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Bis[4′-(3,5-dibromophenyl)-2,2′:6′,2″-terpyridine]ruthenium(II) bis(hexafluorophosphate) acetonitrile disolvate

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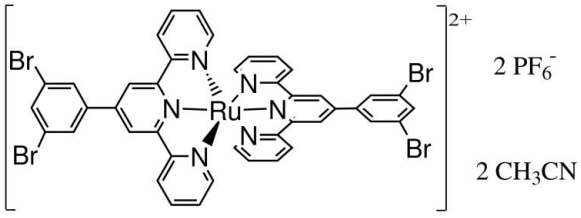
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.025; wR factor = 0.062; data-to-parameter ratio = 10.6.

The title compound, $[Ru(C_{21}H_{13}Br_2N_3)_2](PF_6)_2\cdot 2CH_2CN$, was synthesized to investigate its photophysical properties. The molecule and the crystal structure are both non-centrosymmetric. The Ru atom is in a distorted octahedral coordination geometry. Intermolecular interactions are dominated by π-stacking interactions between aromatic rings, with centroid-centroid distances between 3.7 and 3.9 Å. No bromine–bromine interactions are observed.

Related literature

More details on bromine–bromine interactions in related compounds, such as bis(4-*para*-bromophenylterpyridine) metal complexes, are described by Medlycott *et al.* (2005, 2007) and Reddy *et al.* (2006).



Experimental

Crystal data

$[Ru(C_{21}H_{13}Br_2N_3)_2](PF_6)_2\cdot 2C_2H_3N$
M_r = 1407.45
Triclinic, $P\overline{1}$
a = 8.3158 (1) Å
b = 9.2087 (1) Å
c = 16.2114 (1) Å
α = 89.7346 (5)°
β = 88.7088 (4)°
γ = 83.6367 (5)°
V = 1233.47 (2) Å^3
Z = 1
Cu $K\alpha$ radiation
μ = 7.78 mm^{-1}
T = 100 (2) K
0.10 × 0.05 × 0.02 mm

Data collection

Bruker APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.601, T_{max} = 0.857
19475 measured reflections
7003 independent reflections
6901 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.06
7003 reflections
661 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Absolute structure: Flack (1983), 2532 Friedel pairs
Flack parameter: 0.041 (5)

Table 1
Selected geometric parameters (Å, °).

Ru1—N5	1.983 (3)	Ru1—N1	2.078 (3)
Ru1—N2	1.988 (3)	Ru1—N6	2.082 (4)
Ru1—N4	2.067 (4)	Ru1—N3	2.089 (3)
N5—Ru1—N2	176.91 (17)	N4—Ru1—N6	157.64 (11)
N5—Ru1—N4	79.20 (13)	N1—Ru1—N6	97.48 (12)
N2—Ru1—N4	98.47 (13)	N5—Ru1—N3	103.40 (12)
N5—Ru1—N1	98.77 (12)	N2—Ru1—N3	78.78 (12)
N2—Ru1—N1	78.99 (12)	N4—Ru1—N3	95.84 (12)
N4—Ru1—N1	86.33 (12)	N1—Ru1—N3	157.75 (11)
N5—Ru1—N6	78.44 (13)	N6—Ru1—N3	88.91 (12)
N2—Ru1—N6	103.89 (13)		

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* (Bruker, 1997); software used to prepare material for publication: *UdMX* (local program).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2035).

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supplementary materials

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Bis[4'-(3,5-dibromophenyl)-2,2':6',2''-terpyridine]ruthenium(II) bis(hexafluorophosphate) acetonitrile disolvate

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Comment

The title compound crystallizes in the chiral space group (P1) although the molecule itself is not chiral in solution. Both dibromophenyl rings are almost parallel with a tilt angle of only 5° preventing a S2 axis which can pass through the molecule when the pendant rings are oriented perpendicular to each other.

There are 3 distinct intermolecular π stacking interactions present. The outer pyridyl groups coordinated to the metal atoms interact with their opposite pair forming two distinct stacking interactions 90° apart(fig 2). The distance between the ring centroids are about 3.9 Å, with a perpendicular (centroid-to-plane) distance of about 3.4 Å. The third stacking interaction occurs between opposite dibromophenyl groups of molecules along the c axis. The centroid distance between both phenyl rings is 3.7Å and the perpendicular distance amount to 3.5 Å.

The Br···Br distances varying from 4.2Å to 4.6Å and are much longer than the expected Br···Br short contact distances of 3.4Å to 3.6Å (Medlycott *et al.*, 2007, 2005) (Reddy *et al.*, 2006). Therefore, no intermolecular bromine-bromine interactions occur. There is one Br···F short contact, between Br1 and F3 of 3.1 Å, showing a weak interaction with the hexafluorophosphate anion.

