Ru3—Ru4—C35 | 151.4 (5)  | Ru1—Ru2—C14—C19 | 3.7 (9)    |
| C25—Ru3—Ru4—C35 | 7.1 (4)    | C12—C11—C15—C14 | 0.7 (7)    |
| C23—Ru3—Ru4—C35 | -134.8 (5) | C16—C11—C15—C14 | 179.8 (6)  |
| N3—Ru3—Ru4—C34  | 103.4 (4)  | Ru2—C11—C15—C14 | 62.0 (4)   |
| N4—Ru3—Ru4—C34  | -79.3 (4)  | C12—C11—C15—C20 | 179.3 (6)  |
| C21—Ru3—Ru4—C34 | 146.4 (5)  | C16—C11—C15—C20 | -1.6 (10)  |
| C24—Ru3—Ru4—C34 | 5.8 (5)    | Ru2—C11—C15—C20 | -119.3 (6) |
| C22—Ru3—Ru4—C34 | -139.9 (5) | C12—C11—C15—Ru2 | -61.4 (4)  |
| C25—Ru3—Ru4—C34 | 75.8 (5)   | C16—C11—C15—Ru2 | 117.7 (6)  |
| C23—Ru3—Ru4—C34 | -66.1 (5)  | C13—C14—C15—C11 | 0.7 (7)    |
| N3—Ru3—Ru4—C31  | -32.5 (4)  | C19—C14—C15—C11 | 175.4 (6)  |
| N4—Ru3—Ru4—C31  | 144.8 (4)  | Ru2—C14—C15—C11 | -62.8 (4)  |
| C21—Ru3—Ru4—C31 | 10.5 (5)   | C13—C14—C15—C20 | -177.9 (6) |
| C24—Ru3—Ru4—C31 | -130.1 (5) | C19—C14—C15—C20 | -3.2 (11)  |
| C22—Ru3—Ru4—C31 | 84.2 (5)   | Ru2—C14—C15—C20 | 118.7 (6)  |
| C25—Ru3—Ru4—C31 | -60.1 (5)  | C13—C14—C15—Ru2 | 63.5 (4)   |
| C23—Ru3—Ru4—C31 | 158.0 (5)  | C19—C14—C15—Ru2 | -121.9 (7) |
| N3—Ru3—Ru4—C32  | -105.9 (6) | N2—Ru2—C15—C11  | 144.6 (4)  |
| N4—Ru3—Ru4—C32  | 71.4 (6)   | N1—Ru2—C15—C11  | -87.5 (4)  |
| C21—Ru3—Ru4—C32 | -62.9 (6)  | C14—Ru2—C15—C11 | 118.0 (6)  |
| C24—Ru3—Ru4—C32 | 156.5 (6)  | C12—Ru2—C15—C11 | 37.7 (4)   |
| C22—Ru3—Ru4—C32 | 10.8 (6)   | C13—Ru2—C15—C11 | 79.7 (4)   |
| C25—Ru3—Ru4—C32 | -133.5 (6) | Ru1—Ru2—C15—C11 | -120.5 (4) |
| C23—Ru3—Ru4—C32 | 84.6 (6)   | N2—Ru2—C15—C14  | 26.5 (6)   |
| N3—Ru3—Ru4—C33  | 176.9 (6)  | N1—Ru2—C15—C14  | 154.5 (4)  |
| N4—Ru3—Ru4—C33  | -5.7 (6)   | C12—Ru2—C15—C14 | -80.3 (4)  |
| C21—Ru3—Ru4—C33 | -140.0 (6) | C11—Ru2—C15—C14 | -118.0 (6) |
| C24—Ru3—Ru4—C33 | 79.3 (6)   | C13—Ru2—C15—C14 | -38.4 (4)  |
| C22—Ru3—Ru4—C33 | -66.4 (6)  | Ru1—Ru2—C15—C14 | 121.5 (4)  |
| C25—Ru3—Ru4—C33 | 149.4 (6)  | N2—Ru2—C15—C20  | -95.7 (7)  |
| C23—Ru3—Ru4—C33 | 7.4 (6)    | N1—Ru2—C15—C20  | 32.3 (7)   |
| N2—Ru1—N1—O1    | -173.6 (7) | C14—Ru2—C15—C20 | -122.2 (8) |

## supplementary materials

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|----------------|------------|-----------------|------------|
| C4—Ru1—N1—O1   | -43.7 (9)  | C12—Ru2—C15—C20 | 157.5 (7)  |
| C2—Ru1—N1—O1   | 46.8 (8)   | C11—Ru2—C15—C20 | 119.8 (8)  |
| C5—Ru1—N1—O1   | -19.8 (8)  | C13—Ru2—C15—C20 | -160.6 (7) |
| C1—Ru1—N1—O1   | 18.1 (8)   | Ru1—Ru2—C15—C20 | -0.7 (9)   |
| C3—Ru1—N1—O1   | 18.3 (14)  | N3—Ru3—C21—C25  | -86.9 (4)  |
| Ru2—Ru1—N1—O1  | -175.8 (9) | N4—Ru3—C21—C25  | 143.1 (4)  |
