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Bis[2,6-bis(1*H*-benzimidazol-2-yl)pyridine]ruthenium(II) bis(hexafluoridophosphate) diethyl ether trisolvate

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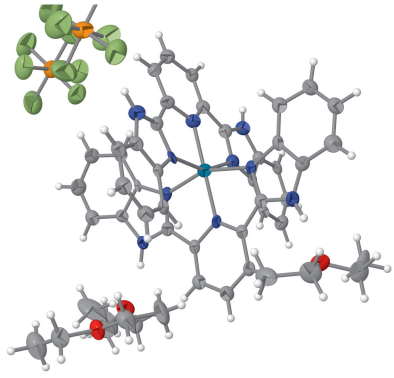
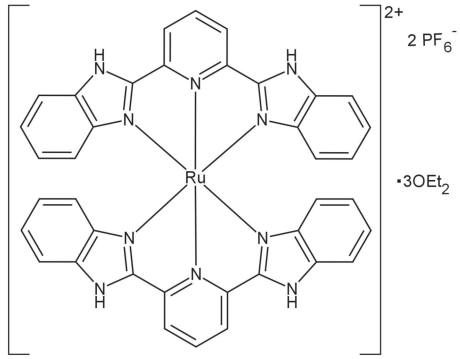
The title compound, $[Ru(C_{19}H_{13}N_5)_2](PF_6)_2\cdot 3C_4H_{10}O$, was obtained from the reaction of $Ru(bimpy)Cl_3$ [bimpy is 2,6-bis(1*H*-benzimidazol-2-yl)pyridine] and bimpy in refluxing ethanol followed by recrystallization from diethyl ether/acetonitrile. At 125 K the complex has orthorhombic ($Pca2_1$) symmetry. It is remarkable that the structure is almost centrosymmetric. However, refinement in space group *Pbcn* leads to disorder and definitely worse results. It is of interest with respect to potential catalytic reduction of CO_2. The structure displays N—H···O, N—H···F hydrogen bonding and significant π–π stacking and C—H···π stacking interactions.

3D view



Chemical scheme



Structure description

Ruthenium(II) complexes that contain polypyridine ligands enjoy enormous popularity in the research community because of their interesting photochemical, electrochemical, and catalytic properties (Juris *et al.*, 1988). Similar to what is found in 2,2′:6′,2″ terpyridine, the triimine structure, 2,6-bis(1*H*-benzimidazol-2-yl)pyridine (bimpy), offers a tridentate pocket for its coordination complexes; however, the imidazole units present a more convenient opportunity for tuning the electronics of donor–acceptor interactions (Groff *et al.*, 2023). Our interest in bimpy complexes of ruthenium stems from reports of their activity in mediation of CO_2 by electrochemical reduction (Chen *et al.*, 2011). This is the first crystal structure of a bis-bimpy complex of Ru^{II} that we are aware of.

The solvated title salt consists of the complex cation, ruthenium(II) bis(bimpy), two hexafluoridophosphate anions and three diethyl ether molecules of solvation (Fig. 1). The two tris-chelating bimpy ligands both coordinate through three of their nitrogen atoms to the central Ru^{II} atom, perpendicular to each other in a meridional fashion, forming a

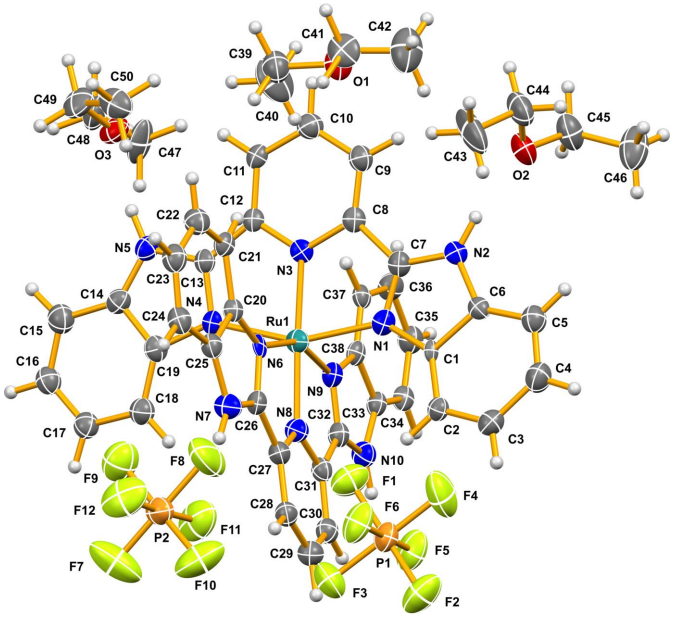


Figure 1
The structures of the molecular entities of the title compound with displacement ellipsoids at the 50% probability level.

slightly distorted octahedral environment. As a result of the $Pca2_1$ space group, all of the Ru—N bonds are unique. The two Ru^{II}—N(pyridinyl) bond lengths are: Ru1—N8 = 1.983 (9) Å and Ru1—N3 = 2.011 (8) Å and the four Ru(II)—N(benzimidazolyl) bonds, Ru1—N1, Ru1—N4, Ru1—N6 and Ru1—N9 are slightly longer and range from 2.046 (13) to 2.104 (12) Å. These same bond lengths in $[Ru(bimpy)(trpy)](ClO_4)_2$ (where trpy = 2,2′:6′,2"-terpyridine) are 2.017 (7) Å and 2.067 (7)–2.072 (7) Å, respectively

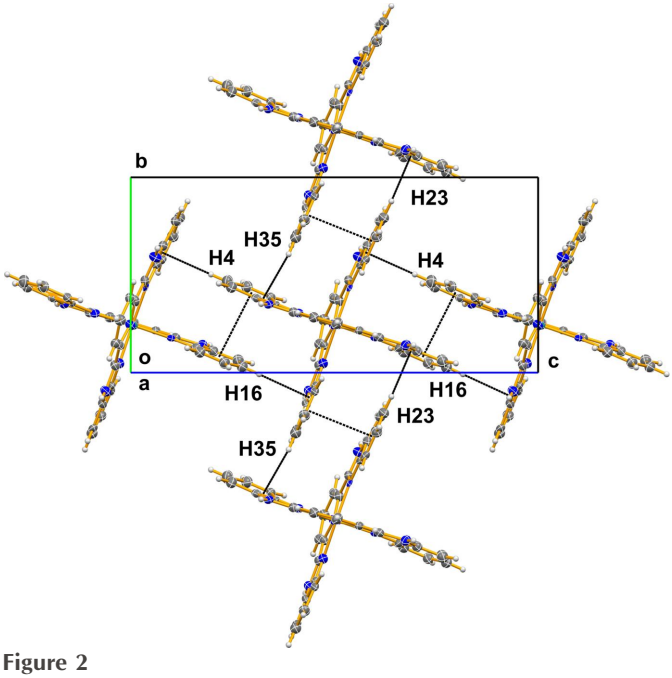


Figure 2
Packing diagram viewed along [100] showing both the C—H···π and π–π interactions (dashed lines).