Experimental

The title compound was synthesized by heating at reflux overnight two equivalents of the 4'-(3,5-dibromophenyl)2,2':6',2''-terpyridine ligand (0.467 g), one equivalent of $RuCl_3$ (0.104 g) and four equivalents of silver nitrate (0.340 g) in ethanol (50 ml). The crude product was filtered over celite and purified by flash chromatography (silica gel, eluant (v/v): 4 acetone, 8 acetonitrile and 1 saturated aqueous solution of KNO_3). The complex was precipitated with KPF_6 and dried under vacuum for a final yield of 51% (0.338 g). The title compound crystallized by isopropyl ether diffusion to an acetonitrile solution of the complex.

Refinement

The H atoms were generated with idealized geometry (sp^2 C—H 0.95 Å, sp^3 C—H 0.98 Å) and were included in the refinement in the riding model approximation; their temperature factors were set to 1.5 times those of the equivalent isotropic temperature factors of the parent site (methyl) and 1.2 times for others. The H atoms of the methyl groups of the acetonitrile molecules were positioned with idealized geometry allowed to rotate but not to tip. The maximum density peak of 1.01 e $Å^{-3}$) is located 0.878 Å from Br4.

Figures

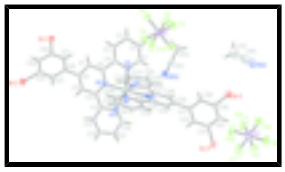

Fig. 1. Ortep view of the title compound. Thermal ellipsoids of non-hydrogen are shown at 50% probability levels.

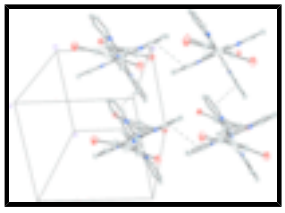

Fig. 2. The packing of the compound, viewed along the c axis, showing the π stacking of the pyridyl groups. H atoms, anions and solvent molecules have been omitted for clarity.

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Crystal data

$[Ru(C_{21}H_{13}Br_2N_3)_2](P_1F_6)_2\cdot 2C_2H_3N$	$Z = 1$
$M_r = 1407.45$	$F_{000} = 686$
Triclinic, $P\overline{1}$	$D_x = 1.895$ Mg m^{-3}
Hall symbol: P -1	Cu $K\alpha$ radiation $\lambda = 1.54178$ Å
$a = 8.3158$ (1) Å	Cell parameters from 17454 reflections
$b = 9.2087$ (1) Å	$\theta = 2.7$–$67.3°$
$c = 16.2114$ (1) Å	$\mu = 7.78$ mm^{-1}
$\alpha = 89.7346$ (5)°	$T = 100$ (2) K
$\beta = 88.7088$ (4)°	Needle-like, red
$\gamma = 83.6367$ (5)°	0.10 × 0.05 × 0.02 mm
$V = 1233.47$ (2) Å^3	

Data collection

Bruker APEX II diffractometer	7003 independent reflections
Radiation source: Micro source	6901 reflections with $I > 2\sigma(I)$
Monochromator: Helios optics	$R_{int} = 0.027$
$T = 100$(2) K	$\theta_{max} = 67.9°$
ω scans	$\theta_{min} = 2.7°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -9\rightarrow 9$
$T_{min} = 0.601$, $T_{max} = 0.857$	$k = -10\rightarrow 10$
19475 measured reflections	$l = -19\rightarrow 19$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.062$

$S = 1.06$

7003 reflections

661 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.01$ e Å^{-3}

$\Delta\rho_{min} = -0.39$ e Å^{-3}

Extinction correction: none

Absolute structure: Flack (1983), 2532 Friedel pairs

Flack parameter: 0.041 (5)

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. 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.

All remaining electron density larger then 0.5 is located less then 0.9 Å from an heavy atom (Br or Ru). Higher symmetry solution, using whole data and only the main molecule, were searched with Platon but none were found.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.05928 (2)	0.69668 (2)	0.094352 (15)	0.01474 (8)
Br1	0.11826 (6)	0.33373 (6)	−0.45785 (3)	0.03716 (14)
Br2	0.36580 (6)	0.88101 (6)	−0.47857 (3)	0.03908 (14)
Br3	−0.34776 (6)	0.45920 (6)	0.64229 (3)	0.04448 (16)
Br4	−0.12003 (6)	1.01619 (6)	0.65312 (3)	0.03841 (14)
N1	0.1580 (3)	0.4799 (4)	0.08447 (18)	0.0148 (7)
N2	0.1171 (4)	0.6848 (4)	−0.02525 (18)	0.0166 (8)
N3	−0.0208 (3)	0.9084 (4)	0.05537 (18)	0.0183 (8)
N4	−0.1640 (4)	0.6186 (4)	0.08997 (19)	0.0202 (8)
N5	−0.0031 (4)	0.6983 (4)	0.21318 (18)	0.0170 (8)
N6	0.2574 (4)	0.7774 (4)	0.14697 (17)	0.0159 (7)
C1	0.1713 (4)	0.3783 (5)	0.1444 (2)	0.0202 (9)
H1A	0.1343	0.4050	0.1986	0.024*
C2	0.2378 (5)	0.2349 (5)	0.1295 (2)	0.0223 (10)
H2A	0.2472	0.1658	0.1733	0.027*
C3	0.2899 (5)	0.1938 (5)	0.0510 (3)	0.0243 (11)
H3A	0.3366	0.0967	0.0399	0.029*
C4	0.2726 (4)	0.2984 (5)	−0.0125 (2)	0.0216 (10)