| N2—Ru1—N1—Ru2  | 2.1 (2)    | C24—Ru3—C21—C25 | 37.5 (4)   |
| C4—Ru1—N1—Ru2  | 132.1 (3)  | C22—Ru3—C21—C25 | 117.8 (5)  |
| C2—Ru1—N1—Ru2  | -137.4 (3) | C23—Ru3—C21—C25 | 80.2 (4)   |
| C5—Ru1—N1—Ru2  | 156.0 (2)  | Ru4—Ru3—C21—C25 | -118.8 (3) |
| C1—Ru1—N1—Ru2  | -166.2 (2) | N3—Ru3—C21—C22  | 155.2 (4)  |
| C3—Ru1—N1—Ru2  | -166.0 (8) | N4—Ru3—C21—C22  | 25.3 (6)   |
| N2—Ru2—N1—O1   | 173.6 (8)  | C24—Ru3—C21—C22 | -80.3 (4)  |
| C15—Ru2—N1—O1  | 20.1 (8)   | C25—Ru3—C21—C22 | -117.8 (5) |
| C14—Ru2—N1—O1  | 42.9 (9)   | C23—Ru3—C21—C22 | -37.7 (4)  |
| C12—Ru2—N1—O1  | -46.6 (8)  | Ru4—Ru3—C21—C22 | 123.4 (4)  |
| C11—Ru2—N1—O1  | -18.1 (8)  | N3—Ru3—C21—C26  | 33.2 (6)   |
| C13—Ru2—N1—O1  | -21.2 (14) | N4—Ru3—C21—C26  | -96.8 (7)  |
| Ru1—Ru2—N1—O1  | 175.7 (9)  | C24—Ru3—C21—C26 | 157.6 (7)  |
| N2—Ru2—N1—Ru1  | -2.1 (2)   | C22—Ru3—C21—C26 | -122.1 (7) |
| C15—Ru2—N1—Ru1 | -155.7 (2) | C25—Ru3—C21—C26 | 120.1 (7)  |
| C14—Ru2—N1—Ru1 | -132.8 (3) | C23—Ru3—C21—C26 | -159.7 (7) |
| C12—Ru2—N1—Ru1 | 137.6 (2)  | Ru4—Ru3—C21—C26 | 1.3 (8)    |
| C11—Ru2—N1—Ru1 | 166.2 (2)  | C25—C21—C22—C23 | 0.9 (7)    |
| C13—Ru2—N1—Ru1 | 163.1 (8)  | C26—C21—C22—C23 | -177.0 (6) |
| N1—Ru2—N2—O2   | -175.0 (7) | Ru3—C21—C22—C23 | 62.9 (4)   |
| C15—Ru2—N2—O2  | -45.3 (10) | C25—C21—C22—C27 | 176.4 (6)  |
| C14—Ru2—N2—O2  | -28.4 (8)  | C26—C21—C22—C27 | -1.5 (10)  |
| C12—Ru2—N2—O2  | 41.9 (8)   | Ru3—C21—C22—C27 | -121.6 (7) |
| C11—Ru2—N2—O2  | 39.1 (11)  | C25—C21—C22—Ru3 | -62.0 (4)  |
| C13—Ru2—N2—O2  | 9.5 (8)    | C26—C21—C22—Ru3 | 120.1 (6)  |
| Ru1—Ru2—N2—O2  | -177.1 (8) | N3—Ru3—C22—C23  | -154.0 (4) |
| N1—Ru2—N2—Ru1  | 2.1 (2)    | N4—Ru3—C22—C23  | 77.5 (4)   |
| C15—Ru2—N2—Ru1 | 131.8 (4)  | C21—Ru3—C22—C23 | -116.9 (6) |
| C14—Ru2—N2—Ru1 | 148.7 (2)  | C24—Ru3—C22—C23 | -36.9 (4)  |
| C12—Ru2—N2—Ru1 | -141.0 (2) | C25—Ru3—C22—C23 | -79.6 (4)  |
| C11—Ru2—N2—Ru1 | -143.8 (6) | Ru4—Ru3—C22—C23 | 122.2 (4)  |
| C13—Ru2—N2—Ru1 | -173.4 (2) | N3—Ru3—C22—C21  | -37.1 (5)  |
| N1—Ru1—N2—O2   | 175.0 (7)  | N4—Ru3—C22—C21  | -165.6 (4) |
| C4—Ru1—N2—O2   | 28.9 (8)   | C24—Ru3—C22—C21 | 80.0 (4)   |
| C2—Ru1—N2—O2   | -41.0 (8)  | C25—Ru3—C22—C21 | 37.2 (4)   |
| C5—Ru1—N2—O2   | 45.2 (9)   | C23—Ru3—C22—C21 | 116.9 (6)  |
| C1—Ru1—N2—O2   | -37.8 (11) | Ru4—Ru3—C22—C21 | -121.0 (4) |
| C3—Ru1—N2—O2   | -8.5 (7)   | N3—Ru3—C22—C27  | 85.7 (7)   |
| Ru2—Ru1—N2—O2  | 177.1 (8)  | N4—Ru3—C22—C27  | -42.8 (7)  |
| N1—Ru1—N2—Ru2  | -2.1 (2)   | C21—Ru3—C22—C27 | 122.8 (8)  |
