Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ_3-Carbonato-$\kappa^3O:O':O''$-tris{(η^6-benzene)[(*R*)-1-(1-aminoethyl)naphthyl-κ^2C^2,N]ruthenium(II)} hexafluoridophosphate dichloromethane solvate

Jean-Baptiste Sortais,[a] Lydia Brelot,[b] Michel Pfeffer[a] and Laurent Barloy[a]*

[a]Institut de Chimie de Strasbourg, Université Louis Pasteur, Laboratoire de Synthèses Métallo-Induites, UMR 7177 CNRS, 4 rue Blaise Pascal, 67070 Strasbourg Cedex, France, and [b]Institut de Chimie de Strasbourg, Université Louis Pasteur, Service de Radiocristallographie, UMR 7177 CNRS, 4 rue Blaise Pascal, 67070 Strasbourg Cedex, France
Correspondence e-mail: barloy@chimie.u-strasbg.fr

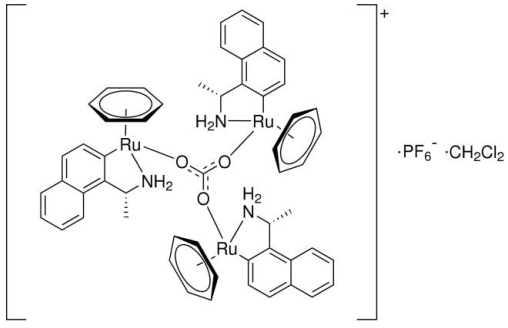
Received 15 November 2007; accepted 6 February 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.011 Å; R factor = 0.053; wR factor = 0.132; data-to-parameter ratio = 19.1.

The title compound, $[Ru_3(C_{12}H_{12}N)_3(CO_3)(C_6H_6)_3]PF_6\cdot CH_2Cl_2$, was obtained unintentionally as the product of an attempted deprotonation of the monomeric parent ruthenium complex $[Ru(C_{12}H_{12}N)(C_6H_6)(C_2H_3N)]PF_6$. The carbonate ligand bridges three half-sandwich cycloruthenated fragments, each of them exhibiting a pseudo-tetrahedral geometry. The configuration of the Ru atoms is *S*. The naphthyl groups of the enantiopure cycloruthenated benzylic amine ligands point in the same direction, adopting a propeller shape.

Related literature

For related literature, see: Cotton *et al.* (1992); Demerseman *et al.* (2006); Lindsay *et al.* (1987); Maurette *et al.* (1999); Sortais *et al.* (2006, 2007).



Experimental

Crystal data

$[Ru_3(C_{12}H_{12}N)_3(CO_3)(C_6H_6)_3]PF_6\cdot CH_2Cl_2$
M_r = 1338.12
Monoclinic, $P2_1$
a = 11.4732 (2) Å
b = 19.1377 (5) Å
c = 12.0169 (2) Å
β = 90.832 (2)°
V = 2638.28 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 173 (2) K
0.12 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
15434 measured reflections
12813 independent reflections
9862 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.132
S = 1.06
12813 reflections
670 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
Absolute structure: Flack (1983), 4881 Friedel pairs
Flack parameter: 0.01 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···F6^{i}	0.92	2.37	3.245 (7)	159
N1—H1B···O3	0.92	2.09	2.860 (7)	141
N2—H2B···O1	0.92	2.38	2.967 (7)	122
N3—H3A···F4^{ii}	0.92	2.36	3.202 (8)	153
N3—H3B···O2	0.92	1.92	2.739 (7)	148

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank André De Cian for his contribution to this work, and the CNRS for financial support. The authors are also indebted to the Ministère de l'Education Nationale for a fellowship granted to JBS.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2047).

References

Cotton, F. A., Labella, L. & Shang, M. (1992). *Inorg. Chem.* **31**, 2385–2389.
Demerseman, B., Mbaye, M. D., Semeril, D., Toupet, L., Bruneau, C. & Dixneuf, P. H. (2006). *Eur. J. Inorg. Chem.* pp. 1174–1181.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Lindsay, A. J., Wilkinson, G., Motevalli, M. & Hursthouse, M. B. (1987). *J. Chem. Soc. Dalton Trans.* pp. 2723–2736.
Maurette, L., Donnadieu, B. & Lavigne, G. (1999). *Angew. Chem. Int. Ed.* **38**, 3707–3710.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

 doi:10.1107/S1600536808003978

Sortais, J.-B., Barloy, L., Sirlin, C., de Vries, A. H. M., de Vries, J. G. & Pfeffer, M. (2006). *Pure Appl. Chem.* **78**, 457–462.
Sortais, J.-B., Pannetier, N., Holuigue, A., Barloy, L., Sirlin, C., Pfeffer, M. & Kyritsakas, N. (2007). *Organometallics*, **26**, 1856–1867.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2008). E**64**, m483–m484 [doi:10.1107/S1600536808003978]

μ_3-Carbonato-$\kappa^3O:O':O''$-tris{(η^6-benzene)[(*R*)-1-(1-aminoethyl)naphthyl-κ^2C^2,N]ruthenium(II)} hexafluoridophosphate dichloromethane solvate

Jean-Baptiste Sortais, Lydia Brelot, Michel Pfeffer and Laurent Barloy

S1. Comment

Chiral cycloruthenated half-sandwich complexes have recently experienced a renewed interest because of their catalytic properties applied to asymmetric synthesis (Sortais *et al.*, 2006). Single crystals of the title compound (I) have been obtained while attempting to isolate catalytic intermediates.

The molecular structure of the compound (I) (Fig. 1) consists of a trinuclear cation comprising three pseudotetrahedral ruthenium (II) centres, which are each coordinated by a bridging μ_3-carbonato ligand, a η^6-benzene ligand and a cyclometallated (*R*)-(+)-1-(1-naphthyl)ethylamine, together with a non-coordinating hexafluorophosphate anion and one molecule of methylene chloride. The complex crystallizes in the $P2_1$ chiral space group, which confirms the presence of a single enantiomer. A partial view showing the coordination sphere of one of the ruthenium atoms is represented Fig. 2, the two others are similar. Its structure is closely related to that of the reported parent complex bearing dimethylphenylphosphine instead of the carbonato ligand (Sortais *et al.*, 2007): S_{Ru} configuration, δ conformation of the metallacycle, axial position of the methyl group. The ruthenium atoms and the four atoms belonging to the carbonato are coplanar, the sum of the three Ru···$C_{carbonato}$···Ru angles reaching 359.89°. The three ruthenium atoms form a nearly equilateral triangle with Ru···Ru distances within the 5.2–5.5 Å range. The benzene ligands lie on one side of the corresponding plane and the cycloruthenated on the other side.

A search in the Cambridge Database revealed no previously reported crystal structure of a carbonato-bridged chemically C_3-symmetric trinuclear ruthenium complex. Related polynuclear carbonato ruthenium complexes where each oxygen atom is ligated to at least one ruthenium atom exhibit metal-metal bonds (Cotton *et al.*, 1992; Lindsay *et al.*, 1987; Maurette *et al.*, 1999). Interestingly, a closely related monomeric half-sandwich complex where a carbonato ligand chelates the Ru center has been recently reported (Demerseman *et al.*, 2006); we notice that in complex (I) the Ru—O bond distances are longer (2.118 (4)–2.132 (4) Å), probably because of steric repulsions.

S2. Experimental

{[(*R*)-1-(1-naphthyl-κC^2)-ethylamine-κN](η^6-benzene) (acetonitrile-κN)ruthenium(II)} hexafluorophosphate (31 mg, 58 μmol) (Sortais *et al.*, 2007) was dissolved in 4 ml dichloromethane with 3.3 mg (1 equiv.) ground potassium hydroxide (containing potassium carbonate as minor impurity). The suspension was heated to reflux for 1.5 h and evaporated to dryness. Analysis of a sample dissolved in CD_2Cl_2 by NMR showed only the signals of the starting material, but single crystals of compound (I) had appeared after letting the tube stand for 3 days at room temperature.

S3. Refinement

The H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

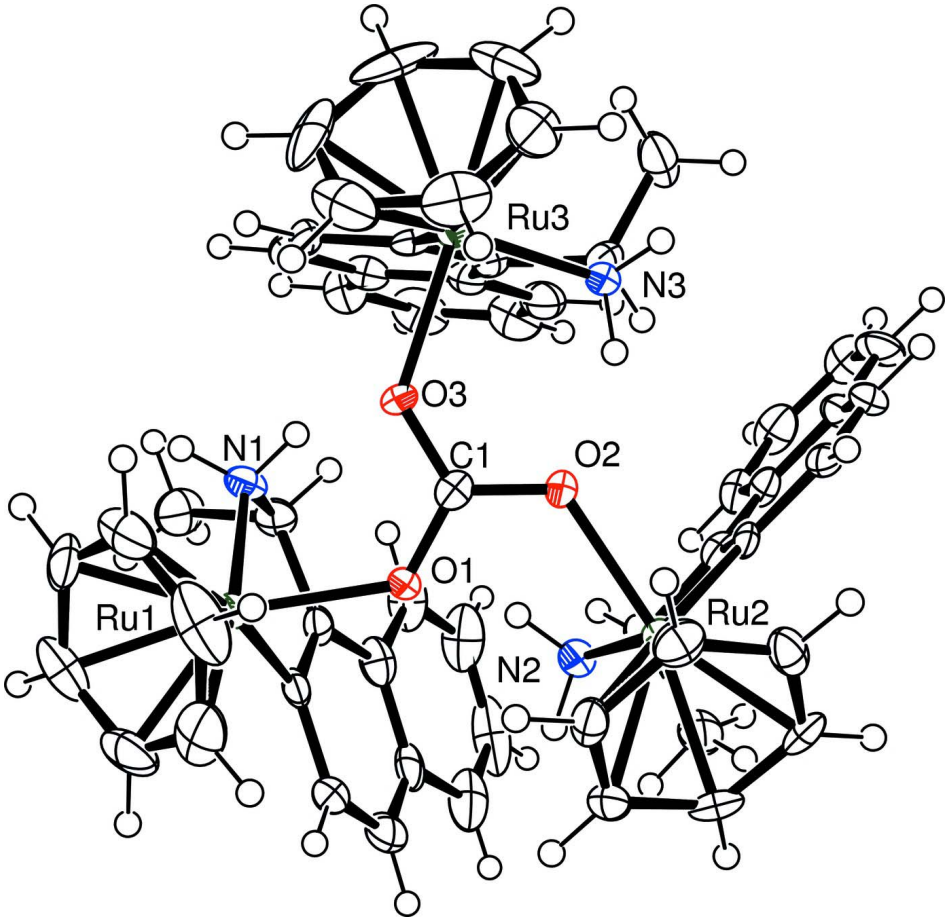


Figure 1

The molecular structure of (I), with selected atom labels and 50% probability displacement ellipsoids for non-H atoms. The counter-anion and solvent have been omitted for clarity.