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O2	0.90 (3)	1.85 (5)	2.730 (18)	166 (17)
N5—H5N···O3	0.91 (3)	1.81 (5)	2.704 (19)	170 (18)
N7—H7N···F8	0.90 (3)	2.58 (7)	3.30 (2)	137 (8)
N7—H7N···F11	0.90 (3)	2.05 (4)	2.93 (2)	167 (10)
N10—H10N···F6^{i}	0.89 (3)	2.16 (3)	3.028 (19)	166 (6)

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

(Singh *et al.*, 2008). While the complex does show hydrogen bonding between the imidazolyl N—H groups and the two hexafluoridophosphate anions and two of the three diethyl ether solvate molecules (Table 1), more interesting are the π–π stacking and C—H···π interactions (Fig. 2). The shortest π–π interactions are between the six-membered (benzene) rings of adjacent benzimidazolyl ligands and range from 3.639 (9) to 3.675 (8) Å. The C—H···π interactions involve a C—H group on these same benzene ring portions of the benzimidazolyl and adjacent benzimidazolyl benzene rings and have carbon to π-ring distances ranging from 3.487 (16) to 3.792 (18) Å.

Synthesis and crystallization

$[Ru(bimpy)_2](PF_6)_2$ was synthesized through reaction of $Ru(bimpy)Cl_3$ (Yu *et al.*, 1999) with bimpy (Xu *et al.*, 2007). Bimpy (0.0646 g, 0.21 mmol) and $Ru(bimpy)Cl_3$ (0.1064 g, 0.21 mmol) were added to a warm solution of aqueous ethanol (75%$_{vol}$). Triethylamine (0.25 ml) was added to the mixture. The solution was refluxed under argon for 24 h, then cooled to room temperature. The insoluble materials were removed by filtration and the complex was precipitated by the addition of a saturated aqueous solution of NH_4PF_6 while cooling at 4°C overnight. The resulting, brown precipitate was filtered and washed with water, air-dried, and then washed with diethyl ether (3 × 10 ml). Crystals of $[Ru(bimpy)_2](PF_6)_2$ were grown by slow diffusion of diethyl ether into an acetonitrile solution of the product, yielding dark-red crystals (0.1555 g, 75%). ^{1}H NMR (400 MHz, DMSO-d_6) (p.p.m.): 15.01 (s, 4H), 8.89 (d, J = 7.9 Hz, 4H), 8.77 (t, J = 7.9 Hz, 2H), 7.59 (d, J = 8.1 Hz, 4H), 7.25 (dd, J = 7.6 Hz, 4H), 7.02 (dd, J =7.6 Hz, 4H), 6.03 (d, J = 8.125 Hz, 4H). ^{13}C NMR (400 MHz, DMSO-d_6) (p.p.m.): 151.51, 149.78, 140.83, 136.70, 133.34, 125.54, 124.69, 122.16, 114.50, 114.28. IR (KBr) (cm^{-1}): 3364 (*br*), 1613 (*w*), 1597 (*w*), 1487 (*w*), 1458 (*w*), 1384 (*w*), 1322, 1297, 1233 (*w*), 1149 (*w*), 1021 (*w*), 851 (s), 760 (*w*), 743 (*s*). ESI–MS: m/z calculated for $C_{38}H_{26}N_{10}Ru$ (M^{2+}): 362.0693, found: 362.0676.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The data were first integrated to a resolution of 0.75 Å but during the final refinement, the data were cut at a resolution of 0.80 Å (θ_{max} = 26.37°) using a *SHEL* instruction to remove some of the noise. The unit cell was determined to be orthorhombic and it was found that the

structure could be refined in either the centrosymmetric space group *Pbcn* or in the non-centrosymmetric space group $Pca2_1$. Ultimately, the non-centrosymmetric space group was chosen, giving an asymmetric unit that contained one complete cation and two complete PF_6 anions. The crystal was also found to be solvated, containing three complete molecules of diethyl ether in the asymmetric unit. The $Pca2_1$ refinement had many atoms that had a tendency to become non-positive definite during the refinement, presumably because it was so close to being centrosymmetric. As a result, the displacement parameters of most atoms were restrained to be more isotropic during the refinement using global ISOR restraints. In addition, a rigid bond restraint was placed over all of the heavy atoms in the structure. The structure was treated as an inversion twin with the BASF parameter refining to 0.45 (12). The error is too large to say if this is different from the 0.50 expected for a centrosymmetric structure but it is possible to say it is not 0 or 1 (expected for a non-twinned non-centrosymmetric structure).

Initial *E* statistics suggested that the correct space group was non-centrosymmetric and the best solution in *SHELXT* was also in a non-centrosymmetric space group. The structure was thus first refined in the non-centrosymmetric space group $Pca2_1$. In this space group the final *R*-factor was high [*R*(reflections) = 0.0920 (9404) and *wR*2(reflections) = 0.1987 (11121)] and there was a level B *checkCIF* alert that the precision of the C—C bonds was low. A level G *checkCIF* alert suggested that there was an 89% fit to a centrosymmetric structure and that the alternative space group *Pbcn* should be used. Refinement in this space group was then carried out, but with much worse results overall. In the centrosymmetric space group, the central ring of the cation and the solvent molecules were all disordered (12% disorder in total). The statistics of the final refinement carried out under similar conditions to the non-centrosymmetric case were also much higher [*R*(reflections) = 0.1494 (5022) and *wR*2(reflections) = 0.3162 (5578)]. For these reasons, refinement in the non-centrosymmetric space group was chosen and the $Pca2_1$ results are presented here.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ru(C_{19}H_{13}N_5)_2](PF_6)_2{\cdot}3C_4H_{10}O$
M_r	1236.05
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	125
a, *b*, *c* (Å)	26.718 (4), 9.8834 (13), 20.648 (3)
V (Å^3)	5452.4 (12)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.44
Crystal size (mm)	0.26 × 0.18 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.027, 0.049
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	54516, 11121, 9404
R_{int}	0.058
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.092, 0.199, 1.18
No. of reflections	11121
No. of parameters	716
No. of restraints	1049
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.08, −1.44
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.45 (12)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

Funding information

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full crystallographic data

IUCrData (2024). **9**, x240269 [https://doi.org/10.1107/S2414314624002694]

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Bis[2,6-bis(1*H*-benzimidazol-2-yl)pyridine]ruthenium(II) bis(hexafluoridophosphate) diethyl ether trisolvate

Crystal data

$[Ru(C_{19}H_{13}N_5)_2](PF_6)_2\cdot 3C_4H_{10}O$
M_r = 1236.05
Orthorhombic, $Pca2_1$
a = 26.718 (4) Å
b = 9.8834 (13) Å
c = 20.648 (3) Å
V = 5452.4 (12) Å^3
Z = 4
$F(000)$ = 2528
D_x = 1.506 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9996 reflections
θ = 2.2–28.3°
μ = 0.44 mm^{-1}
T = 125 K
Rectangular prism, dark brown
0.26 × 0.18 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.027, T_{max} = 0.049
54516 measured reflections
11121 independent reflections
9404 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 26.4°, θ_{min} = 2.1°
h = −33→33
k = −12→12
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.092
$wR(F^2)$ = 0.199
S = 1.18
11121 reflections
716 parameters
1049 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 59.8553P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.44 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.45 (12)