| C4—Ru1—N2—Ru2  | -148.2 (2) | C24—Ru3—C22—C27 | -157.3 (7) |
| C2—Ru1—N2—Ru2  | 141.9 (2)  | C25—Ru3—C22—C27 | 160.0 (7)  |
| C5—Ru1—N2—Ru2  | -132.0 (4) | C23—Ru3—C22—C27 | -120.4 (8) |

|                |            |                 |            |
|----------------|------------|-----------------|------------|
| C1—Ru1—N2—Ru2  | 145.0 (6)  | Ru4—Ru3—C22—C27 | 1.8 (9)    |
| C3—Ru1—N2—Ru2  | 174.4 (2)  | C21—C22—C23—C24 | -1.9 (7)   |
| N4—Ru4—N3—O3   | -176.6 (7) | C27—C22—C23—C24 | -177.6 (6) |
| C35—Ru4—N3—O3  | 21.4 (8)   | Ru3—C22—C23—C24 | 60.3 (4)   |
| C34—Ru4—N3—O3  | 47.1 (8)   | C21—C22—C23—C28 | 177.6 (6)  |
| C31—Ru4—N3—O3  | -16.8 (8)  | C27—C22—C23—C28 | 1.9 (10)   |
| C32—Ru4—N3—O3  | -40.9 (9)  | Ru3—C22—C23—C28 | -120.2 (6) |
| C33—Ru4—N3—O3  | 6.4 (14)   | C21—C22—C23—Ru3 | -62.2 (4)  |
| Ru3—Ru4—N3—O3  | -178.6 (8) | C27—C22—C23—Ru3 | 122.1 (6)  |
| N4—Ru4—N3—Ru3  | 2.0 (2)    | N3—Ru3—C23—C22  | 84.9 (9)   |
| C35—Ru4—N3—Ru3 | -160.0 (2) | N4—Ru3—C23—C22  | -112.6 (4) |
| C34—Ru4—N3—Ru3 | -134.3 (3) | C21—Ru3—C23—C22 | 38.1 (4)   |
| C31—Ru4—N3—Ru3 | 161.8 (2)  | C24—Ru3—C23—C22 | 118.9 (6)  |
| C32—Ru4—N3—Ru3 | 137.7 (3)  | C25—Ru3—C23—C22 | 80.6 (4)   |
| C33—Ru4—N3—Ru3 | -175.0 (9) | Ru4—Ru3—C23—C22 | -122.6 (4) |
| N4—Ru3—N3—O3   | 176.6 (8)  | N3—Ru3—C23—C24  | -34.0 (10) |
| C21—Ru3—N3—O3  | 21.4 (8)   | N4—Ru3—C23—C24  | 128.5 (4)  |
| C24—Ru3—N3—O3  | -46.3 (8)  | C21—Ru3—C23—C24 | -80.8 (4)  |
| C22—Ru3—N3—O3  | 43.9 (9)   | C22—Ru3—C23—C24 | -118.9 (6) |
| C25—Ru3—N3—O3  | -16.9 (8)  | C25—Ru3—C23—C24 | -38.3 (4)  |
| C23—Ru3—N3—O3  | -20.8 (14) | Ru4—Ru3—C23—C24 | 118.6 (4)  |
| Ru4—Ru3—N3—O3  | 178.6 (9)  | N3—Ru3—C23—C28  | -155.0 (8) |
| N4—Ru3—N3—Ru4  | -2.0 (2)   | N4—Ru3—C23—C28  | 7.6 (7)    |
| C21—Ru3—N3—Ru4 | -157.2 (2) | C21—Ru3—C23—C28 | 158.2 (7)  |
| C24—Ru3—N3—Ru4 | 135.1 (3)  | C24—Ru3—C23—C28 | -121.0 (8) |
| C22—Ru3—N3—Ru4 | -134.6 (3) | C22—Ru3—C23—C28 | 120.1 (8)  |
| C25—Ru3—N3—Ru4 | 164.5 (2)  | C25—Ru3—C23—C28 | -159.3 (7) |
| C23—Ru3—N3—Ru4 | 160.6 (7)  | Ru4—Ru3—C23—C28 | -2.4 (9)   |
| N3—Ru3—N4—O4   | -177.9 (8) | C22—C23—C24—C25 | 2.2 (7)    |
| C21—Ru3—N4—O4  | -46.2 (10) | C28—C23—C24—C25 | -177.3 (6) |
| C24—Ru3—N4—O4  | 41.0 (9)   | Ru3—C23—C24—C25 | 62.7 (4)   |
| C22—Ru3—N4—O4  | -29.9 (8)  | C22—C23—C24—C29 | 176.5 (6)  |
| C25—Ru3—N4—O4  | 40.7 (12)  | C28—C23—C24—C29 | -3.0 (11)  |
| C23—Ru3—N4—O4  | 7.2 (8)    | Ru3—C23—C24—C29 | -123.0 (7) |
| Ru4—Ru3—N4—O4  | -179.9 (9) | C22—C23—C24—Ru3 | -60.5 (4)  |