H4A	0.3064	0.2726	−0.0674	0.026*
C5	0.2056 (4)	0.4398 (5)	0.0057 (2)	0.0180 (9)
C6	0.1790 (4)	0.5557 (4)	−0.0570 (2)	0.0160 (9)
C7	0.2061 (4)	0.5403 (5)	−0.1414 (2)	0.0211 (10)
H7A	0.2489	0.4486	−0.1638	0.025*
C8	0.1696 (4)	0.6614 (5)	−0.1934 (2)	0.0186 (9)
C9	0.1080 (4)	0.7944 (5)	−0.1582 (2)	0.0180 (9)
H9A	0.0845	0.8782	−0.1920	0.022*
C10	0.0811 (4)	0.8038 (4)	−0.0736 (2)	0.0161 (9)
C11	0.0059 (4)	0.9314 (5)	−0.0274 (2)	0.0180 (9)
C12	−0.0388 (5)	1.0661 (5)	−0.0633 (2)	0.0213 (9)
H12A	−0.0180	1.0809	−0.1204	0.026*
C13	−0.1141 (5)	1.1788 (5)	−0.0155 (3)	0.0270 (11)
H13A	−0.1461	1.2718	−0.0393	0.032*
C14	−0.1418 (5)	1.1539 (5)	0.0673 (3)	0.0240 (11)
H14A	−0.1948	1.2295	0.1010	0.029*
C15	−0.0926 (4)	1.0195 (5)	0.1010 (2)	0.0235 (10)
H15A	−0.1100	1.0047	0.1584	0.028*
C16	0.1939 (5)	0.6439 (5)	−0.2841 (2)	0.0193 (10)
C17	0.1538 (5)	0.5204 (5)	−0.3221 (2)	0.0239 (11)
H17A	0.1091	0.4470	−0.2904	0.029*
C18	0.1779 (5)	0.5020 (5)	−0.4065 (2)	0.0267 (11)
C19	0.2426 (5)	0.6077 (6)	−0.4544 (2)	0.0278 (12)
H19A	0.2613	0.5949	−0.5121	0.033*
C20	0.2782 (5)	0.7315 (5)	−0.4150 (2)	0.0246 (11)
C21	0.2569 (5)	0.7536 (5)	−0.3312 (2)	0.0229 (10)
H21A	0.2839	0.8405	−0.3061	0.027*
C22	−0.2399 (4)	0.5796 (5)	0.0228 (2)	0.0221 (10)
H22A	−0.1986	0.6031	−0.0302	0.027*
C23	−0.3754 (5)	0.5068 (5)	0.0280 (3)	0.0238 (10)
H23A	−0.4259	0.4791	−0.0207	0.029*
C24	−0.4375 (4)	0.4742 (5)	0.1052 (2)	0.0221 (10)
H24A	−0.5301	0.4227	0.1101	0.027*
C25	−0.3635 (4)	0.5174 (5)	0.1743 (2)	0.0200 (9)
H25A	−0.4056	0.4968	0.2275	0.024*
C26	−0.2277 (4)	0.5909 (4)	0.1665 (2)	0.0166 (9)
C27	−0.1418 (4)	0.6440 (4)	0.2361 (2)	0.0162 (9)
C28	−0.1902 (4)	0.6463 (5)	0.3193 (2)	0.0200 (9)
H28A	−0.2878	0.6088	0.3360	0.024*
C29	−0.0949 (5)	0.7034 (5)	0.3772 (2)	0.0197 (10)
C30	0.0507 (4)	0.7544 (5)	0.3518 (2)	0.0192 (9)
H30A	0.1183	0.7920	0.3911	0.023*
C31	0.0957 (4)	0.7498 (4)	0.2689 (2)	0.0168 (9)
C32	0.2446 (4)	0.7949 (4)	0.2308 (2)	0.0182 (9)
C33	0.3628 (4)	0.8516 (5)	0.2746 (2)	0.0180 (9)
H33A	0.3527	0.8599	0.3329	0.022*
C34	0.4973 (5)	0.8969 (5)	0.2333 (2)	0.0220 (10)
H34A	0.5797	0.9367	0.2627	0.026*
C35	0.5078 (4)	0.8823 (5)	0.1480 (2)	0.0181 (10)