Special details

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

Refinement. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.24603 (3)	0.24442 (12)	0.50446 (12)	0.0272 (2)
P1	0.4281 (2)	0.6827 (5)	0.3798 (2)	0.0392 (11)
P2	0.4255 (2)	0.8396 (6)	0.6165 (2)	0.0438 (12)
F1	0.3806 (5)	0.6486 (12)	0.4238 (6)	0.060 (3)
F2	0.4753 (6)	0.7193 (15)	0.3363 (7)	0.075 (4)
F3	0.4646 (5)	0.6473 (13)	0.4380 (6)	0.064 (3)
F4	0.3917 (6)	0.7185 (16)	0.3226 (6)	0.081 (4)
F5	0.4295 (5)	0.5311 (12)	0.3571 (6)	0.063 (3)
F6	0.4258 (5)	0.8365 (11)	0.4050 (5)	0.060 (3)
F7	0.4672 (6)	0.7920 (16)	0.6616 (9)	0.099 (5)
F8	0.3811 (6)	0.8839 (19)	0.5686 (7)	0.098 (5)
F9	0.3833 (6)	0.7858 (15)	0.6640 (6)	0.074 (4)
F10	0.4666 (6)	0.8928 (15)	0.5686 (8)	0.088 (4)
F11	0.4239 (5)	0.6940 (14)	0.5810 (7)	0.080 (4)
F12	0.4239 (6)	0.9832 (14)	0.6496 (8)	0.083 (4)
O1	0.0440 (5)	0.7937 (12)	0.4605 (6)	0.043 (3)
O2	0.0846 (5)	0.3936 (13)	0.2722 (6)	0.048 (3)
O3	0.0748 (5)	0.1501 (12)	0.7178 (6)	0.042 (3)
N1	0.2297 (5)	0.3044 (12)	0.4120 (6)	0.028 (2)
N2	0.1715 (5)	0.3491 (12)	0.3385 (6)	0.026 (2)
H2N	0.141 (3)	0.352 (18)	0.320 (8)	0.039*
N3	0.1708 (3)	0.2377 (10)	0.5067 (9)	0.0227 (17)
N4	0.2307 (5)	0.1768 (11)	0.5990 (6)	0.021 (2)
N5	0.1704 (6)	0.1409 (14)	0.6749 (6)	0.031 (3)
H5N	0.140 (3)	0.140 (19)	0.694 (8)	0.046*
N6	0.2623 (5)	0.4355 (11)	0.5373 (5)	0.020 (2)
N7	0.3222 (5)	0.5914 (14)	0.5605 (7)	0.036 (3)
H7N	0.3513 (13)	0.636 (9)	0.566 (8)	0.053*
N8	0.3201 (3)	0.2446 (14)	0.4988 (9)	0.030 (2)
N9	0.2618 (5)	0.0479 (13)	0.4726 (6)	0.029 (2)
N10	0.3184 (5)	−0.0946 (14)	0.4384 (7)	0.032 (3)
H10N	0.3482 (12)	−0.129 (7)	0.429 (8)	0.049*
C1	0.2541 (5)	0.3511 (12)	0.3577 (6)	0.016 (2)
C2	0.3034 (6)	0.3852 (15)	0.3447 (7)	0.026 (3)
H2	0.328622	0.370813	0.376313	0.032*
C3	0.3153 (7)	0.4402 (17)	0.2855 (8)	0.037 (3)
H3	0.349201	0.461762	0.275920	0.044*
C4	0.2769 (8)	0.465 (2)	0.2374 (9)	0.044 (4)
H4	0.286593	0.502895	0.196940	0.053*
C5	0.2275 (7)	0.4384 (17)	0.2473 (9)	0.037 (3)
H5	0.202140	0.455960	0.216151	0.044*
C6	0.2178 (6)	0.3816 (14)	0.3086 (7)	0.025 (3)
C7	0.1808 (7)	0.3087 (16)	0.3992 (7)	0.029 (3)
C8	0.1445 (6)	0.2777 (16)	0.4518 (7)	0.026 (3)
C9	0.0937 (7)	0.2833 (18)	0.4488 (8)	0.032 (3)

H9	0.076700	0.306661	0.410022	0.038*
C10	0.0677 (4)	0.2528 (18)	0.5061 (12)	0.036 (2)
H10	0.032208	0.257357	0.506813	0.043*
C11	0.0934 (6)	0.2163 (16)	0.5614 (7)	0.025 (3)
H11	0.075601	0.192158	0.599537	0.030*
C12	0.1461 (6)	0.2152 (16)	0.5609 (7)	0.023 (2)
C13	0.1806 (6)	0.1806 (14)	0.6111 (7)	0.025 (3)
C14	0.2141 (7)	0.1101 (16)	0.7026 (8)	0.031 (3)
C15	0.2286 (8)	0.0600 (18)	0.7645 (9)	0.043 (4)
H15	0.204639	0.047661	0.797942	0.051*
C16	0.2787 (7)	0.0296 (18)	0.7745 (8)	0.037 (3)
H16	0.287942	−0.008088	0.815065	0.045*
C17	0.3151 (7)	0.0501 (17)	0.7303 (8)	0.036 (3)
H17	0.348683	0.026841	0.740472	0.043*
C18	0.3039 (7)	0.1051 (17)	0.6699 (8)	0.034 (3)
H18	0.328848	0.125378	0.638626	0.041*
C19	0.2526 (6)	0.1284 (15)	0.6588 (7)	0.029 (3)
C20	0.2400 (6)	0.5502 (14)	0.5638 (7)	0.022 (3)
C21	0.1872 (6)	0.5763 (14)	0.5768 (6)	0.026 (3)
H21	0.161950	0.511548	0.567312	0.031*
C22	0.1762 (6)	0.6978 (16)	0.6032 (8)	0.036 (3)
H22	0.142021	0.719526	0.610477	0.043*
C23	0.2129 (6)	0.7943 (16)	0.6207 (7)	0.036 (3)
H23	0.202184	0.876976	0.639669	0.043*
C24	0.2631 (7)	0.7742 (18)	0.6115 (8)	0.033 (3)
H24	0.287559	0.838158	0.624789	0.040*
C25	0.2760 (6)	0.6488 (16)	0.5801 (8)	0.029 (3)
C26	0.3113 (6)	0.4726 (14)	0.5348 (7)	0.026 (3)
C27	0.3465 (5)	0.3682 (14)	0.5110 (8)	0.030 (3)
C28	0.3973 (5)	0.3810 (14)	0.4988 (7)	0.030 (3)
H28	0.414240	0.463642	0.506987	0.036*
C29	0.4226 (5)	0.2700 (15)	0.4742 (7)	0.035 (3)
H29	0.457377	0.275983	0.465126	0.042*
C30	0.3968 (5)	0.1492 (15)	0.4628 (6)	0.030 (3)
H30	0.414388	0.071711	0.447839	0.036*
C31	0.3459 (6)	0.1425 (14)	0.4733 (7)	0.028 (3)
C32	0.3105 (6)	0.0362 (15)	0.4618 (7)	0.029 (3)
C33	0.2726 (6)	−0.1596 (15)	0.4308 (7)	0.026 (3)
C34	0.2598 (6)	−0.2854 (16)	0.4076 (7)	0.027 (3)
H34	0.283975	−0.350201	0.394395	0.032*
C35	0.2095 (6)	−0.3095 (17)	0.4051 (8)	0.036 (3)
H35	0.198913	−0.393808	0.387753	0.043*
C36	0.1714 (6)	−0.2182 (16)	0.4265 (8)	0.035 (3)
H36	0.136846	−0.240112	0.423405	0.042*
C37	0.1876 (5)	−0.0952 (14)	0.4520 (6)	0.024 (3)
H37	0.164107	−0.031994	0.468619	0.029*
C38	0.2365 (6)	−0.0668 (14)	0.4530 (7)	0.024 (3)
C39	0.0503 (10)	0.607 (2)	0.5342 (11)	0.075 (7)