| N3—Ru3—N4—Ru4  | 2.0 (2)    | C28—C23—C24—Ru3 | 120.0 (6)  |
| C21—Ru3—N4—Ru4 | 133.7 (4)  | N3—Ru3—C24—C23  | 168.0 (4)  |
| C24—Ru3—N4—Ru4 | -139.1 (2) | N4—Ru3—C24—C23  | -63.4 (5)  |
| C22—Ru3—N4—Ru4 | 150.0 (2)  | C21—Ru3—C24—C23 | 79.2 (4)   |
| C25—Ru3—N4—Ru4 | -139.4 (5) | C22—Ru3—C24—C23 | 36.6 (4)   |
| C23—Ru3—N4—Ru4 | -172.9 (2) | C25—Ru3—C24—C23 | 116.4 (6)  |
| N3—Ru4—N4—O4   | 177.9 (8)  | Ru4—Ru3—C24—C23 | -123.7 (4) |
| C35—Ru4—N4—O4  | -49.2 (11) | N3—Ru3—C24—C25  | 51.7 (5)   |
| C34—Ru4—N4—O4  | -38.8 (9)  | N4—Ru3—C24—C25  | -179.8 (4) |
| C31—Ru4—N4—O4  | 46.7 (11)  | C21—Ru3—C24—C25 | -37.2 (4)  |
| C32—Ru4—N4—O4  | 33.1 (9)   | C22—Ru3—C24—C25 | -79.8 (4)  |
| C33—Ru4—N4—O4  | -3.0 (9)   | C23—Ru3—C24—C25 | -116.4 (6) |
| Ru3—Ru4—N4—O4  | 179.9 (9)  | Ru4—Ru3—C24—C25 | 119.9 (4)  |
| N3—Ru4—N4—Ru3  | -2.0 (2)   | N3—Ru3—C24—C29  | -69.4 (7)  |

## supplementary materials

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|----------------|------------|-----------------|------------|
| C35—Ru4—N4—Ru3 | 130.9 (5)  | N4—Ru3—C24—C29  | 59.1 (7)   |
| C34—Ru4—N4—Ru3 | 141.3 (3)  | C21—Ru3—C24—C29 | -158.3 (7) |
| C31—Ru4—N4—Ru3 | -133.2 (5) | C22—Ru3—C24—C29 | 159.1 (7)  |
| C32—Ru4—N4—Ru3 | -146.8 (3) | C25—Ru3—C24—C29 | -121.1 (8) |
| C33—Ru4—N4—Ru3 | 177.0 (3)  | C23—Ru3—C24—C29 | 122.6 (8)  |
| N1—Ru1—C1—C5   | -99.4 (4)  | Ru4—Ru3—C24—C29 | -1.2 (8)   |
| N2—Ru1—C1—C5   | 113.8 (7)  | C22—C21—C25—C24 | 0.5 (7)    |
| C4—Ru1—C1—C5   | 38.0 (4)   | C26—C21—C25—C24 | 178.4 (6)  |
| C2—Ru1—C1—C5   | 118.2 (6)  | Ru3—C21—C25—C24 | -61.4 (4)  |
| C3—Ru1—C1—C5   | 80.6 (4)   | C22—C21—C25—C30 | -178.6 (6) |
| Ru2—Ru1—C1—C5  | -118.9 (4) | C26—C21—C25—C30 | -0.7 (10)  |
| N1—Ru1—C1—C2   | 142.4 (4)  | Ru3—C21—C25—C30 | 119.5 (6)  |
| N2—Ru1—C1—C2   | -4.4 (8)   | C22—C21—C25—Ru3 | 61.9 (4)   |
| C4—Ru1—C1—C2   | -80.1 (4)  | C26—C21—C25—Ru3 | -120.2 (6) |
| C5—Ru1—C1—C2   | -118.2 (6) | C23—C24—C25—C21 | -1.7 (7)   |
| C3—Ru1—C1—C2   | -37.5 (4)  | C29—C24—C25—C21 | -176.1 (6) |
| Ru2—Ru1—C1—C2  | 122.9 (4)  | Ru3—C24—C25—C21 | 61.5 (4)   |
| N1—Ru1—C1—C6   | 20.6 (6)   | C23—C24—C25—C30 | 177.4 (6)  |
| N2—Ru1—C1—C6   | -126.2 (7) | C29—C24—C25—C30 | 3.0 (10)   |
| C4—Ru1—C1—C6   | 158.1 (6)  | Ru3—C24—C25—C30 | -119.5 (6) |
| C2—Ru1—C1—C6   | -121.8 (7) | C23—C24—C25—Ru3 | -63.2 (4)  |
| C5—Ru1—C1—C6   | 120.0 (7)  | C29—C24—C25—Ru3 | 122.5 (7)  |
| C3—Ru1—C1—C6   | -159.3 (6) | N3—Ru3—C25—C21  | 101.5 (4)  |
| Ru2—Ru1—C1—C6  | 1.1 (8)    | N4—Ru3—C25—C21  | -117.4 (7) |