H35A	0.5970	0.9138	0.1179	0.022*
C36	0.3880 (4)	0.8219 (4)	0.1076 (2)	0.0156 (9)
H36A	0.3975	0.8110	0.0494	0.019*
C37	−0.1458 (5)	0.7154 (5)	0.4666 (2)	0.0223 (11)
C38	−0.2180 (5)	0.6020 (5)	0.5051 (2)	0.0237 (10)
H38A	−0.2384	0.5175	0.4754	0.028*
C39	−0.2583 (5)	0.6177 (5)	0.5879 (3)	0.0290 (12)
C40	−0.2329 (5)	0.7366 (6)	0.6340 (2)	0.0288 (12)
H40A	−0.2621	0.7428	0.6910	0.035*
C41	−0.1627 (5)	0.8477 (5)	0.5939 (2)	0.0257 (11)
C42	−0.1183 (5)	0.8395 (5)	0.5107 (2)	0.0223 (11)
H42A	−0.0703	0.9170	0.4844	0.027*
P1	0.91524 (12)	0.18925 (13)	0.33410 (6)	0.0245 (3)
F1	1.0258 (3)	0.3206 (3)	0.33116 (16)	0.0376 (7)
F2	1.0441 (3)	0.0963 (3)	0.27442 (16)	0.0386 (7)
F3	1.0125 (3)	0.1216 (3)	0.41140 (15)	0.0366 (7)
F4	0.8200 (4)	0.2540 (4)	0.25552 (18)	0.0533 (9)
F5	0.7874 (3)	0.2803 (4)	0.39307 (17)	0.0442 (8)
F6	0.8064 (3)	0.0552 (3)	0.33533 (18)	0.0391 (7)
P2	0.56414 (12)	0.89525 (16)	0.87713 (6)	0.0317 (3)
F7	0.6287 (4)	1.0460 (5)	0.85268 (18)	0.0663 (12)
F8	0.7329 (3)	0.8074 (5)	0.85077 (17)	0.0654 (12)
F9	0.6294 (3)	0.9084 (4)	0.96895 (14)	0.0413 (8)
F10	0.4985 (3)	0.8787 (4)	0.78624 (15)	0.0465 (9)
F11	0.3941 (3)	0.9816 (4)	0.90451 (17)	0.0424 (7)
F12	0.4954 (3)	0.7446 (4)	0.90392 (17)	0.0412 (7)
N50	0.1777 (8)	0.1734 (7)	0.7721 (3)	0.0651 (17)
C50	0.2877 (11)	0.1696 (9)	0.7375 (5)	0.071 (2)
C51	0.4432 (10)	0.1555 (10)	0.6881 (5)	0.084 (3)
H51A	0.5311	0.1806	0.7227	0.126*
H51B	0.4327	0.2219	0.6406	0.126*
H51C	0.4675	0.0547	0.6686	0.126*
N52	0.4003 (6)	0.4943 (6)	0.3489 (3)	0.0504 (14)
C52	0.4083 (6)	0.3754 (7)	0.3625 (3)	0.0398 (14)
C53	0.4195 (7)	0.2178 (6)	0.3814 (4)	0.0566 (18)
H53A	0.4618	0.2003	0.4369	0.085*
H53B	0.4924	0.1639	0.3410	0.085*
H53C	0.3118	0.1846	0.3787	0.085*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01455 (11)	0.01488 (17)	0.01510 (12)	−0.00285 (11)	−0.00092 (9)	−0.00290 (11)
Br1	0.0492 (3)	0.0331 (3)	0.0302 (2)	−0.0078 (3)	−0.00386 (19)	−0.0148 (2)
Br2	0.0558 (3)	0.0436 (3)	0.0207 (2)	−0.0183 (3)	−0.00158 (19)	0.0046 (2)
Br3	0.0552 (3)	0.0416 (4)	0.0379 (3)	−0.0145 (3)	0.0142 (2)	0.0083 (2)
Br4	0.0549 (3)	0.0346 (3)	0.0258 (2)	−0.0057 (2)	0.00264 (19)	−0.0093 (2)
N1	0.0155 (13)	0.0097 (19)	0.0208 (14)	−0.0075 (13)	−0.0038 (11)	−0.0051 (13)

