

Di- μ -nitrosyl-bis[(η^5 -pentamethylcyclopentadienyl)ruthenium(0)]($Ru-Ru$)

Matthew Pearsal,^a Milan Gembicky,^{b*} Paulina Dominiak,^b
Anna Larsen^a and Philip Coppens^b

^aDepartment of Chemistry, CNS 359, Ithaca College, Ithaca, NY 14850, USA, and

^bDepartment of Chemistry, State University of New York at Buffalo, 732 NS Complex, Buffalo, NY 14260, USA

Correspondence e-mail: gembicky@buffalo.edu

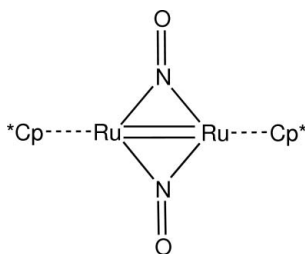
Received 4 September 2007; accepted 14 September 2007

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) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.49$ mm⁻¹
 $T = 90$ (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⁻³
 $\Delta\rho_{min} = -2.33$ e Å⁻³

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).

References

- Bergman, R. G. & Chang, J. (1987). *J. Am. Chem. Soc.* **109**, 4298–4304.
Bernal, I., Korp, J. D. & Reisner, G. M. (1977). *J. Organomet. Chem.* **139**, 321–336.
Bottomley, F. (1983). *Inorg. Chem.* **22**, 2656–2660.
Bruker (2004). APEX2 (Version 2.1-4), SAINT (Version 7.34A) and SADABS (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Burns, R. & Hubbard, J. (1994). *J. Am. Chem. Soc.* **116**, 9514–9520.
Hayton, T. W., Legzdins, P. & Sharp, W. B. (2002). *Chem. Rev.* **102**, 935–991.
Kubat-Martin, K. A., Barr, M. E., Spencer, B. & Dahl, L. (1987). *Organometallics*, **6**, 2570–2579.
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
Sheldrick, G. M. (2000). SHELXTL. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.

supplementary materials

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

Di- μ -nitrosyl-bis[(η^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 α 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° frame-width (ω -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 CH₃ H atoms were treated as part of idealized CH₃ groups with $U_{iso} = 1.5U_{eq}$. 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 - Cp**Ru*(NO)OTf₂ (OTf = OSO₂CF₃) – was prepared according to synthetic methods reported by Burns & Hubbard (1994). 2-Propanol (10 ml) was added with a syringe to Cp**Ru*(NO)OTf₂ (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 Cp**Ru*(NO)OTf₂. 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 ¹H NMR and ¹³C NMR spectroscopy. Alternate routes entailing reductive elimination of Cp**Ru*(NO)Cl₂ or Cp**Ru*(NO)Ph₂ 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 CH₂Cl₂ solutions.

Refinement

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

Figures

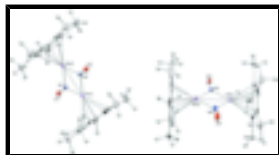


Fig. 1. Molecular structure of title compound, hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

Di- μ -nitrosyl-bis[(η^5 -pentamethylcyclopentadienyl)ruthenium(0)](Ru—Ru)

Crystal data

[Ru₂(C₁₀H₁₅)₂(NO)₂]

$M_r = 532.60$

Triclinic, $P\bar{1}$

Hall symbol: -P 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) Å³

$Z = 4$

$F_{000} = 1072$

$D_x = 1.721$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 7139 reflections

$\theta = 3$ – 28°

$\mu = 1.49$ mm⁻¹

$T = 90$ (1) K

Parallelepiped, red

$0.3 \times 0.2 \times 0.13$ mm

Data collection

Bruker SMART APEXII
diffractometer

Radiation source: rotating anode

Monochromator: graphite

Detector resolution: 8.33 pixels mm⁻¹

$T = 90$ (1) K

ω scans

Absorption correction: multi-scan
(SADABS; Bruker 2004)

$T_{\min} = 0.705$, $T_{\max} = 0.824$

29941 measured reflections

10102 independent reflections

9591 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 28.3^\circ$

$\theta_{\min} = 1.9^\circ$

$h = -14 \rightarrow 14$

$k = -14 \rightarrow 14$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.139$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 11.2766P]$

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

$S = 1.26$ $(\Delta/\sigma)_{\max} = 0.001$
 10102 reflections $\Delta\rho_{\max} = 2.12 \text{ e } \text{Å}^{-3}$
 490 parameters $\Delta\rho_{\min} = -2.33 \text{ e } \text{Å}^{-3}$
 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 $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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

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 (\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

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

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

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

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

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

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

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