| C5—C1—C2—C3    | 1.9 (7)    | C24—Ru3—C25—C21 | -117.9 (5) |
| C6—C1—C2—C3    | -178.3 (6) | C22—Ru3—C25—C21 | -37.5 (4)  |
| Ru1—C1—C2—C3   | 63.5 (4)   | C23—Ru3—C25—C21 | -79.8 (4)  |
| C5—C1—C2—C7    | 175.4 (6)  | Ru4—Ru3—C25—C21 | 122.1 (3)  |
| C6—C1—C2—C7    | -4.8 (10)  | N3—Ru3—C25—C24  | -140.6 (4) |
| Ru1—C1—C2—C7   | -123.0 (6) | N4—Ru3—C25—C24  | 0.5 (8)    |
| C5—C1—C2—Ru1   | -61.5 (4)  | C21—Ru3—C25—C24 | 117.9 (5)  |
| C6—C1—C2—Ru1   | 118.3 (6)  | C22—Ru3—C25—C24 | 80.4 (4)   |
| N1—Ru1—C2—C3   | -166.8 (4) | C23—Ru3—C25—C24 | 38.1 (4)   |
| N2—Ru1—C2—C3   | 61.6 (5)   | Ru4—Ru3—C25—C24 | -120.1 (4) |
| C4—Ru1—C2—C3   | -36.8 (4)  | N3—Ru3—C25—C30  | -18.5 (6)  |
| C5—Ru1—C2—C3   | -80.0 (4)  | N4—Ru3—C25—C30  | 122.6 (7)  |
| C1—Ru1—C2—C3   | -116.6 (6) | C21—Ru3—C25—C30 | -120.0 (7) |
| Ru2—Ru1—C2—C3  | 121.2 (4)  | C24—Ru3—C25—C30 | 122.1 (7)  |
| N1—Ru1—C2—C1   | -50.2 (5)  | C22—Ru3—C25—C30 | -157.5 (6) |
| N2—Ru1—C2—C1   | 178.1 (4)  | C23—Ru3—C25—C30 | 160.2 (6)  |
| C4—Ru1—C2—C1   | 79.8 (4)   | Ru4—Ru3—C25—C30 | 2.1 (7)    |
| C5—Ru1—C2—C1   | 36.6 (4)   | N3—Ru4—C31—C35  | 92.1 (4)   |
| C3—Ru1—C2—C1   | 116.6 (6)  | N4—Ru4—C31—C35  | -137.3 (6) |
| Ru2—Ru1—C2—C1  | -122.2 (4) | C34—Ru4—C31—C35 | -37.6 (4)  |
| N1—Ru1—C2—C7   | 71.8 (7)   | C32—Ru4—C31—C35 | -117.3 (6) |
| N2—Ru1—C2—C7   | -59.9 (7)  | C33—Ru4—C31—C35 | -79.9 (5)  |
| C4—Ru1—C2—C7   | -158.3 (7) | Ru3—Ru4—C31—C35 | 116.4 (4)  |
| C5—Ru1—C2—C7   | 158.6 (7)  | N3—Ru4—C31—C32  | -150.6 (5) |
| C1—Ru1—C2—C7   | 122.0 (8)  | N4—Ru4—C31—C32  | -20.0 (8)  |

|               |            |                 |             |
|---------------|------------|-----------------|-------------|
| C3—Ru1—C2—C7  | -121.5 (8) | C35—Ru4—C31—C32 | 117.3 (6)   |
| Ru2—Ru1—C2—C7 | -0.2 (8)   | C34—Ru4—C31—C32 | 79.6 (5)    |
| C1—C2—C3—C4   | -2.9 (7)   | C33—Ru4—C31—C32 | 37.4 (5)    |
| C7—C2—C3—C4   | -176.5 (6) | Ru3—Ru4—C31—C32 | -126.4 (5)  |
| Ru1—C2—C3—C4  | 60.2 (4)   | N3—Ru4—C31—C36  | -27.8 (8)   |
| C1—C2—C3—C8   | 178.6 (6)  | N4—Ru4—C31—C36  | 102.8 (9)   |
| C7—C2—C3—C8   | 5.0 (10)   | C35—Ru4—C31—C36 | -119.9 (9)  |
| Ru1—C2—C3—C8  | -118.3 (6) | C34—Ru4—C31—C36 | -157.6 (8)  |
| C1—C2—C3—Ru1  | -63.1 (4)  | C32—Ru4—C31—C36 | 122.8 (9)   |
| C7—C2—C3—Ru1  | 123.3 (7)  | C33—Ru4—C31—C36 | 160.2 (8)   |
| N1—Ru1—C3—C2  | 38.1 (10)  | Ru3—Ru4—C31—C36 | -3.6 (10)   |
| N2—Ru1—C3—C2  | -129.9 (4) | C35—C31—C32—C33 | -0.8 (7)    |
| C4—Ru1—C3—C2  | 119.0 (6)  | C36—C31—C32—C33 | 178.7 (7)   |
| C5—Ru1—C3—C2  | 80.2 (4)   | Ru4—C31—C32—C33 | -62.4 (5)   |