N2	0.0155 (14)	0.016 (2)	0.0180 (14)	−0.0017 (14)	−0.0017 (11)	−0.0023 (14)
N3	0.0167 (14)	0.021 (2)	0.0184 (14)	−0.0060 (14)	−0.0023 (11)	−0.0051 (14)
N4	0.0214 (15)	0.017 (2)	0.0223 (15)	−0.0001 (15)	−0.0015 (12)	−0.0021 (14)
N5	0.0186 (15)	0.014 (2)	0.0189 (14)	−0.0036 (14)	−0.0005 (12)	−0.0047 (13)
N6	0.0203 (15)	0.0107 (19)	0.0165 (13)	−0.0015 (14)	0.0009 (11)	−0.0032 (13)
C1	0.0181 (16)	0.022 (3)	0.0208 (17)	−0.0028 (17)	−0.0010 (14)	−0.0005 (17)
C2	0.0220 (19)	0.019 (3)	0.028 (2)	−0.0082 (18)	−0.0046 (15)	0.0034 (18)
C3	0.0250 (18)	0.018 (3)	0.030 (2)	−0.0006 (18)	0.0004 (15)	−0.0017 (18)
C4	0.027 (2)	0.018 (2)	0.0205 (17)	−0.0033 (18)	−0.0007 (15)	−0.0053 (16)
C5	0.0146 (15)	0.020 (2)	0.0198 (17)	−0.0053 (16)	−0.0009 (13)	−0.0006 (16)
C6	0.0136 (15)	0.015 (2)	0.0208 (17)	−0.0059 (16)	−0.0050 (13)	−0.0030 (16)
C7	0.0232 (17)	0.020 (2)	0.0196 (17)	0.0006 (17)	0.0014 (14)	−0.0054 (16)
C8	0.0208 (18)	0.018 (2)	0.0178 (17)	−0.0062 (17)	−0.0026 (14)	−0.0021 (17)
C9	0.0187 (16)	0.017 (2)	0.0189 (16)	−0.0034 (16)	−0.0025 (13)	−0.0010 (16)
C10	0.0152 (16)	0.011 (2)	0.0235 (17)	−0.0086 (16)	−0.0046 (13)	−0.0030 (16)
C11	0.0161 (15)	0.020 (2)	0.0189 (17)	−0.0047 (17)	−0.0035 (13)	−0.0058 (16)
C12	0.0227 (17)	0.020 (3)	0.0213 (17)	−0.0040 (17)	−0.0041 (14)	−0.0029 (17)
C13	0.0302 (19)	0.016 (3)	0.034 (2)	0.0014 (19)	−0.0078 (16)	−0.0019 (19)
C14	0.0218 (19)	0.020 (3)	0.031 (2)	−0.0014 (19)	−0.0041 (16)	−0.0133 (19)
C15	0.0151 (16)	0.034 (3)	0.0214 (17)	−0.0014 (18)	−0.0015 (13)	−0.0055 (18)
C16	0.0237 (18)	0.014 (3)	0.0201 (17)	−0.0032 (18)	−0.0006 (14)	−0.0075 (18)
C17	0.0259 (19)	0.027 (3)	0.0188 (17)	−0.0011 (19)	−0.0027 (15)	−0.0031 (19)
C18	0.033 (2)	0.027 (3)	0.0196 (18)	0.001 (2)	−0.0074 (15)	−0.0116 (18)
C19	0.030 (2)	0.033 (3)	0.0199 (18)	−0.001 (2)	−0.0031 (15)	−0.007 (2)
C20	0.0258 (19)	0.024 (3)	0.0251 (18)	−0.006 (2)	−0.0051 (15)	−0.002 (2)
C21	0.0258 (18)	0.026 (3)	0.0176 (17)	−0.0032 (18)	−0.0043 (14)	0.0003 (17)
C22	0.0180 (17)	0.025 (3)	0.0236 (18)	−0.0029 (18)	−0.0016 (14)	−0.0007 (18)
C23	0.021 (2)	0.020 (3)	0.030 (2)	−0.0011 (19)	−0.0072 (16)	−0.0098 (18)
C24	0.0176 (17)	0.017 (2)	0.033 (2)	−0.0048 (17)	−0.0024 (14)	−0.0045 (18)
C25	0.0150 (15)	0.017 (2)	0.0276 (18)	−0.0021 (16)	−0.0011 (14)	−0.0013 (17)
C26	0.0178 (16)	0.011 (2)	0.0206 (16)	0.0003 (16)	−0.0013 (13)	−0.0048 (15)
C27	0.0157 (16)	0.011 (2)	0.0227 (17)	−0.0043 (16)	−0.0037 (13)	−0.0027 (16)
C28	0.0176 (16)	0.021 (2)	0.0211 (17)	−0.0017 (17)	0.0028 (14)	−0.0011 (16)
C29	0.0211 (18)	0.018 (2)	0.0193 (18)	−0.0001 (18)	0.0002 (14)	−0.0036 (17)
C30	0.0197 (17)	0.018 (2)	0.0191 (17)	−0.0003 (17)	−0.0007 (14)	−0.0043 (16)
C31	0.0159 (16)	0.015 (2)	0.0200 (17)	−0.0021 (16)	−0.0041 (13)	0.0010 (16)
C32	0.0182 (16)	0.015 (2)	0.0206 (17)	0.0002 (16)	0.0009 (14)	−0.0005 (16)
C33	0.0206 (17)	0.017 (2)	0.0169 (16)	−0.0048 (17)	−0.0036 (14)	−0.0048 (16)
C34	0.0201 (17)	0.020 (2)	0.0275 (19)	−0.0063 (18)	−0.0069 (15)	−0.0006 (18)
C35	0.0156 (17)	0.010 (2)	0.0288 (19)	−0.0019 (17)	0.0012 (15)	−0.0023 (17)
C36	0.0181 (16)	0.012 (2)	0.0177 (16)	−0.0040 (16)	−0.0006 (13)	0.0004 (16)
C37	0.0226 (19)	0.024 (3)	0.0199 (18)	−0.0016 (18)	0.0032 (15)	0.0018 (19)
C38	0.0266 (19)	0.021 (3)	0.0241 (18)	−0.0052 (19)	−0.0002 (15)	−0.0042 (18)
C39	0.030 (2)	0.029 (3)	0.027 (2)	−0.003 (2)	0.0072 (16)	0.006 (2)
C40	0.033 (2)	0.034 (3)	0.0181 (18)	0.000 (2)	0.0025 (16)	−0.001 (2)
C41	0.027 (2)	0.026 (3)	0.0241 (19)	−0.0038 (19)	0.0002 (15)	−0.0045 (19)
C42	0.0236 (18)	0.021 (3)	0.0225 (18)	−0.0034 (19)	0.0012 (15)	−0.0021 (19)
P1	0.0310 (5)	0.0211 (7)	0.0215 (4)	−0.0018 (5)	−0.0035 (4)	−0.0038 (4)
F1	0.0522 (15)	0.0246 (16)	0.0377 (13)	−0.0128 (13)	0.0051 (12)	0.0019 (12)