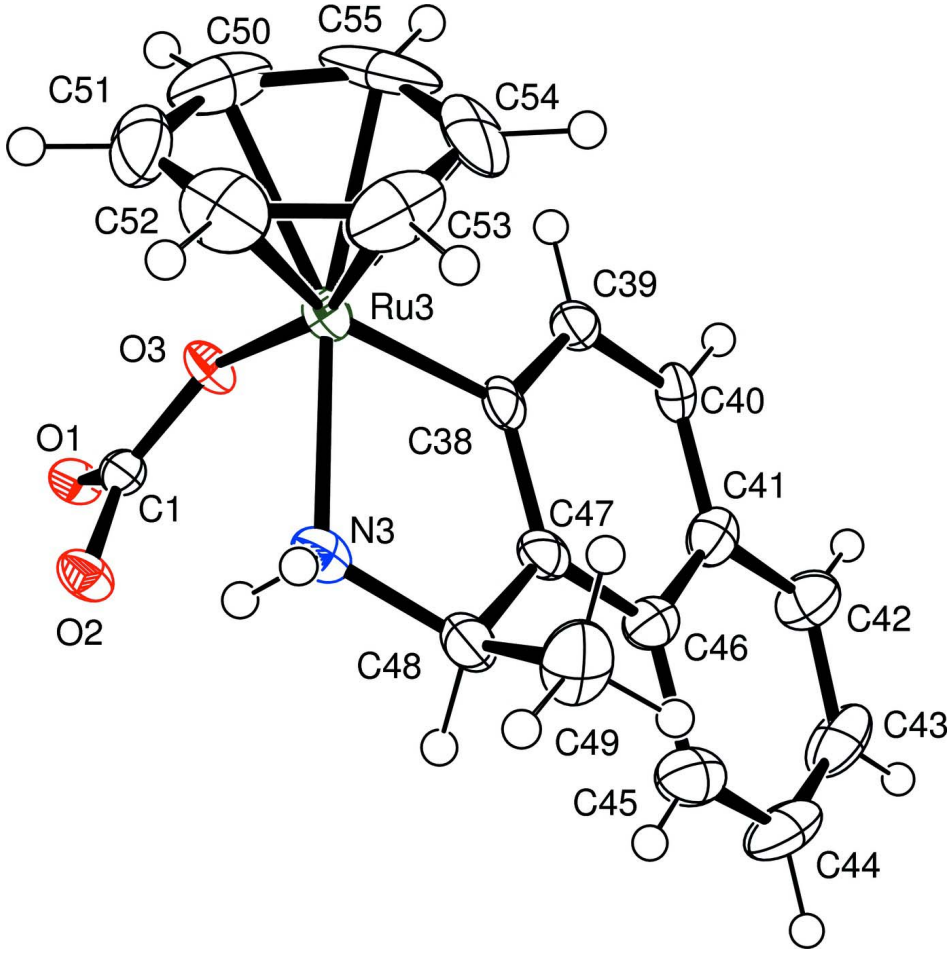


Figure 2

A partial view of the molecular structure of (I), with 50% probability displacement ellipsoids for non-H atoms. Only the Ru3 atom and its ligands are represented.

μ_3-Carbonato-κ^3O:O':O''-tris{(η^6– benzene)[(*R*)-1-(1-aminoethyl)naphthyl- κ^2C^2,*N*]ruthenium(II)} hexafluoridophosphate dichloromethane solvate

Crystal data

$[Ru_3(C_{12}H_{12}N)_3(CO_3)(C_6H_6)_3]PF_6\cdot CH_2Cl_2$
$M_r = 1338.12$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 11.4732\ (2)$ Å
$b = 19.1377\ (5)$ Å
$c = 12.0169\ (2)$ Å
$\beta = 90.832\ (2)°$
$V = 2638.28\ (9)$ Å^3
$Z = 2$
$F(000) = 1344$
$D_x = 1.684$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6871 reflections
$\theta = 1.0$–$30.0°$
$\mu = 1.05$ mm^{-1}
$T = 173$ K
Prism, yellow
0.12 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
φ and ω scans
15434 measured reflections
12813 independent reflections
9862 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.7°$
$h = -16 \rightarrow 16$
$k = -24 \rightarrow 26$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.132$
$S = 1.06$
12813 reflections
670 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.01 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2995 (5)	0.8427 (4)	0.1246 (5)	0.0201 (13)
C2	0.3807 (5)	0.9299 (3)	0.3937 (5)	0.0219 (13)
C3	0.4996 (6)	0.9276 (4)	0.4278 (6)	0.0270 (15)
H3	0.5538	0.9576	0.3928	0.032*
C4	0.5389 (7)	0.8828 (4)	0.5104 (6)	0.0375 (19)
H4	0.6189	0.8830	0.5318	0.045*
C5	0.4618 (6)	0.8371 (4)	0.5629 (5)	0.0294 (16)
C6	0.5008 (8)	0.7871 (5)	0.6434 (6)	0.048 (2)
H6	0.5805	0.7860	0.6659	0.057*
C7	0.4237 (10)	0.7409 (5)	0.6881 (6)	0.058 (3)
H7	0.4506	0.7083	0.7423	0.070*
C8	0.3063 (8)	0.7404 (5)	0.6559 (7)	0.051 (2)
H8	0.2553	0.7067	0.6868	0.061*
C9	0.2642 (8)	0.7874 (4)	0.5810 (6)	0.041 (2)
H9	0.1837	0.7869	0.5615	0.049*
C10	0.3396 (6)	0.8376 (4)	0.5310 (5)	0.0294 (16)

C11	0.3028 (5)	0.8864 (4)	0.4492 (5)	0.0220 (14)
C12	0.1760 (5)	0.8928 (4)	0.4189 (5)	0.0261 (15)
H12	0.1401	0.8453	0.4139	0.031*
C13	0.1102 (6)	0.9370 (5)	0.5027 (6)	0.039 (2)
H13A	0.1150	0.9148	0.5761	0.059*
H13B	0.0283	0.9409	0.4791	0.059*
H13C	0.1450	0.9837	0.5067	0.059*
C14	0.2255 (7)	1.0778 (5)	0.2286 (8)	0.050 (2)
H14	0.1467	1.0869	0.2469	0.060*
C15	0.3115 (9)	1.0883 (5)	0.3096 (7)	0.049 (2)
H15	0.2920	1.1069	0.3803	0.059*
C16	0.4263 (8)	1.0714 (5)	0.2862 (7)	0.045 (2)
H16	0.4849	1.0788	0.3416	0.055*
C17	0.4571 (8)	1.0442 (5)	0.1846 (8)	0.050 (2)
H17	0.5357	1.0315	0.1710	0.060*
C18	0.3705 (10)	1.0354 (5)	0.1007 (7)	0.055 (3)
H18	0.3912	1.0170	0.0303	0.066*
C19	0.2502 (9)	1.0543 (4)	0.1212 (8)	0.055 (3)
H19	0.1915	1.0509	0.0649	0.066*
C20	0.4310 (5)	0.6561 (3)	0.1661 (5)	0.0193 (13)
C21	0.3938 (5)	0.6072 (4)	0.0840 (5)	0.0208 (14)
H21	0.4124	0.6151	0.0083	0.025*
C22	0.3320 (6)	0.5490 (4)	0.1122 (5)	0.0263 (15)
H22	0.3094	0.5172	0.0553	0.032*
C23	0.3005 (6)	0.5347 (4)	0.2225 (5)	0.0245 (14)
C24	0.2331 (6)	0.4752 (4)	0.2510 (6)	0.0357 (17)
H24	0.2115	0.4426	0.1948	0.043*
C25	0.1992 (6)	0.4643 (4)	0.3569 (6)	0.0382 (19)
H25	0.1536	0.4244	0.3742	0.046*
C26	0.2309 (7)	0.5115 (4)	0.4415 (7)	0.0384 (19)
H26	0.2047	0.5043	0.5152	0.046*
C27	0.2986 (6)	0.5674 (4)	0.4181 (5)	0.0290 (16)
H27	0.3221	0.5976	0.4769	0.035*
C28	0.3360 (5)	0.5823 (4)	0.3077 (5)	0.0240 (14)
C29	0.4020 (5)	0.6425 (4)	0.2765 (5)	0.0229 (14)
C30	0.4463 (6)	0.6940 (4)	0.3622 (5)	0.0249 (15)
H30	0.3875	0.7004	0.4220	0.030*
C31	0.5616 (6)	0.6688 (4)	0.4123 (6)	0.0364 (18)
H31A	0.6190	0.6639	0.3532	0.055*
H31B	0.5500	0.6235	0.4485	0.055*
H31C	0.5898	0.7028	0.4674	0.055*
C32	0.6082 (6)	0.7174 (4)	−0.0141 (6)	0.0308 (17)
H32	0.5918	0.6831	−0.0691	0.037*
C33	0.6721 (5)	0.6993 (4)	0.0846 (5)	0.0273 (16)
H33	0.6957	0.6524	0.0977	0.033*
C34	0.6991 (5)	0.7517 (5)	0.1618 (5)	0.0321 (16)
H34	0.7407	0.7400	0.2282	0.039*
C35	0.6650 (5)	0.8231 (4)	0.1422 (6)	0.0307 (17)