| C1—Ru1—C3—C2  | 38.3 (4)   | C35—C31—C32—C37 | -175.3 (7)  |
| Ru2—Ru1—C3—C2 | -122.2 (4) | C36—C31—C32—C37 | 4.2 (12)    |
| N1—Ru1—C3—C4  | -80.9 (10) | Ru4—C31—C32—C37 | 123.1 (8)   |
| N2—Ru1—C3—C4  | 111.1 (4)  | C35—C31—C32—Ru4 | 61.6 (4)    |
| C2—Ru1—C3—C4  | -119.0 (6) | C36—C31—C32—Ru4 | -118.9 (7)  |
| C5—Ru1—C3—C4  | -38.8 (4)  | N3—Ru4—C32—C33  | 157.7 (4)   |
| C1—Ru1—C3—C4  | -80.7 (4)  | N4—Ru4—C32—C33  | -72.9 (5)   |
| Ru2—Ru1—C3—C4 | 118.8 (4)  | C35—Ru4—C32—C33 | 79.6 (5)    |
| N1—Ru1—C3—C8  | 160.2 (8)  | C34—Ru4—C32—C33 | 36.7 (4)    |
| N2—Ru1—C3—C8  | -7.8 (6)   | C31—Ru4—C32—C33 | 117.0 (6)   |
| C4—Ru1—C3—C8  | -118.9 (8) | Ru3—Ru4—C32—C33 | -125.3 (5)  |
| C2—Ru1—C3—C8  | 122.1 (8)  | N3—Ru4—C32—C31  | 40.7 (6)    |
| C5—Ru1—C3—C8  | -157.7 (7) | N4—Ru4—C32—C31  | 170.1 (4)   |
| C1—Ru1—C3—C8  | 160.4 (7)  | C35—Ru4—C32—C31 | -37.4 (4)   |
| Ru2—Ru1—C3—C8 | -0.1 (8)   | C34—Ru4—C32—C31 | -80.3 (5)   |
| C2—C3—C4—C5   | 2.8 (7)    | C33—Ru4—C32—C31 | -117.0 (6)  |
| C8—C3—C4—C5   | -178.7 (6) | Ru3—Ru4—C32—C31 | 117.7 (4)   |
| Ru1—C3—C4—C5  | 63.3 (4)   | N3—Ru4—C32—C37  | -78.9 (12)  |
| C2—C3—C4—C9   | -180.0 (6) | N4—Ru4—C32—C37  | 50.5 (12)   |
| C8—C3—C4—C9   | -1.4 (10)  | C35—Ru4—C32—C37 | -157.0 (12) |
| Ru1—C3—C4—C9  | -119.4 (6) | C34—Ru4—C32—C37 | 160.1 (12)  |
| C2—C3—C4—Ru1  | -60.5 (4)  | C31—Ru4—C32—C37 | -119.6 (13) |
| C8—C3—C4—Ru1  | 118.0 (6)  | C33—Ru4—C32—C37 | 123.4 (13)  |
| N1—Ru1—C4—C3  | 155.3 (4)  | Ru3—Ru4—C32—C37 | -1.9 (15)   |
| N2—Ru1—C4—C3  | -78.7 (4)  | C31—C32—C33—C34 | 1.1 (8)     |
| C2—Ru1—C4—C3  | 36.3 (4)   | C37—C32—C33—C34 | 175.4 (8)   |
| C5—Ru1—C4—C3  | 115.9 (5)  | Ru4—C32—C33—C34 | -60.6 (5)   |
| C1—Ru1—C4—C3  | 79.1 (4)   | C31—C32—C33—C38 | -179.2 (7)  |
| Ru2—Ru1—C4—C3 | -122.9 (4) | C37—C32—C33—C38 | -4.9 (12)   |
| N1—Ru1—C4—C5  | 39.5 (5)   | Ru4—C32—C33—C38 | 119.1 (8)   |
| N2—Ru1—C4—C5  | 165.4 (4)  | C31—C32—C33—Ru4 | 61.7 (5)    |
| C2—Ru1—C4—C5  | -79.6 (4)  | C37—C32—C33—Ru4 | -123.9 (8)  |
| C1—Ru1—C4—C5  | -36.8 (4)  | N3—Ru4—C33—C32  | -63.9 (11)  |
| C3—Ru1—C4—C5  | -115.9 (5) | N4—Ru4—C33—C32  | 119.1 (5)   |
| Ru2—Ru1—C4—C5 | 121.2 (4)  | C35—Ru4—C33—C32 | -80.6 (5)   |

## supplementary materials

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|                 |            |                 |             |
|-----------------|------------|-----------------|-------------|
| N1—Ru1—C4—C9    | -82.9 (7)  | C34—Ru4—C33—C32 | -118.9 (6)  |
| N2—Ru1—C4—C9    | 43.1 (7)   | C31—Ru4—C33—C32 | -38.2 (4)   |