F2	0.0396 (13)	0.0349 (18)	0.0399 (14)	0.0016 (13)	0.0039 (11)	−0.0082 (13)
F3	0.0489 (14)	0.0327 (17)	0.0317 (12)	−0.0180 (13)	−0.0144 (11)	0.0082 (12)
F4	0.0711 (19)	0.045 (2)	0.0407 (14)	0.0144 (17)	−0.0275 (14)	−0.0030 (14)
F5	0.0421 (14)	0.042 (2)	0.0490 (15)	−0.0054 (14)	0.0066 (12)	−0.0238 (14)
F6	0.0328 (12)	0.0324 (18)	0.0536 (15)	−0.0086 (13)	−0.0081 (11)	−0.0102 (13)
P2	0.0220 (5)	0.0555 (9)	0.0197 (5)	−0.0134 (5)	−0.0003 (4)	−0.0055 (5)
F7	0.073 (2)	0.100 (3)	0.0369 (15)	−0.055 (2)	−0.0173 (14)	0.0220 (19)
F8	0.0231 (12)	0.135 (4)	0.0355 (14)	0.0025 (18)	0.0015 (11)	−0.0110 (17)
F9	0.0375 (13)	0.069 (2)	0.0221 (11)	−0.0276 (14)	−0.0040 (10)	0.0018 (13)
F10	0.0344 (13)	0.083 (3)	0.0232 (11)	−0.0109 (15)	−0.0071 (10)	−0.0110 (14)
F11	0.0390 (14)	0.045 (2)	0.0430 (14)	−0.0045 (14)	0.0005 (11)	−0.0157 (13)
F12	0.0399 (14)	0.0401 (19)	0.0450 (15)	−0.0084 (13)	−0.0095 (11)	−0.0051 (14)
N50	0.092 (4)	0.058 (4)	0.044 (3)	−0.004 (3)	0.009 (3)	0.011 (3)
C50	0.100 (6)	0.054 (5)	0.060 (4)	−0.014 (4)	−0.010 (4)	0.011 (4)
C51	0.091 (5)	0.082 (6)	0.082 (5)	−0.018 (5)	0.002 (4)	0.020 (5)
N52	0.057 (3)	0.044 (3)	0.048 (2)	0.002 (2)	0.024 (2)	0.010 (2)
C52	0.042 (3)	0.044 (4)	0.032 (2)	−0.004 (2)	0.016 (2)	−0.006 (2)
C53	0.038 (3)	0.033 (4)	0.097 (5)	−0.003 (3)	0.020 (3)	−0.006 (3)

Geometric parameters (Å, °)

Ru1—N5	1.983 (3)	C22—C23	1.375 (7)
Ru1—N2	1.988 (3)	C22—H22a	0.95
Ru1—N4	2.067 (4)	C23—C24	1.387 (6)
Ru1—N1	2.078 (3)	C23—H23a	0.95
Ru1—N6	2.082 (4)	C24—C25	1.371 (6)
Ru1—N3	2.089 (3)	C24—H24a	0.95
Br1—C18	1.882 (5)	C25—C26	1.383 (6)
Br2—C20	1.914 (4)	C25—H25a	0.95
Br3—C39	1.913 (5)	C26—C27	1.463 (6)
Br4—C41	1.899 (5)	C27—C28	1.398 (5)
N1—C1	1.343 (5)	C28—C29	1.385 (7)
N1—C5	1.368 (5)	C28—H28a	0.95
N2—C6	1.342 (5)	C29—C30	1.399 (6)
N2—C10	1.355 (5)	C29—C37	1.502 (5)
N3—C15	1.342 (5)	C30—C31	1.385 (5)
N3—C11	1.374 (4)	C30—H30a	0.95
N4—C22	1.341 (6)	C31—C32	1.471 (5)
N4—C26	1.372 (5)	C32—C33	1.376 (6)
N5—C27	1.351 (5)	C33—C34	1.393 (6)
N5—C31	1.357 (6)	C33—H33a	0.95
N6—C36	1.349 (5)	C34—C35	1.390 (6)
N6—C32	1.370 (5)	C34—H34a	0.95
C1—C2	1.394 (6)	C35—C36	1.374 (6)
C1—H1a	0.95	C35—H35a	0.95
C2—C3	1.376 (6)	C36—H36a	0.95
C2—H2a	0.95	C37—C42	1.394 (7)
C3—C4	1.405 (5)	C37—C38	1.398 (6)
C3—H3a	0.95	C38—C39	1.380 (6)