H39A	0.052672	0.582148	0.580088	0.113*
H39B	0.020112	0.565792	0.515506	0.113*
H39C	0.079855	0.572996	0.511162	0.113*
C40	0.0475 (8)	0.7574 (19)	0.5278 (8)	0.048 (4)
H40A	0.017872	0.791796	0.551371	0.057*
H40B	0.077751	0.799017	0.547017	0.057*
C41	0.0408 (7)	0.9406 (15)	0.4498 (9)	0.046 (4)
H41A	0.010402	0.977684	0.470652	0.055*
H41B	0.070461	0.986418	0.468538	0.055*
C42	0.0390 (9)	0.961 (2)	0.3828 (10)	0.073 (6)
H42A	0.036900	1.058186	0.373676	0.110*
H42B	0.069346	0.923976	0.362836	0.110*
H42C	0.009558	0.915281	0.364940	0.110*
C43	0.0841 (11)	0.614 (3)	0.3205 (11)	0.087 (9)
H43A	0.065395	0.699277	0.321833	0.131*
H43B	0.085209	0.574427	0.364004	0.131*
H43C	0.118219	0.631189	0.305314	0.131*
C44	0.0579 (8)	0.515 (2)	0.2740 (9)	0.057 (5)
H44A	0.023291	0.498075	0.288902	0.068*
H44B	0.056384	0.554979	0.230065	0.068*
C45	0.0627 (8)	0.298 (2)	0.2275 (8)	0.051 (4)
H45A	0.025870	0.299040	0.232993	0.062*
H45B	0.074628	0.206030	0.238549	0.062*
C46	0.0748 (9)	0.326 (2)	0.1574 (9)	0.069 (6)
H46A	0.058863	0.257949	0.129959	0.104*
H46B	0.062365	0.416238	0.145643	0.104*
H46C	0.111179	0.323123	0.151205	0.104*
C47	0.0695 (9)	−0.089 (2)	0.6989 (9)	0.060 (6)
H47A	0.056533	−0.174994	0.715149	0.090*
H47B	0.055627	−0.070924	0.655783	0.090*
H47C	0.106089	−0.093155	0.696159	0.090*
C48	0.0544 (8)	0.024 (2)	0.7447 (8)	0.052 (4)
H48A	0.017518	0.030157	0.747938	0.062*
H48B	0.068217	0.007822	0.788502	0.062*
C49	0.0599 (7)	0.2660 (18)	0.7536 (10)	0.053 (4)
H49A	0.081330	0.276570	0.792397	0.063*
H49B	0.024761	0.256431	0.767869	0.063*
C50	0.0654 (7)	0.3909 (17)	0.7089 (9)	0.049 (4)
H50A	0.055352	0.472484	0.732478	0.074*
H50B	0.100400	0.399676	0.695133	0.074*
H50C	0.044044	0.379613	0.670697	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.0292 (4)	0.0228 (4)	0.0298 (4)	−0.0012 (5)	−0.0013 (8)	−0.0070 (5)
P1	0.047 (3)	0.039 (2)	0.031 (2)	0.001 (2)	0.004 (2)	−0.0052 (18)
P2	0.039 (3)	0.050 (3)	0.043 (2)	−0.001 (2)	−0.002 (2)	−0.013 (2)

F1	0.055 (6)	0.054 (6)	0.070 (7)	−0.001 (5)	0.019 (5)	0.005 (5)
F2	0.079 (8)	0.071 (8)	0.074 (8)	−0.012 (7)	0.038 (6)	−0.004 (6)
F3	0.066 (7)	0.072 (8)	0.054 (6)	0.000 (6)	−0.023 (5)	0.000 (5)
F4	0.102 (9)	0.089 (9)	0.053 (7)	−0.024 (8)	−0.027 (6)	0.022 (6)
F5	0.088 (9)	0.048 (6)	0.052 (6)	−0.007 (6)	0.014 (6)	−0.022 (5)
F6	0.090 (9)	0.041 (5)	0.048 (6)	0.000 (5)	0.020 (6)	−0.012 (5)
F7	0.082 (9)	0.066 (8)	0.150 (12)	−0.008 (7)	−0.063 (9)	0.011 (8)
F8	0.074 (8)	0.149 (12)	0.069 (8)	0.001 (8)	−0.026 (7)	0.035 (8)
F9	0.080 (8)	0.073 (8)	0.068 (7)	−0.013 (7)	0.013 (6)	0.003 (6)
F10	0.078 (8)	0.067 (8)	0.120 (10)	0.003 (7)	0.051 (8)	−0.001 (8)
F11	0.084 (9)	0.080 (7)	0.078 (8)	−0.019 (7)	0.012 (7)	−0.042 (7)
F12	0.088 (10)	0.050 (6)	0.112 (10)	−0.002 (6)	0.022 (8)	−0.030 (7)
O1	0.061 (7)	0.028 (5)	0.040 (6)	0.004 (5)	−0.003 (5)	0.003 (5)
O2	0.051 (8)	0.055 (7)	0.037 (6)	−0.003 (6)	−0.016 (5)	−0.004 (5)
O3	0.038 (6)	0.042 (6)	0.046 (7)	0.002 (5)	0.010 (5)	−0.014 (5)
N1	0.034 (4)	0.021 (4)	0.028 (4)	−0.006 (4)	0.003 (3)	0.000 (3)
N2	0.030 (4)	0.019 (4)	0.028 (4)	0.002 (4)	−0.002 (3)	0.002 (3)
N3	0.028 (3)	0.012 (3)	0.028 (3)	−0.004 (3)	−0.001 (4)	0.002 (3)
N4	0.029 (4)	0.013 (4)	0.021 (4)	−0.003 (3)	0.001 (3)	−0.002 (3)
N5	0.033 (4)	0.030 (5)	0.029 (4)	0.001 (4)	0.005 (3)	0.004 (4)
N6	0.030 (4)	0.020 (4)	0.010 (4)	0.005 (3)	−0.005 (3)	0.007 (3)
N7	0.034 (4)	0.030 (4)	0.042 (5)	0.000 (4)	−0.002 (4)	−0.008 (4)
N8	0.030 (3)	0.029 (3)	0.030 (4)	0.002 (3)	−0.001 (4)	−0.006 (3)
N9	0.034 (4)	0.028 (4)	0.024 (4)	0.000 (3)	0.001 (4)	−0.002 (4)
N10	0.035 (4)	0.031 (4)	0.032 (5)	0.002 (4)	−0.002 (4)	−0.005 (4)
C1	0.028 (4)	0.009 (4)	0.011 (4)	0.002 (3)	−0.001 (3)	0.002 (3)
C2	0.030 (4)	0.025 (5)	0.024 (4)	−0.001 (4)	0.001 (4)	−0.003 (4)
C3	0.037 (5)	0.038 (5)	0.035 (5)	0.001 (4)	0.006 (4)	0.000 (4)
C4	0.048 (5)	0.050 (6)	0.034 (5)	−0.001 (4)	0.005 (4)	0.002 (4)
C5	0.042 (5)	0.036 (5)	0.032 (5)	0.002 (4)	−0.001 (4)	0.002 (4)
C6	0.028 (4)	0.021 (5)	0.027 (4)	0.002 (4)	−0.003 (3)	−0.003 (4)
C7	0.034 (4)	0.026 (5)	0.027 (4)	−0.003 (4)	0.000 (4)	0.000 (4)
C8	0.034 (4)	0.016 (4)	0.028 (4)	−0.001 (4)	0.000 (4)	0.002 (4)
C9	0.036 (4)	0.029 (5)	0.030 (5)	0.000 (4)	−0.002 (4)	0.001 (4)
C10	0.035 (4)	0.035 (4)	0.036 (4)	0.003 (4)	0.000 (4)	0.005 (4)
C11	0.032 (4)	0.019 (5)	0.025 (4)	0.000 (4)	0.004 (4)	−0.001 (4)
C12	0.030 (4)	0.016 (4)	0.024 (4)	0.001 (4)	0.000 (3)	−0.001 (4)
C13	0.031 (4)	0.021 (5)	0.023 (4)	−0.001 (4)	−0.001 (3)	−0.004 (4)
C14	0.032 (4)	0.030 (5)	0.031 (4)	−0.002 (4)	0.003 (4)	−0.002 (4)
C15	0.046 (5)	0.045 (6)	0.038 (5)	0.001 (4)	−0.002 (4)	−0.003 (4)
C16	0.042 (5)	0.036 (5)	0.034 (5)	0.003 (4)	−0.004 (4)	0.001 (4)
C17	0.038 (5)	0.035 (5)	0.033 (5)	0.004 (4)	−0.001 (4)	0.000 (4)
C18	0.037 (5)	0.033 (5)	0.033 (5)	−0.001 (4)	0.000 (4)	−0.001 (4)
C19	0.036 (4)	0.024 (5)	0.028 (5)	−0.001 (4)	−0.001 (4)	0.007 (4)
C20	0.029 (4)	0.017 (4)	0.021 (5)	0.001 (3)	−0.001 (4)	0.004 (4)
C21	0.032 (4)	0.022 (4)	0.022 (5)	0.000 (4)	0.002 (4)	0.006 (4)
C22	0.038 (5)	0.035 (5)	0.036 (5)	0.004 (4)	−0.003 (4)	−0.001 (4)
C23	0.044 (5)	0.031 (5)	0.032 (5)	0.003 (4)	−0.002 (4)	−0.003 (4)