| C2—Ru1—C4—C9    | 158.1 (7)  | Ru3—Ru4—C33—C32 | 123.5 (5)   |
| C5—Ru1—C4—C9    | -122.4 (8) | N3—Ru4—C33—C34  | 55.0 (12)   |
| C1—Ru1—C4—C9    | -159.2 (7) | N4—Ru4—C33—C34  | -122.0 (4)  |
| C3—Ru1—C4—C9    | 121.8 (8)  | C35—Ru4—C33—C34 | 38.3 (4)    |
| Ru2—Ru1—C4—C9   | -1.2 (9)   | C31—Ru4—C33—C34 | 80.8 (4)    |
| C2—C1—C5—C4     | -0.2 (7)   | C32—Ru4—C33—C34 | 118.9 (6)   |
| C6—C1—C5—C4     | 180.0 (6)  | Ru3—Ru4—C33—C34 | -117.6 (4)  |
| Ru1—C1—C5—C4    | -61.3 (4)  | N3—Ru4—C33—C38  | 174.2 (9)   |
| C2—C1—C5—C10    | -178.6 (6) | N4—Ru4—C33—C38  | -2.8 (10)   |
| C6—C1—C5—C10    | 1.6 (10)   | C35—Ru4—C33—C38 | 157.5 (11)  |
| Ru1—C1—C5—C10   | 120.4 (6)  | C34—Ru4—C33—C38 | 119.2 (12)  |
| C2—C1—C5—Ru1    | 61.1 (4)   | C31—Ru4—C33—C38 | -160.1 (11) |
| C6—C1—C5—Ru1    | -118.7 (6) | C32—Ru4—C33—C38 | -121.9 (12) |
| C3—C4—C5—C1     | -1.6 (7)   | Ru3—Ru4—C33—C38 | 1.5 (13)    |
| C9—C4—C5—C1     | -178.8 (6) | C32—C33—C34—C35 | -1.0 (7)    |
| Ru1—C4—C5—C1    | 62.2 (4)   | C38—C33—C34—C35 | 179.3 (7)   |
| C3—C4—C5—C10    | 176.7 (6)  | Ru4—C33—C34—C35 | -62.0 (4)   |
| C9—C4—C5—C10    | -0.5 (10)  | C32—C33—C34—C39 | -175.8 (7)  |
| Ru1—C4—C5—C10   | -119.5 (7) | C38—C33—C34—C39 | 4.5 (11)    |
| C3—C4—C5—Ru1    | -63.8 (4)  | Ru4—C33—C34—C39 | 123.1 (7)   |
| C9—C4—C5—Ru1    | 119.0 (6)  | C32—C33—C34—Ru4 | 61.1 (5)    |
| N1—Ru1—C5—C1    | 89.1 (4)   | C38—C33—C34—Ru4 | -118.6 (7)  |
| N2—Ru1—C5—C1    | -142.7 (4) | N3—Ru4—C34—C33  | -160.4 (4)  |
| C4—Ru1—C5—C1    | -117.6 (5) | N4—Ru4—C34—C33  | 70.4 (5)    |
| C2—Ru1—C5—C1    | -37.5 (4)  | C35—Ru4—C34—C33 | -116.6 (6)  |
| C3—Ru1—C5—C1    | -79.4 (4)  | C31—Ru4—C34—C33 | -79.4 (5)   |
| Ru2—Ru1—C5—C1   | 122.2 (4)  | C32—Ru4—C34—C33 | -36.5 (5)   |
| N1—Ru1—C5—C4    | -153.4 (4) | Ru3—Ru4—C34—C33 | 127.0 (5)   |
| N2—Ru1—C5—C4    | -25.2 (6)  | N3—Ru4—C34—C35  | -43.8 (5)   |
| C2—Ru1—C5—C4    | 80.1 (4)   | N4—Ru4—C34—C35  | -173.0 (4)  |
| C1—Ru1—C5—C4    | 117.6 (5)  | C31—Ru4—C34—C35 | 37.2 (4)    |
| C3—Ru1—C5—C4    | 38.2 (4)   | C32—Ru4—C34—C35 | 80.1 (5)    |
| Ru2—Ru1—C5—C4   | -120.2 (4) | C33—Ru4—C34—C35 | 116.6 (6)   |
| N1—Ru1—C5—C10   | -30.6 (7)  | Ru3—Ru4—C34—C35 | -116.5 (4)  |
| N2—Ru1—C5—C10   | 97.6 (7)   | N3—Ru4—C34—C39  | 74.7 (8)    |
| C4—Ru1—C5—C10   | 122.8 (8)  | N4—Ru4—C34—C39  | -54.5 (8)   |
| C2—Ru1—C5—C10   | -157.2 (7) | C35—Ru4—C34—C39 | 118.5 (9)   |
| C1—Ru1—C5—C10   | -119.7 (8) | C31—Ru4—C34—C39 | 155.7 (9)   |
| C3—Ru1—C5—C10   | 160.9 (8)  | C32—Ru4—C34—C39 | -161.4 (9)  |