H35	0.6865	0.8585	0.1939	0.037*
C36	0.6011 (6)	0.8398 (4)	0.0483 (6)	0.0295 (16)
H36	0.5780	0.8868	0.0352	0.035*
C37	0.5697 (6)	0.7867 (4)	−0.0290 (6)	0.0319 (17)
H37	0.5220	0.7981	−0.0917	0.038*
C38	−0.0018 (5)	0.7922 (4)	0.1656 (5)	0.0210 (14)
C39	−0.0630 (5)	0.8442 (4)	0.2251 (5)	0.0228 (14)
H39	−0.0807	0.8875	0.1901	0.027*
C40	−0.0973 (5)	0.8328 (4)	0.3329 (5)	0.0236 (14)
H40	−0.1398	0.8681	0.3704	0.028*
C41	−0.0710 (6)	0.7704 (4)	0.3883 (5)	0.0276 (16)
C42	−0.1033 (7)	0.7603 (4)	0.5014 (6)	0.0367 (18)
H42	−0.1451	0.7956	0.5396	0.044*
C43	−0.0734 (7)	0.6995 (5)	0.5543 (6)	0.042 (2)
H43	−0.0939	0.6933	0.6299	0.051*
C44	−0.0146 (8)	0.6472 (5)	0.5006 (6)	0.044 (2)
H44	0.0051	0.6056	0.5397	0.053*
C45	0.0157 (6)	0.6541 (4)	0.3920 (6)	0.0366 (18)
H45	0.0550	0.6171	0.3556	0.044*
C46	−0.0113 (6)	0.7170 (4)	0.3325 (5)	0.0251 (14)
C47	0.0225 (5)	0.7292 (4)	0.2197 (5)	0.0227 (14)
C48	0.0813 (6)	0.6732 (4)	0.1515 (6)	0.0286 (16)
H48	0.1427	0.6501	0.1987	0.034*
C49	−0.0024 (7)	0.6186 (4)	0.1104 (7)	0.042 (2)
H49A	−0.0612	0.6403	0.0616	0.063*
H49B	−0.0408	0.5968	0.1739	0.063*
H49C	0.0401	0.5829	0.0688	0.063*
C50	0.0522 (9)	0.8959 (5)	−0.1028 (7)	0.053 (3)
H50	0.0912	0.9393	−0.0929	0.063*
C51	0.1030 (7)	0.8457 (6)	−0.1663 (6)	0.044 (2)
H51	0.1732	0.8556	−0.2041	0.053*
C52	0.0537 (8)	0.7825 (5)	−0.1752 (6)	0.045 (2)
H52	0.0903	0.7479	−0.2193	0.053*
C53	−0.0490 (8)	0.7661 (5)	−0.1221 (7)	0.050 (2)
H53	−0.0800	0.7202	−0.1265	0.060*
C54	−0.1065 (6)	0.8179 (7)	−0.0621 (6)	0.059 (3)
H54	−0.1792	0.8083	−0.0283	0.070*
C55	−0.0543 (10)	0.8858 (6)	−0.0522 (7)	0.062 (3)
H55	−0.0913	0.9223	−0.0125	0.075*
C56	0.6094 (7)	0.4920 (5)	0.2644 (7)	0.046 (2)
H56A	0.6005	0.4719	0.3398	0.055*
H56B	0.5462	0.5265	0.2523	0.055*
N1	0.1666 (4)	0.9289 (3)	0.3070 (4)	0.0247 (12)
H1A	0.1069	0.9609	0.3098	0.030*
H1B	0.1462	0.8960	0.2543	0.030*
N2	0.4657 (5)	0.7614 (3)	0.3023 (4)	0.0262 (13)
H2A	0.5237	0.7858	0.3389	0.031*
H2B	0.3986	0.7876	0.3054	0.031*

N3	0.1387 (4)	0.7088 (3)	0.0559 (4)	0.0232 (12)
H3A	0.1368	0.6791	−0.0044	0.028*
H3B	0.2157	0.7164	0.0744	0.028*
O1	0.3648 (3)	0.8835 (2)	0.1831 (3)	0.0203 (9)
O2	0.3397 (4)	0.7824 (2)	0.0963 (4)	0.0234 (10)
O3	0.1951 (3)	0.8604 (2)	0.0977 (3)	0.0218 (10)
F1	0.0698 (6)	0.5255 (4)	0.8771 (4)	0.093 (2)
F2	0.2357 (5)	0.4880 (4)	0.8156 (7)	0.110 (3)
F3	0.2403 (6)	0.5770 (4)	0.6939 (5)	0.089 (2)
F4	0.2240 (5)	0.5996 (3)	0.8724 (4)	0.0723 (18)
F5	0.0723 (5)	0.6159 (3)	0.7598 (6)	0.086 (2)
F6	0.0852 (5)	0.5061 (3)	0.6993 (4)	0.0566 (15)
P1	0.15655 (17)	0.55228 (11)	0.78605 (15)	0.0312 (4)
Cl1	0.5964 (2)	0.42565 (14)	0.1657 (2)	0.0600 (6)
Cl2	0.74437 (19)	0.53430 (14)	0.2568 (2)	0.0589 (6)
Ru1	0.31904 (4)	0.98086 (3)	0.25393 (4)	0.02012 (12)
Ru2	0.51234 (4)	0.74976 (3)	0.13391 (4)	0.01916 (12)
Ru3	0.06260 (4)	0.80527 (3)	0.00783 (4)	0.02022 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.021 (3)	0.024 (4)	0.016 (3)	0.003 (3)	0.002 (2)	0.003 (3)
C2	0.027 (3)	0.012 (3)	0.027 (3)	0.000 (3)	0.001 (2)	−0.004 (3)
C3	0.024 (3)	0.020 (4)	0.037 (4)	−0.003 (3)	−0.001 (3)	−0.002 (3)
C4	0.039 (4)	0.030 (5)	0.043 (4)	0.002 (4)	−0.019 (3)	−0.009 (4)
C5	0.046 (4)	0.021 (4)	0.021 (3)	0.008 (3)	−0.003 (3)	−0.010 (3)
C6	0.079 (6)	0.040 (6)	0.023 (4)	0.024 (5)	−0.014 (4)	−0.006 (4)
C7	0.128 (9)	0.028 (5)	0.019 (4)	0.019 (6)	0.015 (5)	0.006 (4)
C8	0.074 (7)	0.036 (5)	0.044 (5)	0.011 (5)	0.025 (4)	0.011 (4)
C9	0.061 (5)	0.027 (5)	0.034 (4)	0.006 (4)	0.021 (4)	0.009 (3)
C10	0.045 (4)	0.026 (4)	0.017 (3)	0.002 (3)	0.007 (3)	−0.004 (3)
C11	0.025 (3)	0.017 (3)	0.024 (3)	0.002 (3)	0.004 (2)	−0.004 (3)
C12	0.021 (3)	0.026 (4)	0.032 (4)	−0.007 (3)	0.007 (3)	0.002 (3)
C13	0.035 (4)	0.054 (6)	0.030 (4)	0.005 (4)	0.006 (3)	−0.012 (4)
C14	0.038 (5)	0.019 (4)	0.092 (7)	0.011 (4)	0.001 (4)	0.000 (5)
C15	0.076 (7)	0.026 (5)	0.046 (5)	−0.018 (4)	0.007 (4)	−0.008 (4)
C16	0.053 (5)	0.028 (5)	0.055 (5)	−0.020 (4)	−0.016 (4)	0.008 (4)
C17	0.046 (5)	0.027 (5)	0.078 (6)	−0.005 (4)	0.020 (4)	0.017 (5)
C18	0.111 (9)	0.026 (5)	0.028 (4)	−0.016 (5)	0.015 (5)	0.011 (4)
C19	0.075 (7)	0.021 (5)	0.068 (6)	−0.010 (5)	−0.047 (5)	0.017 (5)
C20	0.017 (3)	0.013 (3)	0.029 (3)	0.005 (2)	0.001 (2)	−0.001 (3)
C21	0.019 (3)	0.025 (4)	0.019 (3)	0.004 (3)	−0.004 (2)	−0.002 (3)
C22	0.025 (3)	0.026 (4)	0.028 (3)	−0.001 (3)	−0.009 (3)	−0.008 (3)
C23	0.024 (3)	0.019 (4)	0.030 (3)	−0.002 (3)	−0.006 (3)	−0.002 (3)
C24	0.030 (4)	0.027 (4)	0.050 (4)	−0.015 (3)	−0.008 (3)	0.001 (4)
C25	0.036 (4)	0.027 (4)	0.052 (5)	−0.002 (3)	0.006 (3)	0.016 (4)
C26	0.035 (4)	0.033 (5)	0.047 (5)	0.005 (4)	0.011 (3)	0.013 (4)