C24	0.041 (5)	0.027 (5)	0.031 (5)	0.002 (4)	−0.005 (4)	−0.001 (4)
C25	0.034 (5)	0.029 (4)	0.025 (5)	0.002 (4)	−0.003 (4)	0.000 (4)
C26	0.030 (4)	0.026 (4)	0.021 (4)	−0.001 (3)	0.001 (4)	−0.001 (4)
C27	0.029 (4)	0.035 (4)	0.025 (5)	0.000 (3)	−0.002 (4)	−0.001 (4)
C28	0.031 (4)	0.033 (4)	0.027 (5)	−0.002 (4)	−0.001 (4)	0.000 (4)
C29	0.033 (5)	0.036 (5)	0.036 (5)	0.001 (4)	0.000 (4)	0.000 (4)
C30	0.034 (4)	0.030 (4)	0.026 (5)	0.002 (4)	−0.001 (4)	0.003 (4)
C31	0.032 (4)	0.027 (4)	0.024 (5)	0.001 (3)	−0.004 (4)	−0.005 (4)
C32	0.034 (4)	0.029 (4)	0.024 (5)	0.000 (4)	−0.001 (4)	−0.004 (4)
C33	0.033 (4)	0.025 (4)	0.021 (5)	0.002 (3)	0.001 (4)	−0.003 (4)
C34	0.036 (5)	0.020 (4)	0.024 (5)	0.005 (4)	0.000 (4)	0.005 (4)
C35	0.041 (5)	0.033 (5)	0.034 (5)	−0.002 (4)	0.001 (4)	0.001 (4)
C36	0.038 (5)	0.033 (5)	0.035 (5)	−0.006 (4)	0.003 (4)	−0.001 (4)
C37	0.031 (4)	0.023 (4)	0.018 (4)	0.003 (4)	−0.003 (4)	0.003 (4)
C38	0.033 (4)	0.020 (4)	0.018 (4)	0.000 (3)	0.003 (4)	0.005 (4)
C39	0.101 (18)	0.049 (10)	0.075 (14)	−0.004 (11)	−0.028 (13)	0.031 (10)
C40	0.054 (10)	0.049 (9)	0.039 (8)	0.005 (8)	−0.004 (7)	−0.002 (7)
C41	0.061 (11)	0.019 (6)	0.059 (9)	0.003 (7)	−0.005 (8)	−0.012 (6)
C42	0.113 (19)	0.053 (12)	0.054 (9)	0.014 (12)	−0.002 (11)	0.001 (9)
C43	0.11 (2)	0.085 (15)	0.064 (15)	0.028 (14)	−0.053 (14)	−0.038 (13)
C44	0.061 (12)	0.066 (10)	0.043 (11)	0.010 (9)	−0.020 (9)	−0.017 (8)
C45	0.066 (12)	0.048 (9)	0.040 (8)	−0.011 (9)	−0.013 (8)	0.006 (7)
C46	0.112 (18)	0.052 (12)	0.043 (9)	0.024 (12)	0.002 (10)	0.002 (8)
C47	0.096 (17)	0.051 (9)	0.031 (9)	−0.032 (10)	0.022 (10)	0.003 (7)
C48	0.060 (12)	0.068 (9)	0.027 (9)	−0.003 (9)	0.009 (8)	0.001 (7)
C49	0.056 (10)	0.054 (8)	0.048 (9)	0.018 (8)	0.013 (9)	−0.012 (7)
C50	0.050 (10)	0.036 (8)	0.061 (11)	0.004 (7)	−0.012 (8)	−0.017 (7)

Geometric parameters (Å, º)

Ru1—N8	1.983 (9)	C16—C17	1.35 (2)
Ru1—N3	2.011 (8)	C16—H16	0.9500
Ru1—N1	2.046 (13)	C17—C18	1.39 (2)
Ru1—N6	2.053 (12)	C17—H17	0.9500
Ru1—N9	2.094 (13)	C18—C19	1.41 (2)
Ru1—N4	2.104 (12)	C18—H18	0.9500
P1—F5	1.570 (12)	C20—C25	1.41 (2)
P1—F4	1.571 (14)	C20—C21	1.46 (2)
P1—F3	1.586 (12)	C21—C22	1.35 (2)
P1—F2	1.591 (13)	C21—H21	0.9500
P1—F1	1.597 (12)	C22—C23	1.41 (2)
P1—F6	1.607 (12)	C22—H22	0.9500
P2—F7	1.525 (15)	C23—C24	1.37 (2)
P2—F10	1.569 (15)	C23—H23	0.9500
P2—F12	1.575 (14)	C24—C25	1.44 (2)
P2—F9	1.586 (14)	C24—H24	0.9500
P2—F8	1.607 (14)	C26—C27	1.48 (2)
P2—F11	1.615 (13)	C27—C28	1.386 (19)