C4—C5	1.389 (6)	C38—H38a	0.95
C4—H4a	0.95	C39—C40	1.368 (8)
C5—C6	1.473 (5)	C40—C41	1.385 (7)
C6—C7	1.386 (5)	C40—H40a	0.95
C7—C8	1.406 (5)	C41—C42	1.390 (6)
C7—H7a	0.95	C42—H42a	0.95
C8—C9	1.394 (6)	P1—F5	1.585 (3)
C8—C16	1.485 (5)	P1—F3	1.593 (2)
C9—C10	1.386 (5)	P1—F4	1.594 (3)
C9—H9a	0.95	P1—F1	1.599 (3)
C10—C11	1.469 (6)	P1—F2	1.605 (3)
C11—C12	1.384 (5)	P1—F6	1.609 (4)
C12—C13	1.382 (6)	P2—F7	1.588 (4)
C12—H12a	0.95	P2—F8	1.591 (3)
C13—C14	1.381 (6)	P2—F10	1.597 (3)
C13—H13a	0.95	P2—F11	1.598 (3)
C14—C15	1.375 (6)	P2—F9	1.606 (3)
C14—H14a	0.95	P2—F12	1.612 (4)
C15—H15a	0.95	N50—C50	1.060 (9)
C16—C17	1.373 (7)	C50—C51	1.499 (12)
C16—C21	1.404 (6)	C51—H51a	0.98
C17—C18	1.387 (5)	C51—H51b	0.98
C17—H17a	0.95	C51—H51c	0.98
C18—C19	1.389 (7)	N52—C52	1.111 (7)
C19—C20	1.373 (8)	C52—C53	1.475 (8)
C19—H19a	0.95	C53—H53a	0.98
C20—C21	1.380 (6)	C53—H53b	0.98
C21—H21a	0.95	C53—H53c	0.98
N5—Ru1—N2	176.91 (17)	C25—C24—C23	119.2 (4)
N5—Ru1—N4	79.20 (13)	C25—C24—H24A	120.4
N2—Ru1—N4	98.47 (13)	C23—C24—H24A	120.4
N5—Ru1—N1	98.77 (12)	C24—C25—C26	120.0 (3)
N2—Ru1—N1	78.99 (12)	C24—C25—H25A	120
N4—Ru1—N1	86.33 (12)	C26—C25—H25A	120
N5—Ru1—N6	78.44 (13)	N4—C26—C25	120.4 (4)
N2—Ru1—N6	103.89 (13)	N4—C26—C27	115.3 (3)
N4—Ru1—N6	157.64 (11)	C25—C26—C27	124.3 (3)
N1—Ru1—N6	97.48 (12)	N5—C27—C28	119.6 (4)
N5—Ru1—N3	103.40 (12)	N5—C27—C26	113.1 (3)
N2—Ru1—N3	78.78 (12)	C28—C27—C26	127.3 (4)
N4—Ru1—N3	95.84 (12)	C29—C28—C27	119.6 (4)
N1—Ru1—N3	157.75 (11)	C29—C28—H28A	120.2
N6—Ru1—N3	88.91 (12)	C27—C28—H28A	120.2
C1—N1—C5	118.8 (3)	C28—C29—C30	119.4 (3)
C1—N1—RU1	127.6 (3)	C28—C29—C37	121.6 (4)
C5—N1—RU1	113.5 (2)	C30—C29—C37	119.0 (4)
C6—N2—C10	121.7 (3)	C31—C30—C29	119.6 (4)
C6—N2—RU1	118.9 (2)	C31—C30—H30A	120.2
C10—N2—RU1	119.2 (3)	C29—C30—H30A	120.2