C27	0.032 (4)	0.028 (4)	0.027 (3)	0.009 (3)	0.003 (3)	−0.001 (3)
C28	0.022 (3)	0.021 (4)	0.029 (3)	0.007 (3)	0.002 (3)	0.002 (3)
C29	0.020 (3)	0.027 (4)	0.022 (3)	0.005 (3)	0.002 (2)	0.001 (3)
C30	0.033 (4)	0.023 (4)	0.019 (3)	−0.002 (3)	0.003 (3)	−0.001 (3)
C31	0.044 (5)	0.037 (5)	0.028 (4)	0.005 (4)	−0.013 (3)	−0.004 (4)
C32	0.030 (4)	0.027 (4)	0.035 (4)	−0.006 (3)	0.013 (3)	−0.010 (3)
C33	0.014 (3)	0.033 (4)	0.036 (4)	0.009 (3)	0.004 (3)	0.006 (3)
C34	0.013 (3)	0.046 (5)	0.037 (4)	−0.003 (3)	−0.006 (2)	0.004 (4)
C35	0.020 (3)	0.031 (4)	0.041 (4)	−0.004 (3)	0.001 (3)	−0.011 (3)
C36	0.024 (3)	0.018 (4)	0.047 (4)	−0.001 (3)	0.013 (3)	0.001 (3)
C37	0.027 (4)	0.040 (5)	0.029 (4)	0.002 (3)	0.003 (3)	0.004 (3)
C38	0.011 (3)	0.028 (4)	0.024 (3)	−0.003 (3)	−0.003 (2)	0.000 (3)
C39	0.019 (3)	0.017 (4)	0.033 (3)	0.000 (3)	0.000 (3)	0.000 (3)
C40	0.017 (3)	0.027 (4)	0.027 (3)	−0.002 (3)	0.007 (2)	−0.004 (3)
C41	0.027 (3)	0.032 (4)	0.023 (3)	−0.008 (3)	−0.003 (3)	0.002 (3)
C42	0.045 (4)	0.035 (5)	0.030 (4)	0.000 (4)	0.003 (3)	0.005 (4)
C43	0.057 (5)	0.050 (6)	0.020 (4)	−0.017 (4)	−0.001 (3)	0.011 (4)
C44	0.060 (5)	0.037 (5)	0.035 (4)	−0.010 (4)	−0.013 (4)	0.017 (4)
C45	0.036 (4)	0.031 (5)	0.042 (4)	−0.003 (4)	−0.013 (3)	0.003 (4)
C46	0.026 (3)	0.025 (4)	0.024 (3)	−0.004 (3)	−0.006 (3)	0.002 (3)
C47	0.016 (3)	0.023 (4)	0.029 (3)	0.000 (3)	−0.005 (2)	0.000 (3)
C48	0.019 (3)	0.028 (4)	0.038 (4)	0.003 (3)	0.001 (3)	0.000 (3)
C49	0.047 (5)	0.027 (4)	0.052 (5)	−0.006 (4)	0.012 (4)	−0.011 (4)
C50	0.074 (7)	0.033 (5)	0.051 (5)	−0.017 (5)	−0.032 (5)	0.016 (4)
C51	0.037 (4)	0.068 (7)	0.027 (4)	−0.005 (4)	0.006 (3)	0.009 (4)
C52	0.052 (5)	0.057 (6)	0.024 (4)	0.009 (5)	−0.004 (3)	−0.014 (4)
C53	0.064 (6)	0.041 (6)	0.044 (5)	−0.027 (5)	−0.027 (4)	0.008 (4)
C54	0.019 (4)	0.132 (11)	0.025 (4)	0.011 (5)	−0.008 (3)	0.020 (6)
C55	0.083 (7)	0.077 (8)	0.027 (4)	0.063 (7)	−0.021 (4)	−0.010 (5)
C56	0.045 (5)	0.036 (5)	0.057 (5)	0.007 (4)	0.018 (4)	0.004 (4)
N1	0.022 (3)	0.027 (3)	0.025 (3)	−0.007 (2)	0.000 (2)	−0.005 (3)
N2	0.025 (3)	0.022 (4)	0.031 (3)	0.000 (2)	−0.003 (2)	−0.003 (3)
N3	0.019 (3)	0.019 (3)	0.032 (3)	0.000 (2)	−0.005 (2)	−0.005 (3)
O1	0.018 (2)	0.016 (2)	0.026 (2)	0.0002 (18)	−0.0048 (17)	−0.0036 (19)
O2	0.019 (2)	0.018 (2)	0.033 (2)	0.0031 (18)	−0.0012 (18)	−0.005 (2)
O3	0.013 (2)	0.024 (3)	0.029 (2)	0.0024 (18)	−0.0031 (16)	−0.005 (2)
F1	0.136 (6)	0.097 (6)	0.046 (3)	−0.046 (5)	0.032 (3)	−0.005 (3)
F2	0.069 (4)	0.042 (4)	0.219 (8)	0.009 (4)	−0.056 (5)	0.001 (5)
F3	0.115 (5)	0.082 (5)	0.072 (4)	−0.066 (4)	0.045 (3)	−0.030 (4)
F4	0.106 (5)	0.052 (4)	0.058 (3)	−0.011 (3)	−0.043 (3)	−0.014 (3)
F5	0.064 (4)	0.034 (3)	0.158 (6)	0.011 (3)	−0.037 (4)	−0.001 (4)
F6	0.076 (4)	0.044 (3)	0.049 (3)	−0.031 (3)	−0.009 (2)	−0.006 (2)
P1	0.0385 (11)	0.0268 (11)	0.0282 (9)	−0.0024 (8)	−0.0040 (8)	−0.0021 (8)
Cl1	0.0737 (16)	0.0425 (14)	0.0635 (14)	0.0017 (13)	−0.0093 (12)	−0.0031 (12)
Cl2	0.0362 (11)	0.0526 (15)	0.0879 (17)	−0.0006 (11)	0.0012 (10)	0.0091 (14)
Ru1	0.0205 (2)	0.0170 (3)	0.0229 (2)	−0.0008 (2)	−0.00081 (18)	−0.0004 (2)
Ru2	0.0149 (2)	0.0201 (3)	0.0225 (2)	0.0010 (2)	−0.00019 (17)	−0.0030 (2)
Ru3	0.0163 (2)	0.0223 (3)	0.0221 (2)	0.0002 (2)	−0.00065 (17)	−0.0025 (2)

Geometric parameters (Å, º)

C1—O3	1.281 (7)	C33—H33	0.9500
C1—O1	1.284 (8)	C34—C35	1.440 (11)
C1—O2	1.291 (8)	C34—Ru2	2.165 (6)
C2—C11	1.398 (9)	C34—H34	0.9500
C2—C3	1.419 (9)	C35—C36	1.373 (10)
C2—Ru1	2.059 (6)	C35—Ru2	2.245 (7)
C3—C4	1.382 (10)	C35—H35	0.9500
C3—H3	0.9500	C36—C37	1.419 (10)
C4—C5	1.400 (11)	C36—Ru2	2.257 (7)
C4—H4	0.9500	C36—H36	0.9500
C5—C6	1.427 (10)	C37—Ru2	2.191 (7)
C5—C10	1.449 (10)	C37—H37	0.9500
C6—C7	1.367 (13)	C38—C47	1.397 (9)
C6—H6	0.9500	C38—C39	1.417 (9)
C7—C8	1.396 (13)	C38—Ru3	2.060 (6)
C7—H7	0.9500	C39—C40	1.376 (9)
C8—C9	1.356 (11)	C39—H39	0.9500
C8—H8	0.9500	C40—C41	1.399 (10)
C9—C10	1.431 (10)	C40—H40	0.9500
C9—H9	0.9500	C41—C46	1.405 (10)
C10—C11	1.415 (9)	C41—C42	1.427 (9)
C11—C12	1.500 (9)	C42—C43	1.367 (11)
C12—N1	1.514 (8)	C42—H42	0.9500
C12—C13	1.523 (9)	C43—C44	1.374 (12)
C12—H12	1.0000	C43—H43	0.9500
C13—H13A	0.9800	C44—C45	1.361 (11)
C13—H13B	0.9800	C44—H44	0.9500
C13—H13C	0.9800	C45—C46	1.432 (10)
C14—C15	1.391 (12)	C45—H45	0.9500
C14—C19	1.399 (13)	C46—C47	1.433 (9)
C14—Ru1	2.162 (8)	C47—C48	1.513 (9)
C14—H14	0.9500	C48—N3	1.497 (9)
C15—C16	1.388 (12)	C48—C49	1.499 (10)
C15—Ru1	2.165 (9)	C48—H48	1.0000
C15—H15	0.9500	C49—H49A	0.9800
C16—C17	1.379 (12)	C49—H49B	0.9800
C16—Ru1	2.158 (8)	C49—H49C	0.9800
C16—H16	0.9500	C50—C51	1.361 (13)
C17—C18	1.415 (13)	C50—C55	1.387 (14)
C17—Ru1	2.171 (8)	C50—Ru3	2.187 (8)
C17—H17	0.9500	C50—H50	0.9500
C18—C19	1.451 (14)	C51—C52	1.339 (13)
C18—Ru1	2.205 (7)	C51—Ru3	2.284 (7)
C18—H18	0.9500	C51—H51	0.9500
C19—Ru1	2.260 (8)	C52—C53	1.383 (12)
C19—H19	0.9500	C52—Ru3	2.243 (7)

C20—C29	1.397 (8)	C52—H52	0.9500
C20—C21	1.421 (9)	C53—C54	1.398 (14)
C20—Ru2	2.060 (6)	C53—Ru3	2.140 (7)
C21—C22	1.366 (9)	C53—H53	0.9500
C21—H21	0.9500	C54—C55	1.434 (16)
C22—C23	1.405 (9)	C54—Ru3	2.117 (7)
C22—H22	0.9500	C54—H54	0.9500
C23—C24	1.421 (10)	C55—Ru3	2.160 (8)
C23—C28	1.427 (9)	C55—H55	0.9500
C24—C25	1.352 (10)	C56—Cl1	1.742 (9)
C24—H24	0.9500	C56—Cl2	1.751 (8)
C25—C26	1.405 (11)	C56—H56A	0.9900
C25—H25	0.9500	C56—H56B	0.9900
C26—C27	1.353 (10)	N1—Ru1	2.119 (5)
C26—H26	0.9500	N1—H1A	0.9200
C27—C28	1.429 (9)	N1—H1B	0.9200
C27—H27	0.9500	N2—Ru2	2.112 (5)
C28—C29	1.432 (10)	N2—H2A	0.9200
C29—C30	1.508 (9)	N2—H2B	0.9200
C30—N2	1.495 (9)	N3—Ru3	2.119 (6)
C30—C31	1.523 (10)	N3—H3A	0.9200
C30—H30	1.0000	N3—H3B	0.9200
C31—H31A	0.9800	O1—Ru1	2.118 (4)
C31—H31B	0.9800	O2—Ru2	2.119 (4)
C31—H31C	0.9800	O3—Ru3	2.132 (4)
C32—C37	1.409 (10)	F1—P1	1.576 (6)
C32—C33	1.428 (10)	F2—P1	1.566 (7)
C32—Ru2	2.193 (7)	F3—P1	1.551 (5)
C32—H32	0.9500	F4—P1	1.572 (5)
C33—C34	1.397 (10)	F5—P1	1.584 (6)
C33—Ru2	2.162 (6)	F6—P1	1.585 (5)

O3—C1—O1	120.9 (6)	C47—C48—H48	108.7
O3—C1—O2	120.4 (6)	C48—C49—H49A	109.5
O1—C1—O2	118.7 (5)	C48—C49—H49B	109.5
C11—C2—C3	117.5 (6)	H49A—C49—H49B	109.5
C11—C2—Ru1	117.2 (5)	C48—C49—H49C	109.5
C3—C2—Ru1	124.6 (5)	H49A—C49—H49C	109.5
C4—C3—C2	121.9 (7)	H49B—C49—H49C	109.5
C4—C3—H3	119.0	C51—C50—C55	122.3 (9)
C2—C3—H3	119.0	C51—C50—Ru3	76.2 (5)
C3—C4—C5	120.6 (7)	C55—C50—Ru3	70.3 (5)
C3—C4—H4	119.7	C51—C50—H50	118.9
C5—C4—H4	119.7	C55—C50—H50	118.9
C4—C5—C6	122.0 (7)	Ru3—C50—H50	126.6
C4—C5—C10	119.5 (6)	C52—C51—C50	119.9 (8)
C6—C5—C10	118.5 (7)	C52—C51—Ru3	71.1 (5)
C7—C6—C5	120.1 (9)	C50—C51—Ru3	68.4 (4)