O1—C40	1.44 (2)	C28—C29	1.385 (19)
O1—C41	1.472 (19)	C28—H28	0.9500
O2—C44	1.40 (2)	C29—C30	1.40 (2)
O2—C45	1.44 (2)	C29—H29	0.9500
O3—C49	1.419 (19)	C30—C31	1.38 (2)
O3—C48	1.47 (2)	C30—H30	0.9500
N1—C7	1.34 (2)	C31—C32	1.43 (2)
N1—C1	1.377 (17)	C33—C34	1.38 (2)
N2—C7	1.340 (19)	C33—C38	1.41 (2)
N2—C6	1.42 (2)	C34—C35	1.37 (2)
N2—H2N	0.90 (3)	C34—H34	0.9500
N3—C12	1.32 (2)	C35—C36	1.43 (2)
N3—C8	1.39 (2)	C35—H35	0.9500
N4—C13	1.36 (2)	C36—C37	1.39 (2)
N4—C19	1.449 (19)	C36—H36	0.9500
N5—C14	1.34 (2)	C37—C38	1.34 (2)
N5—C13	1.402 (19)	C37—H37	0.9500
N5—H5N	0.91 (3)	C39—C40	1.50 (3)
N6—C26	1.36 (2)	C39—H39A	0.9800
N6—C20	1.392 (18)	C39—H39B	0.9800
N7—C26	1.321 (19)	C39—H39C	0.9800
N7—C25	1.42 (2)	C40—H40A	0.9900
N7—H7N	0.90 (3)	C40—H40B	0.9900
N8—C31	1.330 (19)	C41—C42	1.40 (3)
N8—C27	1.432 (18)	C41—H41A	0.9900
N9—C32	1.32 (2)	C41—H41B	0.9900
N9—C38	1.380 (19)	C42—H42A	0.9800
N10—C33	1.39 (2)	C42—H42B	0.9800
N10—C32	1.396 (19)	C42—H42C	0.9800
N10—H10N	0.89 (3)	C43—C44	1.54 (3)
C1—C2	1.38 (2)	C43—H43A	0.9800
C1—C6	1.435 (19)	C43—H43B	0.9800
C2—C3	1.38 (2)	C43—H43C	0.9800
C2—H2	0.9500	C44—H44A	0.9900
C3—C4	1.45 (3)	C44—H44B	0.9900
C3—H3	0.9500	C45—C46	1.51 (2)
C4—C5	1.36 (3)	C45—H45A	0.9900
C4—H4	0.9500	C45—H45B	0.9900
C5—C6	1.41 (2)	C46—H46A	0.9800
C5—H5	0.9500	C46—H46B	0.9800
C7—C8	1.49 (2)	C46—H46C	0.9800
C8—C9	1.36 (2)	C47—C48	1.52 (3)
C9—C10	1.40 (3)	C47—H47A	0.9800
C9—H9	0.9500	C47—H47B	0.9800
C10—C11	1.38 (3)	C47—H47C	0.9800
C10—H10	0.9500	C48—H48A	0.9900
C11—C12	1.41 (2)	C48—H48B	0.9900
C11—H11	0.9500	C49—C50	1.55 (3)

C12—C13	1.43 (2)	C49—H49A	0.9900
C14—C19	1.38 (2)	C49—H49B	0.9900
C14—C15	1.42 (2)	C50—H50A	0.9800
C15—C16	1.39 (3)	C50—H50B	0.9800
C15—H15	0.9500	C50—H50C	0.9800

N8—Ru1—N3	177.3 (7)	C14—C19—C18	126.6 (15)
N8—Ru1—N1	99.1 (7)	C14—C19—N4	107.5 (14)
N3—Ru1—N1	79.5 (6)	C18—C19—N4	125.9 (15)
N8—Ru1—N6	78.9 (5)	N6—C20—C25	111.4 (13)
N3—Ru1—N6	103.5 (5)	N6—C20—C21	129.0 (13)
N1—Ru1—N6	95.0 (5)	C25—C20—C21	119.6 (13)
N8—Ru1—N9	77.3 (6)	C22—C21—C20	116.2 (14)
N3—Ru1—N9	100.3 (5)	C22—C21—H21	121.9
N1—Ru1—N9	91.0 (5)	C20—C21—H21	121.9
N6—Ru1—N9	156.1 (3)	C21—C22—C23	123.5 (16)
N8—Ru1—N4	104.5 (6)	C21—C22—H22	118.2
N3—Ru1—N4	76.9 (6)	C23—C22—H22	118.2
N1—Ru1—N4	156.4 (4)	C24—C23—C22	123.1 (16)
N6—Ru1—N4	91.5 (4)	C24—C23—H23	118.5
N9—Ru1—N4	92.1 (5)	C22—C23—H23	118.5
F5—P1—F4	90.2 (8)	C23—C24—C25	115.0 (16)
F5—P1—F3	90.1 (7)	C23—C24—H24	122.5
F4—P1—F3	179.6 (10)	C25—C24—H24	122.5
F5—P1—F2	91.7 (8)	C20—C25—N7	104.4 (13)
F4—P1—F2	90.8 (9)	C20—C25—C24	122.6 (15)
F3—P1—F2	89.5 (8)	N7—C25—C24	133.0 (15)
F5—P1—F1	89.2 (7)	N7—C26—N6	115.8 (14)
F4—P1—F1	89.1 (8)	N7—C26—C27	127.8 (14)
F3—P1—F1	90.6 (7)	N6—C26—C27	115.9 (12)
F2—P1—F1	179.1 (8)	C28—C27—N8	121.8 (12)
F5—P1—F6	178.3 (7)	C28—C27—C26	128.3 (13)
F4—P1—F6	90.4 (8)	N8—C27—C26	109.9 (12)
F3—P1—F6	89.3 (7)	C29—C28—C27	118.2 (13)
F2—P1—F6	89.9 (7)	C29—C28—H28	120.9
F1—P1—F6	89.1 (6)	C27—C28—H28	120.9
F7—P2—F10	88.7 (10)	C28—C29—C30	119.8 (13)
F7—P2—F12	91.9 (9)	C28—C29—H29	120.1
F10—P2—F12	89.5 (8)	C30—C29—H29	120.1
F7—P2—F9	92.3 (10)	C31—C30—C29	120.0 (14)
F10—P2—F9	179.0 (9)	C31—C30—H30	120.0
F12—P2—F9	90.8 (8)	C29—C30—H30	120.0
F7—P2—F8	177.9 (10)	N8—C31—C30	122.4 (13)
F10—P2—F8	92.1 (9)	N8—C31—C32	106.3 (13)
F12—P2—F8	90.1 (10)	C30—C31—C32	131.2 (14)
F9—P2—F8	86.9 (8)	N9—C32—N10	106.7 (14)
F7—P2—F11	91.2 (9)	N9—C32—C31	123.7 (14)
F10—P2—F11	91.7 (8)	N10—C32—C31	129.6 (15)