| Ru2—Ru1—C5—C10  | 2.6 (9)    | C33—Ru4—C34—C39 | -124.9 (9)  |
| N2—Ru2—C11—C15  | -113.6 (7) | Ru3—Ru4—C34—C39 | 2.1 (10)    |
| N1—Ru2—C11—C15  | 100.8 (4)  | C32—C31—C35—C34 | 0.2 (7)     |
| C14—Ru2—C11—C15 | -37.3 (4)  | C36—C31—C35—C34 | -179.3 (6)  |
| C12—Ru2—C11—C15 | -117.3 (6) | Ru4—C31—C35—C34 | 62.3 (4)    |
| C13—Ru2—C11—C15 | -80.2 (4)  | C32—C31—C35—C40 | 179.4 (6)   |
| Ru1—Ru2—C11—C15 | 119.4 (4)  | C36—C31—C35—C40 | -0.1 (10)   |
| N2—Ru2—C11—C12  | 3.8 (8)    | Ru4—C31—C35—C40 | -118.5 (6)  |

|                 |            |                 |            |
|-----------------|------------|-----------------|------------|
| N1—Ru2—C11—C12  | -141.8 (4) | C32—C31—C35—Ru4 | -62.1 (5)  |
| C15—Ru2—C11—C12 | 117.3 (6)  | C36—C31—C35—Ru4 | 118.3 (7)  |
| C14—Ru2—C11—C12 | 80.0 (4)   | C33—C34—C35—C31 | 0.5 (7)    |
| C13—Ru2—C11—C12 | 37.1 (4)   | C39—C34—C35—C31 | 175.6 (6)  |
| Ru1—Ru2—C11—C12 | -123.3 (4) | Ru4—C34—C35—C31 | -62.6 (4)  |
| N2—Ru2—C11—C16  | 126.0 (7)  | C33—C34—C35—C40 | -178.7 (6) |
| N1—Ru2—C11—C16  | -19.6 (6)  | C39—C34—C35—C40 | -3.6 (10)  |
| C15—Ru2—C11—C16 | -120.4 (7) | Ru4—C34—C35—C40 | 118.2 (6)  |
| C14—Ru2—C11—C16 | -157.8 (6) | C33—C34—C35—Ru4 | 63.1 (5)   |
| C12—Ru2—C11—C16 | 122.2 (7)  | C39—C34—C35—Ru4 | -121.8 (6) |
| C13—Ru2—C11—C16 | 159.3 (6)  | N3—Ru4—C35—C31  | -94.8 (4)  |
| Ru1—Ru2—C11—C16 | -1.0 (7)   | N4—Ru4—C35—C31  | 132.7 (6)  |
| C15—C11—C12—C13 | -1.8 (7)   | C34—Ru4—C35—C31 | 117.7 (6)  |
| C16—C11—C12—C13 | 179.1 (6)  | C32—Ru4—C35—C31 | 37.9 (5)   |
| Ru2—C11—C12—C13 | -62.9 (4)  | C33—Ru4—C35—C31 | 80.0 (5)   |
| C15—C11—C12—C17 | -175.7 (6) | Ru3—Ru4—C35—C31 | -120.4 (4) |
| C16—C11—C12—C17 | 5.2 (10)   | N3—Ru4—C35—C34  | 147.5 (4)  |
| Ru2—C11—C12—C17 | 123.3 (6)  | N4—Ru4—C35—C34  | 15.0 (8)   |
| C15—C11—C12—Ru2 | 61.1 (4)   | C31—Ru4—C35—C34 | -117.7 (6) |
| C16—C11—C12—Ru2 | -118.0 (6) | C32—Ru4—C35—C34 | -79.8 (5)  |
| N2—Ru2—C12—C13  | -61.0 (4)  | C33—Ru4—C35—C34 | -37.7 (5)  |
| N1—Ru2—C12—C13  | 167.7 (4)  | Ru3—Ru4—C35—C34 | 121.8 (4)  |
| C15—Ru2—C12—C13 | 80.1 (4)   | N3—Ru4—C35—C40  | 25.9 (6)   |
| C14—Ru2—C12—C13 | 37.4 (4)   | N4—Ru4—C35—C40  | -106.7 (7) |
| C11—Ru2—C12—C13 | 117.5 (6)  | C34—Ru4—C35—C40 | -121.6 (8) |
| Ru1—Ru2—C12—C13 | -122.9 (4) | C31—Ru4—C35—C40 | 120.6 (8)  |
| N2—Ru2—C12—C11  | -178.4 (4) | C32—Ru4—C35—C40 | 158.6 (7)  |
| N1—Ru2—C12—C11  | 50.2 (5)   | C33—Ru4—C35—C40 | -159.4 (7) |
| C15—Ru2—C12—C11 | -37.4 (4)  | Ru3—Ru4—C35—C40 | 0.2 (7)    |

Fig. 1