C7—C6—H6	119.9	C52—C51—H51	120.1
C5—C6—H6	119.9	C50—C51—H51	120.1
C6—C7—C8	121.5 (8)	Ru3—C51—H51	133.6
C6—C7—H7	119.2	C51—C52—C53	122.0 (8)
C8—C7—H7	119.2	C51—C52—Ru3	74.5 (5)
C9—C8—C7	120.8 (8)	C53—C52—Ru3	67.6 (4)
C9—C8—H8	119.6	C51—C52—H52	119.0
C7—C8—H8	119.6	C53—C52—H52	119.0
C8—C9—C10	120.8 (8)	Ru3—C52—H52	131.9
C8—C9—H9	119.6	C52—C53—C54	119.2 (9)
C10—C9—H9	119.6	C52—C53—Ru3	75.7 (5)
C11—C10—C9	124.0 (7)	C54—C53—Ru3	69.9 (4)
C11—C10—C5	117.7 (6)	C52—C53—H53	120.4
C9—C10—C5	118.2 (7)	C54—C53—H53	120.4
C2—C11—C10	122.6 (6)	Ru3—C53—H53	125.7
C2—C11—C12	117.4 (6)	C53—C54—C55	119.0 (8)
C10—C11—C12	120.0 (6)	C53—C54—Ru3	71.7 (4)
C11—C12—N1	108.0 (5)	C55—C54—Ru3	72.0 (5)
C11—C12—C13	111.9 (6)	C53—C54—H54	120.5
N1—C12—C13	107.7 (6)	C55—C54—H54	120.5
C11—C12—H12	109.7	Ru3—C54—H54	127.8
N1—C12—H12	109.7	C50—C55—C54	117.3 (8)
C13—C12—H12	109.7	C50—C55—Ru3	72.5 (5)
C12—C13—H13A	109.5	C54—C55—Ru3	68.8 (5)
C12—C13—H13B	109.5	C50—C55—H55	121.3
H13A—C13—H13B	109.5	C54—C55—H55	121.3
C12—C13—H13C	109.5	Ru3—C55—H55	129.6
H13A—C13—H13C	109.5	Cl1—C56—Cl2	111.6 (4)
H13B—C13—H13C	109.5	Cl1—C56—H56A	109.3
C15—C14—C19	122.7 (8)	Cl2—C56—H56A	109.3
C15—C14—Ru1	71.3 (5)	Cl1—C56—H56B	109.3
C19—C14—Ru1	75.4 (5)	Cl2—C56—H56B	109.3
C15—C14—H14	118.6	H56A—C56—H56B	108.0
C19—C14—H14	118.6	C12—N1—Ru1	115.6 (4)
Ru1—C14—H14	126.7	C12—N1—H1A	108.4
C16—C15—C14	119.3 (8)	Ru1—N1—H1A	108.4
C16—C15—Ru1	71.0 (5)	C12—N1—H1B	108.4
C14—C15—Ru1	71.1 (5)	Ru1—N1—H1B	108.4
C16—C15—H15	120.3	H1A—N1—H1B	107.4
C14—C15—H15	120.3	C30—N2—Ru2	114.4 (4)
Ru1—C15—H15	130.0	C30—N2—H2A	108.7
C17—C16—C15	121.6 (8)	Ru2—N2—H2A	108.7
C17—C16—Ru1	71.9 (5)	C30—N2—H2B	108.7
C15—C16—Ru1	71.6 (5)	Ru2—N2—H2B	108.7
C17—C16—H16	119.2	H2A—N2—H2B	107.6
C15—C16—H16	119.2	C48—N3—Ru3	114.9 (4)
Ru1—C16—H16	129.9	C48—N3—H3A	108.5
C16—C17—C18	119.3 (8)	Ru3—N3—H3A	108.5

C16—C17—Ru1	70.9 (5)	C48—N3—H3B	108.5
C18—C17—Ru1	72.4 (5)	Ru3—N3—H3B	108.5
C16—C17—H17	120.4	H3A—N3—H3B	107.5
C18—C17—H17	120.4	C1—O1—Ru1	127.5 (4)
Ru1—C17—H17	128.5	C1—O2—Ru2	122.9 (4)
C17—C18—C19	120.6 (8)	C1—O3—Ru3	130.9 (4)
C17—C18—Ru1	69.8 (4)	F3—P1—F2	92.2 (4)
C19—C18—Ru1	73.1 (5)	F3—P1—F4	89.5 (3)
C17—C18—H18	119.7	F2—P1—F4	91.4 (3)
C19—C18—H18	119.7	F3—P1—F1	178.3 (4)
Ru1—C18—H18	129.9	F2—P1—F1	87.6 (4)
C14—C19—C18	116.3 (7)	F4—P1—F1	92.3 (3)
C14—C19—Ru1	67.8 (5)	F3—P1—F5	90.3 (4)
C18—C19—Ru1	69.0 (4)	F2—P1—F5	177.5 (4)
C14—C19—H19	121.8	F4—P1—F5	89.0 (3)
C18—C19—H19	121.8	F1—P1—F5	89.9 (4)
Ru1—C19—H19	134.2	F3—P1—F6	91.2 (3)
C29—C20—C21	117.6 (6)	F2—P1—F6	90.2 (3)
C29—C20—Ru2	117.1 (5)	F4—P1—F6	178.3 (3)
C21—C20—Ru2	125.1 (5)	F1—P1—F6	87.1 (3)
C22—C21—C20	121.1 (6)	F5—P1—F6	89.4 (3)
C22—C21—H21	119.4	C2—Ru1—O1	80.0 (2)
C20—C21—H21	119.4	C2—Ru1—N1	78.9 (2)
C21—C22—C23	122.3 (6)	O1—Ru1—N1	85.3 (2)
C21—C22—H22	118.8	C2—Ru1—C16	92.6 (3)
C23—C22—H22	118.8	O1—Ru1—C16	129.5 (3)
C22—C23—C24	122.2 (6)	N1—Ru1—C16	142.6 (3)
C22—C23—C28	118.5 (6)	C2—Ru1—C14	133.2 (3)
C24—C23—C28	119.3 (6)	O1—Ru1—C14	145.5 (3)
C25—C24—C23	121.0 (7)	N1—Ru1—C14	92.0 (3)
C25—C24—H24	119.5	C16—Ru1—C14	67.4 (4)
C23—C24—H24	119.5	C2—Ru1—C15	102.3 (3)
C24—C25—C26	120.4 (7)	O1—Ru1—C15	166.3 (3)
C24—C25—H25	119.8	N1—Ru1—C15	108.4 (3)
C26—C25—H25	119.8	C16—Ru1—C15	37.5 (3)
C27—C26—C25	120.1 (7)	C14—Ru1—C15	37.5 (3)
C27—C26—H26	120.0	C2—Ru1—C17	109.5 (3)
C25—C26—H26	120.0	O1—Ru1—C17	98.7 (3)
C26—C27—C28	122.2 (7)	N1—Ru1—C17	171.2 (3)
C26—C27—H27	118.9	C16—Ru1—C17	37.2 (3)
C28—C27—H27	118.9	C14—Ru1—C17	80.2 (3)
C23—C28—C27	116.9 (7)	C15—Ru1—C17	67.7 (3)
C23—C28—C29	118.2 (6)	C2—Ru1—C18	144.4 (3)
C27—C28—C29	124.8 (6)	O1—Ru1—C18	90.6 (3)
C20—C29—C28	122.2 (6)	N1—Ru1—C18	134.9 (3)
C20—C29—C30	116.4 (6)	C16—Ru1—C18	67.1 (3)
C28—C29—C30	121.4 (5)	C14—Ru1—C18	67.3 (4)
N2—C30—C29	106.6 (5)	C15—Ru1—C18	79.7 (3)

N2—C30—C31	109.2 (6)	C17—Ru1—C18	37.7 (3)
C29—C30—C31	110.2 (6)	C2—Ru1—C19	169.4 (3)
N2—C30—H30	110.3	O1—Ru1—C19	110.5 (3)
C29—C30—H30	110.3	N1—Ru1—C19	102.9 (3)
C31—C30—H30	110.3	C16—Ru1—C19	79.6 (3)
C30—C31—H31A	109.5	C14—Ru1—C19	36.8 (4)
C30—C31—H31B	109.5	C15—Ru1—C19	67.2 (3)
H31A—C31—H31B	109.5	C17—Ru1—C19	68.3 (4)
C30—C31—H31C	109.5	C18—Ru1—C19	37.9 (4)
H31A—C31—H31C	109.5	C20—Ru2—N2	77.8 (2)
H31B—C31—H31C	109.5	C20—Ru2—O2	82.6 (2)
C37—C32—C33	119.4 (7)	N2—Ru2—O2	85.66 (19)
C37—C32—Ru2	71.2 (4)	C20—Ru2—C33	92.9 (3)
C33—C32—Ru2	69.7 (4)	N2—Ru2—C33	122.5 (2)
C37—C32—H32	120.3	O2—Ru2—C33	150.1 (2)
C33—C32—H32	120.3	C20—Ru2—C34	115.9 (3)
Ru2—C32—H32	131.6	N2—Ru2—C34	96.5 (2)
C34—C33—C32	118.9 (7)	O2—Ru2—C34	161.5 (3)
C34—C33—Ru2	71.3 (4)	C33—Ru2—C34	37.7 (3)
C32—C33—Ru2	72.1 (4)	C20—Ru2—C37	126.3 (3)
C34—C33—H33	120.6	N2—Ru2—C37	154.9 (3)
C32—C33—H33	120.6	O2—Ru2—C37	90.4 (2)
Ru2—C33—H33	128.2	C33—Ru2—C37	68.5 (3)
C33—C34—C35	121.0 (6)	C34—Ru2—C37	79.8 (3)
C33—C34—Ru2	71.0 (4)	C20—Ru2—C32	98.1 (3)
C35—C34—Ru2	74.0 (4)	N2—Ru2—C32	160.6 (3)
C33—C34—H34	119.5	O2—Ru2—C32	112.9 (2)
C35—C34—H34	119.5	C33—Ru2—C32	38.3 (3)
Ru2—C34—H34	127.6	C34—Ru2—C32	67.9 (3)
C36—C35—C34	119.7 (7)	C37—Ru2—C32	37.5 (3)
C36—C35—Ru2	72.7 (4)	C20—Ru2—C35	153.0 (3)
C34—C35—Ru2	67.9 (4)	N2—Ru2—C35	95.8 (2)
C36—C35—H35	120.1	O2—Ru2—C35	123.5 (2)
C34—C35—H35	120.1	C33—Ru2—C35	68.1 (3)
Ru2—C35—H35	132.1	C34—Ru2—C35	38.1 (3)
C35—C36—C37	119.9 (7)	C37—Ru2—C35	66.0 (3)
C35—C36—Ru2	71.8 (4)	C32—Ru2—C35	79.2 (3)
C37—C36—Ru2	68.9 (4)	C20—Ru2—C36	163.4 (2)
C35—C36—H36	120.1	N2—Ru2—C36	118.6 (2)
C37—C36—H36	120.1	O2—Ru2—C36	96.0 (2)
Ru2—C36—H36	132.2	C33—Ru2—C36	80.0 (3)
C32—C37—C36	120.9 (7)	C34—Ru2—C36	66.7 (3)
C32—C37—Ru2	71.3 (4)	C37—Ru2—C36	37.2 (3)
C36—C37—Ru2	73.9 (4)	C32—Ru2—C36	67.1 (3)
C32—C37—H37	119.5	C35—Ru2—C36	35.5 (3)
C36—C37—H37	119.5	C38—Ru3—C54	92.3 (3)
Ru2—C37—H37	127.3	C38—Ru3—N3	78.2 (2)
C47—C38—C39	117.9 (5)	C54—Ru3—N3	125.4 (4)