F12—P2—F11	176.6 (9)	C34—C33—N10	132.5 (14)
F9—P2—F11	87.9 (7)	C34—C33—C38	122.2 (15)
F8—P2—F11	86.7 (9)	N10—C33—C38	105.3 (13)
C40—O1—C41	113.2 (13)	C35—C34—C33	114.5 (15)
C44—O2—C45	111.9 (14)	C35—C34—H34	122.7
C49—O3—C48	112.5 (13)	C33—C34—H34	122.7
C7—N1—C1	106.9 (13)	C34—C35—C36	125.3 (16)
C7—N1—Ru1	113.7 (10)	C34—C35—H35	117.3
C1—N1—Ru1	139.2 (11)	C36—C35—H35	117.3
C7—N2—C6	108.2 (13)	C37—C36—C35	116.4 (15)
C7—N2—H2N	125 (10)	C37—C36—H36	121.8
C6—N2—H2N	127 (10)	C35—C36—H36	121.8
C12—N3—C8	119.1 (9)	C38—C37—C36	119.5 (14)
C12—N3—Ru1	121.7 (12)	C38—C37—H37	120.2
C8—N3—Ru1	118.5 (11)	C36—C37—H37	120.2
C13—N4—C19	104.5 (12)	C37—C38—N9	131.0 (14)
C13—N4—Ru1	110.7 (10)	C37—C38—C33	121.8 (14)
C19—N4—Ru1	144.8 (11)	N9—C38—C33	107.2 (13)
C14—N5—C13	107.2 (14)	C40—C39—H39A	109.5
C14—N5—H5N	127 (10)	C40—C39—H39B	109.5
C13—N5—H5N	126 (10)	H39A—C39—H39B	109.5
C26—N6—C20	101.9 (12)	C40—C39—H39C	109.5
C26—N6—Ru1	116.0 (9)	H39A—C39—H39C	109.5
C20—N6—Ru1	142.1 (11)	H39B—C39—H39C	109.5
C26—N7—C25	106.2 (13)	O1—C40—C39	109.7 (15)
C26—N7—H7N	132 (3)	O1—C40—H40A	109.7
C25—N7—H7N	122 (3)	C39—C40—H40A	109.7
C31—N8—C27	117.5 (10)	O1—C40—H40B	109.7
C31—N8—Ru1	122.6 (10)	C39—C40—H40B	109.7
C27—N8—Ru1	118.8 (9)	H40A—C40—H40B	108.2
C32—N9—C38	111.1 (13)	C42—C41—O1	107.0 (14)
C32—N9—Ru1	109.4 (10)	C42—C41—H41A	110.3
C38—N9—Ru1	139.0 (11)	O1—C41—H41A	110.3
C33—N10—C32	109.5 (13)	C42—C41—H41B	110.3
C33—N10—H10N	126 (2)	O1—C41—H41B	110.3
C32—N10—H10N	125 (3)	H41A—C41—H41B	108.6
N1—C1—C2	133.6 (13)	C41—C42—H42A	109.5
N1—C1—C6	109.0 (13)	C41—C42—H42B	109.5
C2—C1—C6	117.0 (12)	H42A—C42—H42B	109.5
C3—C2—C1	119.3 (15)	C41—C42—H42C	109.5
C3—C2—H2	120.3	H42A—C42—H42C	109.5
C1—C2—H2	120.3	H42B—C42—H42C	109.5
C2—C3—C4	120.7 (17)	C44—C43—H43A	109.5
C2—C3—H3	119.6	C44—C43—H43B	109.5
C4—C3—H3	119.6	H43A—C43—H43B	109.5
C5—C4—C3	123.4 (18)	C44—C43—H43C	109.5
C5—C4—H4	118.3	H43A—C43—H43C	109.5
C3—C4—H4	118.3	H43B—C43—H43C	109.5

C4—C5—C6	113.0 (17)	O2—C44—C43	109.4 (16)
C4—C5—H5	123.5	O2—C44—H44A	109.8
C6—C5—H5	123.5	C43—C44—H44A	109.8
C5—C6—N2	129.8 (15)	O2—C44—H44B	109.8
C5—C6—C1	126.5 (16)	C43—C44—H44B	109.8
N2—C6—C1	103.6 (12)	H44A—C44—H44B	108.2
N1—C7—N2	112.1 (14)	O2—C45—C46	113.8 (16)
N1—C7—C8	119.1 (14)	O2—C45—H45A	108.8
N2—C7—C8	128.7 (16)	C46—C45—H45A	108.8
C9—C8—N3	123.6 (14)	O2—C45—H45B	108.8
C9—C8—C7	127.4 (15)	C46—C45—H45B	108.8
N3—C8—C7	109.0 (14)	H45A—C45—H45B	107.7
C8—C9—C10	116.5 (15)	C45—C46—H46A	109.5
C8—C9—H9	121.7	C45—C46—H46B	109.5
C10—C9—H9	121.7	H46A—C46—H46B	109.5
C11—C10—C9	120.5 (10)	C45—C46—H46C	109.5
C11—C10—H10	119.8	H46A—C46—H46C	109.5
C9—C10—H10	119.8	H46B—C46—H46C	109.5
C10—C11—C12	119.5 (14)	C48—C47—H47A	109.5
C10—C11—H11	120.2	C48—C47—H47B	109.5
C12—C11—H11	120.2	H47A—C47—H47B	109.5
N3—C12—C11	120.4 (14)	C48—C47—H47C	109.5
N3—C12—C13	109.5 (14)	H47A—C47—H47C	109.5
C11—C12—C13	129.9 (15)	H47B—C47—H47C	109.5
N4—C13—N5	110.8 (14)	O3—C48—C47	106.8 (13)
N4—C13—C12	120.5 (14)	O3—C48—H48A	110.4
N5—C13—C12	128.7 (15)	C47—C48—H48A	110.4
N5—C14—C19	110.0 (15)	O3—C48—H48B	110.4
N5—C14—C15	134.5 (16)	C47—C48—H48B	110.4
C19—C14—C15	115.5 (17)	H48A—C48—H48B	108.6
C16—C15—C14	118.1 (18)	O3—C49—C50	107.9 (15)
C16—C15—H15	121.0	O3—C49—H49A	110.1
C14—C15—H15	121.0	C50—C49—H49A	110.1
C17—C16—C15	124.2 (18)	O3—C49—H49B	110.1
C17—C16—H16	117.9	C50—C49—H49B	110.1
C15—C16—H16	117.9	H49A—C49—H49B	108.4
C16—C17—C18	120.6 (18)	C49—C50—H50A	109.5
C16—C17—H17	119.7	C49—C50—H50B	109.5
C18—C17—H17	119.7	H50A—C50—H50B	109.5
C17—C18—C19	114.7 (16)	C49—C50—H50C	109.5
C17—C18—H18	122.6	H50A—C50—H50C	109.5
C19—C18—H18	122.6	H50B—C50—H50C	109.5

C7—N1—C1—C2	170.7 (15)	Ru1—N6—C20—C21	−3 (2)
Ru1—N1—C1—C2	−4 (3)	N6—C20—C21—C22	179.8 (14)
C7—N1—C1—C6	−1.8 (16)	C25—C20—C21—C22	1 (2)
Ru1—N1—C1—C6	−176.8 (11)	C20—C21—C22—C23	−3 (2)
N1—C1—C2—C3	−174.8 (15)	C21—C22—C23—C24	1 (2)

C6—C1—C2—C3	−3 (2)	C22—C23—C24—C25	2 (2)
C1—C2—C3—C4	1 (2)	N6—C20—C25—N7	1.8 (17)
C2—C3—C4—C5	0 (3)	C21—C20—C25—N7	−179.5 (13)
C3—C4—C5—C6	−1 (3)	N6—C20—C25—C24	−176.6 (13)
C4—C5—C6—N2	174.9 (16)	C21—C20—C25—C24	2 (2)
C4—C5—C6—C1	−1 (2)	C26—N7—C25—C20	1.0 (17)
C7—N2—C6—C5	−174.4 (16)	C26—N7—C25—C24	179.2 (17)
C7—N2—C6—C1	1.9 (15)	C23—C24—C25—C20	−4 (2)
N1—C1—C6—C5	176.4 (14)	C23—C24—C25—N7	178.2 (17)
C2—C1—C6—C5	3 (2)	C25—N7—C26—N6	−3.7 (19)
N1—C1—C6—N2	−0.1 (14)	C25—N7—C26—C27	−175.4 (15)
C2—C1—C6—N2	−174.0 (12)	C20—N6—C26—N7	4.6 (17)
C1—N1—C7—N2	3.2 (17)	Ru1—N6—C26—N7	−175.0 (10)
Ru1—N1—C7—N2	179.6 (10)	C20—N6—C26—C27	177.3 (12)
C1—N1—C7—C8	−173.6 (13)	Ru1—N6—C26—C27	−2.3 (16)
Ru1—N1—C7—C8	2.9 (18)	C31—N8—C27—C28	−2 (2)
C6—N2—C7—N1	−3.3 (18)	Ru1—N8—C27—C28	−170.4 (12)
C6—N2—C7—C8	173.1 (15)	C31—N8—C27—C26	175.9 (14)
C12—N3—C8—C9	−6 (3)	Ru1—N8—C27—C26	7.5 (19)
Ru1—N3—C8—C9	−176.8 (13)	N7—C26—C27—C28	−14 (3)
C12—N3—C8—C7	174.9 (11)	N6—C26—C27—C28	174.6 (15)
Ru1—N3—C8—C7	4.3 (16)	N7—C26—C27—N8	168.6 (16)
N1—C7—C8—C9	176.6 (16)	N6—C26—C27—N8	−3.1 (19)
N2—C7—C8—C9	0 (3)	N8—C27—C28—C29	0 (2)
N1—C7—C8—N3	−5 (2)	C26—C27—C28—C29	−177.6 (15)
N2—C7—C8—N3	179.2 (15)	C27—C28—C29—C30	0 (2)
N3—C8—C9—C10	3 (3)	C28—C29—C30—C31	3 (2)
C7—C8—C9—C10	−178.2 (16)	C27—N8—C31—C30	5 (2)
C8—C9—C10—C11	−1 (3)	Ru1—N8—C31—C30	172.6 (11)
C9—C10—C11—C12	3 (3)	C27—N8—C31—C32	−175.9 (14)
C8—N3—C12—C11	7 (2)	Ru1—N8—C31—C32	−8.0 (19)
Ru1—N3—C12—C11	177.5 (11)	C29—C30—C31—N8	−5 (2)
C8—N3—C12—C13	−177.8 (11)	C29—C30—C31—C32	175.5 (15)
Ru1—N3—C12—C13	−7.5 (17)	C38—N9—C32—N10	−4.2 (18)
C10—C11—C12—N3	−6 (2)	Ru1—N9—C32—N10	−177.8 (10)
C10—C11—C12—C13	−179.5 (16)	C38—N9—C32—C31	175.8 (14)
C19—N4—C13—N5	1.4 (15)	Ru1—N9—C32—C31	2.3 (19)
Ru1—N4—C13—N5	−177.6 (9)	C33—N10—C32—N9	4.3 (18)
C19—N4—C13—C12	−175.6 (13)	C33—N10—C32—C31	−175.8 (15)
Ru1—N4—C13—C12	5.4 (17)	N8—C31—C32—N9	3 (2)
C14—N5—C13—N4	−0.9 (17)	C30—C31—C32—N9	−177.4 (15)
C14—N5—C13—C12	175.8 (15)	N8—C31—C32—N10	−176.7 (16)
N3—C12—C13—N4	1 (2)	C30—C31—C32—N10	3 (3)
C11—C12—C13—N4	175.2 (15)	C32—N10—C33—C34	177.4 (16)
N3—C12—C13—N5	−175.7 (14)	C32—N10—C33—C38	−2.7 (17)
C11—C12—C13—N5	−1 (3)	N10—C33—C34—C35	−177.1 (16)
C13—N5—C14—C19	0.0 (18)	C38—C33—C34—C35	3 (2)
C13—N5—C14—C15	−177.4 (18)	C33—C34—C35—C36	−2 (2)

N5—C14—C15—C16	175.0 (18)	C34—C35—C36—C37	0 (2)
C19—C14—C15—C16	−2 (2)	C35—C36—C37—C38	3 (2)
C14—C15—C16—C17	3 (3)	C36—C37—C38—N9	176.7 (14)
C15—C16—C17—C18	0 (3)	C36—C37—C38—C33	−2 (2)
C16—C17—C18—C19	−3 (2)	C32—N9—C38—C37	−176.3 (15)
N5—C14—C19—C18	−179.3 (16)	Ru1—N9—C38—C37	−6 (3)
C15—C14—C19—C18	−1 (3)	C32—N9—C38—C33	2.6 (17)
N5—C14—C19—N4	0.9 (18)	Ru1—N9—C38—C33	173.4 (12)
C15—C14—C19—N4	178.9 (13)	C34—C33—C38—C37	−1 (2)
C17—C18—C19—C14	4 (2)	N10—C33—C38—C37	179.2 (14)
C17—C18—C19—N4	−176.0 (14)	C34—C33—C38—N9	−180.0 (14)
C13—N4—C19—C14	−1.4 (16)	N10—C33—C38—N9	0.1 (16)
Ru1—N4—C19—C14	176.9 (12)	C41—O1—C40—C39	179.7 (15)
C13—N4—C19—C18	178.8 (15)	C40—O1—C41—C42	178.4 (18)
Ru1—N4—C19—C18	−3 (3)	C45—O2—C44—C43	−178.1 (18)
C26—N6—C20—C25	−3.7 (15)	C44—O2—C45—C46	78 (2)
Ru1—N6—C20—C25	175.7 (11)	C49—O3—C48—C47	175.3 (17)
C26—N6—C20—C21	177.7 (14)	C48—O3—C49—C50	−158.7 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O2	0.90 (3)	1.85 (5)	2.730 (18)	166 (17)
N5—H5*N*···O3	0.91 (3)	1.81 (5)	2.704 (19)	170 (18)
N7—H7*N*···F8	0.90 (3)	2.58 (7)	3.30 (2)	137 (8)
N7—H7*N*···F11	0.90 (3)	2.05 (4)	2.93 (2)	167 (10)
N10—H10*N*···F6^{i}	0.89 (3)	2.16 (3)	3.028 (19)	166 (6)

Symmetry code: (i) *x*, *y*−1, *z*.