C47—C38—Ru3	117.5 (5)	C38—Ru3—O3	81.8 (2)
C39—C38—Ru3	124.5 (5)	C54—Ru3—O3	141.9 (4)
C40—C39—C38	121.0 (6)	N3—Ru3—O3	90.30 (19)
C40—C39—H39	119.5	C38—Ru3—C53	114.2 (3)
C38—C39—H39	119.5	C54—Ru3—C53	38.3 (4)
C39—C40—C41	121.3 (6)	N3—Ru3—C53	97.7 (3)
C39—C40—H40	119.3	O3—Ru3—C53	163.2 (3)
C41—C40—H40	119.3	C38—Ru3—C55	99.5 (3)
C40—C41—C46	119.8 (6)	C54—Ru3—C55	39.2 (4)
C40—C41—C42	120.7 (7)	N3—Ru3—C55	164.6 (4)
C46—C41—C42	119.5 (7)	O3—Ru3—C55	104.5 (4)
C43—C42—C41	119.4 (7)	C53—Ru3—C55	69.2 (4)
C43—C42—H42	120.3	C38—Ru3—C50	129.7 (4)
C41—C42—H42	120.3	C54—Ru3—C50	68.1 (4)
C42—C43—C44	121.6 (7)	N3—Ru3—C50	151.0 (3)
C42—C43—H43	119.2	O3—Ru3—C50	87.0 (2)
C44—C43—H43	119.2	C53—Ru3—C50	78.9 (3)
C45—C44—C43	120.8 (8)	C55—Ru3—C50	37.2 (4)
C45—C44—H44	119.6	C38—Ru3—C52	150.1 (3)
C43—C44—H44	119.6	C54—Ru3—C52	66.7 (3)
C44—C45—C46	120.3 (8)	N3—Ru3—C52	96.4 (3)
C44—C45—H45	119.8	O3—Ru3—C52	127.9 (3)
C46—C45—H45	119.8	C53—Ru3—C52	36.7 (3)
C41—C46—C45	118.4 (6)	C55—Ru3—C52	78.0 (3)
C41—C46—C47	118.3 (6)	C50—Ru3—C52	63.7 (4)
C45—C46—C47	123.3 (7)	C38—Ru3—C51	164.6 (3)
C38—C47—C46	121.7 (6)	C54—Ru3—C51	78.1 (3)
C38—C47—C48	116.5 (6)	N3—Ru3—C51	117.2 (3)
C46—C47—C48	121.7 (6)	O3—Ru3—C51	98.2 (3)
N3—C48—C49	110.5 (6)	C53—Ru3—C51	65.0 (3)
N3—C48—C47	107.4 (6)	C55—Ru3—C51	65.5 (3)
C49—C48—C47	112.6 (5)	C50—Ru3—C51	35.4 (3)
N3—C48—H48	108.8	C52—Ru3—C51	34.4 (3)
C49—C48—H48	108.8		

C11—C2—C3—C4	1.8 (10)	C17—C18—Ru1—C19	132.7 (8)
Ru1—C2—C3—C4	−168.3 (6)	C14—C19—Ru1—C2	−23 (2)
C2—C3—C4—C5	0.8 (11)	C18—C19—Ru1—C2	109.2 (18)
C3—C4—C5—C6	175.9 (7)	C14—C19—Ru1—O1	165.5 (5)
C3—C4—C5—C10	−0.8 (11)	C18—C19—Ru1—O1	−62.5 (5)
C4—C5—C6—C7	−176.4 (7)	C14—C19—Ru1—N1	75.8 (5)
C10—C5—C6—C7	0.4 (10)	C18—C19—Ru1—N1	−152.2 (5)
C5—C6—C7—C8	0.9 (12)	C14—C19—Ru1—C16	−66.1 (6)
C6—C7—C8—C9	−1.9 (13)	C18—C19—Ru1—C16	65.9 (5)
C7—C8—C9—C10	1.5 (12)	C18—C19—Ru1—C14	132.0 (8)
C8—C9—C10—C11	177.5 (7)	C14—C19—Ru1—C15	−29.1 (5)
C8—C9—C10—C5	−0.3 (10)	C18—C19—Ru1—C15	102.9 (6)
C4—C5—C10—C11	−1.7 (9)	C14—C19—Ru1—C17	−103.0 (6)

C6—C5—C10—C11	−178.6 (6)	C18—C19—Ru1—C17	28.9 (5)
C4—C5—C10—C9	176.2 (6)	C14—C19—Ru1—C18	−132.0 (8)
C6—C5—C10—C9	−0.7 (9)	C29—C20—Ru2—N2	−8.2 (5)
C3—C2—C11—C10	−4.5 (10)	C21—C20—Ru2—N2	166.5 (6)
Ru1—C2—C11—C10	166.3 (5)	C29—C20—Ru2—O2	−95.3 (5)
C3—C2—C11—C12	175.6 (6)	C21—C20—Ru2—O2	79.4 (5)
Ru1—C2—C11—C12	−13.6 (8)	C29—C20—Ru2—C33	114.4 (5)
C9—C10—C11—C2	−173.2 (6)	C21—C20—Ru2—C33	−70.9 (5)
C5—C10—C11—C2	4.5 (10)	C29—C20—Ru2—C34	83.3 (5)
C9—C10—C11—C12	6.7 (10)	C21—C20—Ru2—C34	−102.1 (5)
C5—C10—C11—C12	−175.6 (6)	C29—C20—Ru2—C37	179.7 (4)
C2—C11—C12—N1	18.7 (8)	C21—C20—Ru2—C37	−5.6 (6)
C10—C11—C12—N1	−161.2 (6)	C29—C20—Ru2—C32	152.5 (5)
C2—C11—C12—C13	−99.7 (7)	C21—C20—Ru2—C32	−32.8 (6)
C10—C11—C12—C13	80.4 (8)	C29—C20—Ru2—C35	70.5 (7)
C19—C14—C15—C16	−3.7 (13)	C21—C20—Ru2—C35	−114.9 (6)
Ru1—C14—C15—C16	54.1 (8)	C29—C20—Ru2—C36	178.5 (7)
C19—C14—C15—Ru1	−57.7 (8)	C21—C20—Ru2—C36	−6.9 (12)
C14—C15—C16—C17	−0.2 (13)	C30—N2—Ru2—C20	22.1 (4)
Ru1—C15—C16—C17	54.0 (8)	C30—N2—Ru2—O2	105.5 (4)
C14—C15—C16—Ru1	−54.2 (7)	C30—N2—Ru2—C33	−63.6 (5)
C15—C16—C17—C18	2.1 (13)	C30—N2—Ru2—C34	−93.0 (5)
Ru1—C16—C17—C18	55.9 (7)	C30—N2—Ru2—C37	−172.9 (5)
C15—C16—C17—Ru1	−53.8 (7)	C30—N2—Ru2—C32	−57.6 (9)
C16—C17—C18—C19	−0.4 (13)	C30—N2—Ru2—C35	−131.3 (4)
Ru1—C17—C18—C19	54.8 (7)	C30—N2—Ru2—C36	−160.0 (4)
C16—C17—C18—Ru1	−55.2 (7)	C1—O2—Ru2—C20	139.6 (5)
C15—C14—C19—C18	5.2 (13)	C1—O2—Ru2—N2	61.3 (5)
Ru1—C14—C19—C18	−50.7 (7)	C1—O2—Ru2—C33	−137.4 (5)
C15—C14—C19—Ru1	55.9 (8)	C1—O2—Ru2—C34	−36.3 (9)
C17—C18—C19—C14	−3.1 (12)	C1—O2—Ru2—C37	−93.8 (5)
Ru1—C18—C19—C14	50.2 (7)	C1—O2—Ru2—C32	−124.7 (5)
C17—C18—C19—Ru1	−53.2 (7)	C1—O2—Ru2—C35	−32.7 (5)
C29—C20—C21—C22	0.1 (9)	C1—O2—Ru2—C36	−57.0 (5)
Ru2—C20—C21—C22	−174.6 (5)	C34—C33—Ru2—C20	−130.4 (4)
C20—C21—C22—C23	0.8 (10)	C32—C33—Ru2—C20	99.4 (4)
C21—C22—C23—C24	178.1 (7)	C34—C33—Ru2—N2	−52.9 (5)
C21—C22—C23—C28	−0.8 (10)	C32—C33—Ru2—N2	176.8 (4)
C22—C23—C24—C25	−176.8 (7)	C34—C33—Ru2—O2	149.3 (5)
C28—C23—C24—C25	2.0 (11)	C32—C33—Ru2—O2	19.1 (7)
C23—C24—C25—C26	−0.5 (12)	C32—C33—Ru2—C34	−130.2 (7)
C24—C25—C26—C27	−2.0 (12)	C34—C33—Ru2—C37	101.5 (5)
C25—C26—C27—C28	2.8 (11)	C32—C33—Ru2—C37	−28.7 (4)
C22—C23—C28—C27	177.7 (6)	C34—C33—Ru2—C32	130.2 (7)
C24—C23—C28—C27	−1.2 (9)	C34—C33—Ru2—C35	29.7 (4)
C22—C23—C28—C29	0.0 (9)	C32—C33—Ru2—C35	−100.5 (5)
C24—C23—C28—C29	−178.9 (6)	C34—C33—Ru2—C36	64.7 (4)
C26—C27—C28—C23	−1.2 (10)	C32—C33—Ru2—C36	−65.6 (4)

C26—C27—C28—C29	176.3 (7)	C33—C34—Ru2—C20	57.7 (5)
C21—C20—C29—C28	−0.9 (9)	C35—C34—Ru2—C20	−170.6 (4)
Ru2—C20—C29—C28	174.2 (5)	C33—C34—Ru2—N2	137.3 (4)
C21—C20—C29—C30	177.9 (6)	C35—C34—Ru2—N2	−91.0 (4)
Ru2—C20—C29—C30	−7.0 (7)	C33—C34—Ru2—O2	−126.8 (7)
C23—C28—C29—C20	0.8 (9)	C35—C34—Ru2—O2	4.9 (9)
C27—C28—C29—C20	−176.7 (6)	C35—C34—Ru2—C33	131.7 (6)
C23—C28—C29—C30	−177.9 (6)	C33—C34—Ru2—C37	−67.8 (4)
C27—C28—C29—C30	4.6 (10)	C35—C34—Ru2—C37	63.9 (4)
C20—C29—C30—N2	24.0 (8)	C33—C34—Ru2—C32	−30.7 (4)
C28—C29—C30—N2	−157.2 (6)	C35—C34—Ru2—C32	101.0 (5)
C20—C29—C30—C31	−94.4 (7)	C33—C34—Ru2—C35	−131.7 (6)
C28—C29—C30—C31	84.4 (8)	C33—C34—Ru2—C36	−104.3 (4)
C37—C32—C33—C34	−2.8 (9)	C35—C34—Ru2—C36	27.4 (4)
Ru2—C32—C33—C34	−55.7 (5)	C32—C37—Ru2—C20	−47.9 (5)
C37—C32—C33—Ru2	52.9 (6)	C36—C37—Ru2—C20	−179.4 (4)
C32—C33—C34—C35	−0.8 (9)	C32—C37—Ru2—N2	150.4 (5)
Ru2—C33—C34—C35	−56.9 (5)	C36—C37—Ru2—N2	19.0 (8)
C32—C33—C34—Ru2	56.1 (5)	C32—C37—Ru2—O2	−129.0 (4)
C33—C34—C35—C36	2.4 (10)	C36—C37—Ru2—O2	99.5 (4)
Ru2—C34—C35—C36	−53.1 (6)	C32—C37—Ru2—C33	29.3 (4)
C33—C34—C35—Ru2	55.5 (5)	C36—C37—Ru2—C33	−102.2 (5)
C34—C35—C36—C37	−0.3 (10)	C32—C37—Ru2—C34	66.8 (5)
Ru2—C35—C36—C37	−51.2 (6)	C36—C37—Ru2—C34	−64.7 (4)
C34—C35—C36—Ru2	50.9 (5)	C36—C37—Ru2—C32	−131.5 (6)
C33—C32—C37—C36	4.9 (10)	C32—C37—Ru2—C35	104.0 (5)
Ru2—C32—C37—C36	57.1 (6)	C36—C37—Ru2—C35	−27.4 (4)
C33—C32—C37—Ru2	−52.2 (6)	C32—C37—Ru2—C36	131.5 (6)
C35—C36—C37—C32	−3.3 (10)	C37—C32—Ru2—C20	142.8 (4)
Ru2—C36—C37—C32	−55.9 (6)	C33—C32—Ru2—C20	−84.4 (4)
C35—C36—C37—Ru2	52.5 (6)	C37—C32—Ru2—N2	−140.9 (7)
C47—C38—C39—C40	0.1 (9)	C33—C32—Ru2—N2	−8.1 (10)
Ru3—C38—C39—C40	−176.1 (5)	C37—C32—Ru2—O2	57.4 (5)
C38—C39—C40—C41	1.4 (10)	C33—C32—Ru2—O2	−169.8 (4)
C39—C40—C41—C46	−1.9 (10)	C37—C32—Ru2—C33	−132.8 (6)
C39—C40—C41—C42	177.6 (6)	C37—C32—Ru2—C34	−102.5 (5)
C40—C41—C42—C43	−178.2 (7)	C33—C32—Ru2—C34	30.3 (4)
C46—C41—C42—C43	1.3 (11)	C33—C32—Ru2—C37	132.8 (6)
C41—C42—C43—C44	−1.1 (12)	C37—C32—Ru2—C35	−64.5 (4)
C42—C43—C44—C45	−0.2 (13)	C33—C32—Ru2—C35	68.3 (4)
C43—C44—C45—C46	1.3 (12)	C37—C32—Ru2—C36	−29.4 (4)
C40—C41—C46—C45	179.2 (6)	C33—C32—Ru2—C36	103.3 (5)
C42—C41—C46—C45	−0.3 (10)	C36—C35—Ru2—C20	152.2 (5)
C40—C41—C46—C47	1.0 (9)	C34—C35—Ru2—C20	18.8 (8)
C42—C41—C46—C47	−178.6 (6)	C36—C35—Ru2—N2	−133.4 (4)
C44—C45—C46—C41	−0.9 (10)	C34—C35—Ru2—N2	93.3 (4)
C44—C45—C46—C47	177.2 (7)	C36—C35—Ru2—O2	−44.8 (5)
C39—C38—C47—C46	−1.0 (9)	C34—C35—Ru2—O2	−178.1 (3)

Ru3—C38—C47—C46	175.5 (5)	C36—C35—Ru2—C33	103.9 (4)
C39—C38—C47—C48	176.3 (6)	C34—C35—Ru2—C33	−29.5 (4)
Ru3—C38—C47—C48	−7.2 (7)	C36—C35—Ru2—C34	133.4 (6)
C41—C46—C47—C38	0.5 (9)	C36—C35—Ru2—C37	28.6 (4)
C45—C46—C47—C38	−177.7 (6)	C34—C35—Ru2—C37	−104.7 (5)
C41—C46—C47—C48	−176.7 (6)	C36—C35—Ru2—C32	65.6 (4)
C45—C46—C47—C48	5.2 (10)	C34—C35—Ru2—C32	−67.8 (4)
C38—C47—C48—N3	21.1 (8)	C34—C35—Ru2—C36	−133.4 (6)
C46—C47—C48—N3	−161.6 (5)	C35—C36—Ru2—C20	−131.9 (8)
C38—C47—C48—C49	−100.8 (7)	C37—C36—Ru2—C20	1.7 (11)
C46—C47—C48—C49	76.5 (8)	C35—C36—Ru2—N2	55.5 (5)
C55—C50—C51—C52	−4.5 (13)	C37—C36—Ru2—N2	−171.0 (4)
Ru3—C50—C51—C52	51.1 (8)	C35—C36—Ru2—O2	143.8 (4)
C55—C50—C51—Ru3	−55.6 (7)	C37—C36—Ru2—O2	−82.6 (4)
C50—C51—C52—C53	0.4 (13)	C35—C36—Ru2—C33	−66.2 (4)
Ru3—C51—C52—C53	50.3 (7)	C37—C36—Ru2—C33	67.4 (4)
C50—C51—C52—Ru3	−49.8 (7)	C35—C36—Ru2—C34	−29.2 (4)
C51—C52—C53—C54	3.4 (12)	C37—C36—Ru2—C34	104.4 (5)
Ru3—C52—C53—C54	56.7 (6)	C35—C36—Ru2—C37	−133.6 (6)
C51—C52—C53—Ru3	−53.3 (8)	C35—C36—Ru2—C32	−103.9 (5)
C52—C53—C54—C55	−3.3 (11)	C37—C36—Ru2—C32	29.7 (4)
Ru3—C53—C54—C55	56.3 (6)	C37—C36—Ru2—C35	133.6 (6)
C52—C53—C54—Ru3	−59.6 (7)	C47—C38—Ru3—C54	119.8 (6)
C51—C50—C55—C54	4.5 (12)	C39—C38—Ru3—C54	−64.0 (6)
Ru3—C50—C55—C54	−53.8 (6)	C47—C38—Ru3—N3	−5.9 (4)
C51—C50—C55—Ru3	58.3 (7)	C39—C38—Ru3—N3	170.3 (5)
C53—C54—C55—C50	−0.5 (11)	C47—C38—Ru3—O3	−98.0 (5)
Ru3—C54—C55—C50	55.7 (7)	C39—C38—Ru3—O3	78.2 (5)
C53—C54—C55—Ru3	−56.2 (6)	C47—C38—Ru3—C53	87.3 (5)
C11—C12—N1—Ru1	−15.9 (7)	C39—C38—Ru3—C53	−96.6 (6)
C13—C12—N1—Ru1	105.3 (5)	C47—C38—Ru3—C55	158.5 (6)
C29—C30—N2—Ru2	−30.4 (6)	C39—C38—Ru3—C55	−25.3 (6)
C31—C30—N2—Ru2	88.6 (5)	C47—C38—Ru3—C50	−177.1 (5)
C49—C48—N3—Ru3	97.5 (6)	C39—C38—Ru3—C50	−0.9 (7)
C47—C48—N3—Ru3	−25.7 (6)	C47—C38—Ru3—C52	76.3 (7)
O3—C1—O1—Ru1	3.7 (8)	C39—C38—Ru3—C52	−107.6 (8)
O2—C1—O1—Ru1	−174.1 (4)	C47—C38—Ru3—C51	170.9 (9)
O3—C1—O2—Ru2	178.5 (4)	C39—C38—Ru3—C51	−13.0 (14)
O1—C1—O2—Ru2	−3.7 (7)	C53—C54—Ru3—C38	−127.7 (6)
O1—C1—O3—Ru3	−177.6 (4)	C55—C54—Ru3—C38	102.2 (5)
O2—C1—O3—Ru3	0.2 (8)	C53—C54—Ru3—N3	−50.5 (6)
C11—C2—Ru1—O1	−84.1 (5)	C55—C54—Ru3—N3	179.3 (4)
C3—C2—Ru1—O1	86.0 (6)	C53—C54—Ru3—O3	152.8 (5)
C11—C2—Ru1—N1	3.0 (5)	C55—C54—Ru3—O3	22.6 (7)
C3—C2—Ru1—N1	173.1 (6)	C55—C54—Ru3—C53	−130.1 (7)
C11—C2—Ru1—C16	146.3 (5)	C53—C54—Ru3—C55	130.1 (7)
C3—C2—Ru1—C16	−43.6 (6)	C53—C54—Ru3—C50	100.0 (6)
C11—C2—Ru1—C14	85.2 (6)	C55—C54—Ru3—C50	−30.1 (5)

C3—C2—Ru1—C14	−104.7 (6)	C53—C54—Ru3—C52	30.4 (5)
C11—C2—Ru1—C15	109.7 (5)	C55—C54—Ru3—C52	−99.8 (6)
C3—C2—Ru1—C15	−80.2 (6)	C53—C54—Ru3—C51	64.5 (6)
C11—C2—Ru1—C17	−179.9 (5)	C55—C54—Ru3—C51	−65.6 (5)
C3—C2—Ru1—C17	−9.8 (7)	C48—N3—Ru3—C38	18.2 (4)
C11—C2—Ru1—C18	−161.0 (5)	C48—N3—Ru3—C54	−66.2 (5)
C3—C2—Ru1—C18	9.1 (9)	C48—N3—Ru3—O3	99.7 (4)
C11—C2—Ru1—C19	103.8 (18)	C48—N3—Ru3—C53	−95.1 (5)
C3—C2—Ru1—C19	−86.1 (19)	C48—N3—Ru3—C55	−64.6 (12)
C1—O1—Ru1—C2	125.6 (5)	C48—N3—Ru3—C50	−176.0 (5)
C1—O1—Ru1—N1	46.1 (5)	C48—N3—Ru3—C52	−132.1 (5)
C1—O1—Ru1—C16	−149.2 (5)	C48—N3—Ru3—C51	−160.9 (5)
C1—O1—Ru1—C14	−40.6 (7)	C1—O3—Ru3—C38	103.6 (5)
C1—O1—Ru1—C15	−133.5 (11)	C1—O3—Ru3—C54	−173.3 (5)
C1—O1—Ru1—C17	−125.9 (5)	C1—O3—Ru3—N3	25.5 (5)
C1—O1—Ru1—C18	−88.9 (5)	C1—O3—Ru3—C53	−93.2 (12)
C1—O1—Ru1—C19	−55.9 (6)	C1—O3—Ru3—C55	−158.7 (5)
C12—N1—Ru1—C2	7.8 (5)	C1—O3—Ru3—C50	−125.6 (6)
C12—N1—Ru1—O1	88.5 (5)	C1—O3—Ru3—C52	−72.8 (6)
C12—N1—Ru1—C16	−71.9 (7)	C1—O3—Ru3—C51	−92.0 (6)
C12—N1—Ru1—C14	−126.0 (5)	C52—C53—Ru3—C38	−170.8 (5)
C12—N1—Ru1—C15	−91.6 (5)	C54—C53—Ru3—C38	60.1 (6)
C12—N1—Ru1—C18	174.7 (5)	C52—C53—Ru3—C54	129.0 (8)
C12—N1—Ru1—C19	−161.5 (5)	C52—C53—Ru3—N3	−90.4 (6)
C17—C16—Ru1—C2	119.6 (5)	C54—C53—Ru3—N3	140.6 (6)
C15—C16—Ru1—C2	−106.9 (5)	C52—C53—Ru3—O3	27.4 (14)
C17—C16—Ru1—O1	40.3 (6)	C54—C53—Ru3—O3	−101.7 (12)
C15—C16—Ru1—O1	173.9 (4)	C52—C53—Ru3—C55	97.9 (6)
C17—C16—Ru1—N1	−165.4 (5)	C54—C53—Ru3—C55	−31.1 (6)
C15—C16—Ru1—N1	−31.8 (7)	C52—C53—Ru3—C50	60.5 (6)
C17—C16—Ru1—C14	−104.1 (6)	C54—C53—Ru3—C50	−68.6 (6)
C15—C16—Ru1—C14	29.5 (5)	C54—C53—Ru3—C52	−129.0 (8)
C17—C16—Ru1—C15	−133.6 (8)	C52—C53—Ru3—C51	26.1 (5)
C15—C16—Ru1—C17	133.6 (8)	C54—C53—Ru3—C51	−103.0 (6)
C17—C16—Ru1—C18	−30.2 (5)	C50—C55—Ru3—C38	148.3 (5)
C15—C16—Ru1—C18	103.4 (6)	C54—C55—Ru3—C38	−81.9 (5)
C17—C16—Ru1—C19	−67.7 (6)	C50—C55—Ru3—C54	−129.7 (8)
C15—C16—Ru1—C19	65.9 (6)	C50—C55—Ru3—N3	−131.7 (11)
C15—C14—Ru1—C2	41.7 (7)	C54—C55—Ru3—N3	−2.0 (14)
C19—C14—Ru1—C2	174.4 (5)	C50—C55—Ru3—O3	64.5 (6)
C15—C14—Ru1—O1	−157.1 (4)	C54—C55—Ru3—O3	−165.8 (4)
C19—C14—Ru1—O1	−24.4 (8)	C50—C55—Ru3—C53	−99.2 (6)
C15—C14—Ru1—N1	118.3 (5)	C54—C55—Ru3—C53	30.5 (5)
C19—C14—Ru1—N1	−109.0 (5)	C54—C55—Ru3—C50	129.7 (8)
C15—C14—Ru1—C16	−29.5 (5)	C50—C55—Ru3—C52	−62.0 (6)
C19—C14—Ru1—C16	103.2 (6)	C54—C55—Ru3—C52	67.7 (5)
C19—C14—Ru1—C15	132.7 (8)	C50—C55—Ru3—C51	−28.1 (5)
C15—C14—Ru1—C17	−65.9 (6)	C54—C55—Ru3—C51	101.6 (5)

C19—C14—Ru1—C17	66.7 (6)	C51—C50—Ru3—C38	−174.5 (4)
C15—C14—Ru1—C18	−103.0 (6)	C55—C50—Ru3—C38	−42.3 (7)
C19—C14—Ru1—C18	29.7 (5)	C51—C50—Ru3—C54	−100.6 (6)
C15—C14—Ru1—C19	−132.7 (8)	C55—C50—Ru3—C54	31.6 (6)
C16—C15—Ru1—C2	78.0 (5)	C51—C50—Ru3—N3	23.6 (9)
C14—C15—Ru1—C2	−150.3 (5)	C55—C50—Ru3—N3	155.8 (6)
C16—C15—Ru1—O1	−20.2 (14)	C51—C50—Ru3—O3	108.8 (5)
C14—C15—Ru1—O1	111.5 (12)	C55—C50—Ru3—O3	−119.0 (6)
C16—C15—Ru1—N1	160.3 (5)	C51—C50—Ru3—C53	−62.2 (6)
C14—C15—Ru1—N1	−68.1 (5)	C55—C50—Ru3—C53	70.1 (6)
C14—C15—Ru1—C16	131.7 (8)	C51—C50—Ru3—C55	−132.2 (8)
C16—C15—Ru1—C14	−131.7 (8)	C51—C50—Ru3—C52	−26.7 (5)
C16—C15—Ru1—C17	−28.2 (5)	C55—C50—Ru3—C52	105.5 (6)
C14—C15—Ru1—C17	103.5 (6)	C55—C50—Ru3—C51	132.2 (8)
C16—C15—Ru1—C18	−65.7 (5)	C51—C52—Ru3—C38	152.0 (6)
C14—C15—Ru1—C18	66.0 (6)	C53—C52—Ru3—C38	16.9 (10)
C16—C15—Ru1—C19	−103.1 (6)	C51—C52—Ru3—C54	103.5 (7)
C14—C15—Ru1—C19	28.5 (5)	C53—C52—Ru3—C54	−31.6 (6)
C16—C17—Ru1—C2	−67.2 (6)	C51—C52—Ru3—N3	−130.6 (5)
C18—C17—Ru1—C2	162.1 (5)	C53—C52—Ru3—N3	94.3 (6)
C16—C17—Ru1—O1	−149.6 (5)	C51—C52—Ru3—O3	−35.2 (6)
C18—C17—Ru1—O1	79.6 (6)	C53—C52—Ru3—O3	−170.3 (5)
C18—C17—Ru1—C16	−130.7 (8)	C51—C52—Ru3—C53	135.1 (8)
C16—C17—Ru1—C14	65.4 (6)	C51—C52—Ru3—C55	64.0 (6)
C18—C17—Ru1—C14	−65.4 (6)	C53—C52—Ru3—C55	−71.1 (7)
C16—C17—Ru1—C15	28.4 (5)	C51—C52—Ru3—C50	27.4 (5)
C18—C17—Ru1—C15	−102.3 (6)	C53—C52—Ru3—C50	−107.7 (7)
C16—C17—Ru1—C18	130.7 (8)	C53—C52—Ru3—C51	−135.1 (8)
C16—C17—Ru1—C19	101.7 (6)	C52—C51—Ru3—C38	−118.4 (11)
C18—C17—Ru1—C19	−29.1 (6)	C50—C51—Ru3—C38	16.1 (14)
C17—C18—Ru1—C2	−29.9 (8)	C52—C51—Ru3—C54	−65.9 (6)
C19—C18—Ru1—C2	−162.6 (5)	C50—C51—Ru3—C54	68.7 (6)
C17—C18—Ru1—O1	−103.5 (6)	C52—C51—Ru3—N3	58.0 (6)
C19—C18—Ru1—O1	123.8 (5)	C50—C51—Ru3—N3	−167.4 (5)
C17—C18—Ru1—N1	172.6 (5)	C52—C51—Ru3—O3	152.6 (5)
C19—C18—Ru1—N1	39.9 (7)	C50—C51—Ru3—O3	−72.8 (5)
C17—C18—Ru1—C16	29.8 (5)	C52—C51—Ru3—C53	−27.7 (5)
C19—C18—Ru1—C16	−102.9 (6)	C50—C51—Ru3—C53	106.8 (6)
C17—C18—Ru1—C14	103.8 (6)	C52—C51—Ru3—C55	−105.1 (6)
C19—C18—Ru1—C14	−28.9 (5)	C50—C51—Ru3—C55	29.5 (6)
C17—C18—Ru1—C15	66.8 (6)	C52—C51—Ru3—C50	−134.5 (8)
C19—C18—Ru1—C15	−65.9 (5)	C50—C51—Ru3—C52	134.5 (8)
C19—C18—Ru1—C17	−132.7 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F6^{i}	0.92	2.37	3.245 (7)	159

N1—H1*B*···O3	0.92	2.09	2.860 (7)	141
N2—H2*B*···O1	0.92	2.38	2.967 (7)	122
N3—H3*A*···F4^{ii}	0.92	2.36	3.202 (8)	153
N3—H3*B*···O2	0.92	1.92	2.739 (7)	148

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