C15—N3—C11	118.6 (3)	N5—C31—C30	119.7 (3)
C15—N3—RU1	127.9 (2)	N5—C31—C32	112.8 (3)
C11—N3—RU1	113.6 (3)	C30—C31—C32	127.6 (4)
C22—N4—C26	119.1 (4)	N6—C32—C33	121.6 (3)
C22—N4—RU1	127.3 (2)	N6—C32—C31	114.9 (4)
C26—N4—RU1	113.2 (3)	C33—C32—C31	123.5 (3)
C27—N5—C31	122.1 (3)	C32—C33—C34	119.9 (3)
C27—N5—RU1	118.4 (3)	C32—C33—H33A	120
C31—N5—RU1	119.5 (2)	C34—C33—H33A	120
C36—N6—C32	118.0 (4)	C35—C34—C33	118.3 (4)
C36—N6—RU1	127.5 (2)	C35—C34—H34A	120.9
C32—N6—RU1	114.4 (2)	C33—C34—H34A	120.9
N1—C1—C2	122.1 (3)	C36—C35—C34	119.4 (4)
N1—C1—H1A	118.9	C36—C35—H35A	120.3
C2—C1—H1A	118.9	C34—C35—H35A	120.3
C3—C2—C1	119.7 (3)	N6—C36—C35	122.8 (3)
C3—C2—H2A	120.2	N6—C36—H36A	118.6
C1—C2—H2A	120.2	C35—C36—H36A	118.6
C2—C3—C4	118.6 (4)	C42—C37—C38	120.6 (4)
C2—C3—H3A	120.7	C42—C37—C29	119.3 (4)
C4—C3—H3A	120.7	C38—C37—C29	120.1 (4)
C5—C4—C3	119.4 (3)	C39—C38—C37	117.4 (5)
C5—C4—H4A	120.3	C39—C38—H38A	121.3
C3—C4—H4A	120.3	C37—C38—H38A	121.3
N1—C5—C4	121.3 (3)	C40—C39—C38	124.2 (4)
N1—C5—C6	115.4 (3)	C40—C39—BR3	118.0 (3)
C4—C5—C6	123.2 (3)	C38—C39—BR3	117.7 (4)
N2—C6—C7	120.4 (3)	C39—C40—C41	116.9 (4)
N2—C6—C5	113.0 (3)	C39—C40—H40A	121.5
C7—C6—C5	126.5 (4)	C41—C40—H40A	121.5
C6—C7—C8	119.5 (4)	C40—C41—C42	122.1 (5)
C6—C7—H7A	120.3	C40—C41—BR4	120.0 (3)
C8—C7—H7A	120.3	C42—C41—BR4	117.9 (4)
C9—C8—C7	118.6 (3)	C41—C42—C37	118.7 (4)
C9—C8—C16	121.9 (3)	C41—C42—H42A	120.7
C7—C8—C16	119.5 (4)	C37—C42—H42A	120.7
C10—C9—C8	119.7 (3)	F5—P1—F3	91.04 (15)
C10—C9—H9A	120.1	F5—P1—F4	90.19 (16)
C8—C9—H9A	120.1	F3—P1—F4	178.70 (18)
N2—C10—C9	120.1 (3)	F5—P1—F1	90.91 (17)
N2—C10—C11	113.1 (3)	F3—P1—F1	89.85 (15)
C9—C10—C11	126.8 (3)	F4—P1—F1	90.55 (18)
N3—C11—C12	121.1 (3)	F5—P1—F2	179.7 (2)
N3—C11—C10	115.4 (3)	F3—P1—F2	88.94 (14)
C12—C11—C10	123.5 (3)	F4—P1—F2	89.82 (15)
C13—C12—C11	119.6 (3)	F1—P1—F2	89.43 (16)
C13—C12—H12A	120.2	F5—P1—F6	90.37 (17)
C11—C12—H12A	120.2	F3—P1—F6	90.41 (15)
C14—C13—C12	118.7 (4)	F4—P1—F6	89.17 (18)

C14—C13—H13A	120.6	F1—P1—F6	178.69 (16)
C12—C13—H13A	120.6	F2—P1—F6	89.29 (17)
C15—C14—C13	119.9 (4)	F7—P2—F8	91.2 (2)
C15—C14—H14A	120	F7—P2—F10	90.82 (18)
C13—C14—H14A	120	F8—P2—F10	90.54 (15)
N3—C15—C14	122.1 (3)	F7—P2—F11	89.6 (2)
N3—C15—H15A	119	F8—P2—F11	179.2 (2)
C14—C15—H15A	119	F10—P2—F11	89.81 (15)
C17—C16—C21	119.8 (4)	F7—P2—F9	90.38 (18)
C17—C16—C8	120.0 (4)	F8—P2—F9	89.23 (15)
C21—C16—C8	120.3 (4)	F10—P2—F9	178.8 (2)
C16—C17—C18	120.5 (4)	F11—P2—F9	90.40 (15)
C16—C17—H17A	119.8	F7—P2—F12	178.4 (2)
C18—C17—H17A	119.8	F8—P2—F12	90.2 (2)
C17—C18—C19	121.0 (5)	F10—P2—F12	89.99 (18)
C17—C18—BR1	119.8 (4)	F11—P2—F12	89.01 (16)
C19—C18—BR1	119.2 (3)	F9—P2—F12	88.81 (16)
C20—C19—C18	117.2 (4)	N50—C50—C51	176.9 (10)
C20—C19—H19A	121.4	C50—C51—H51A	109.5
C18—C19—H19A	121.4	C50—C51—H51B	109.5
C19—C20—C21	123.6 (4)	H51A—C51—H51B	109.5
C19—C20—BR2	118.8 (3)	C50—C51—H51C	109.5
C21—C20—BR2	117.6 (4)	H51A—C51—H51C	109.5
C20—C21—C16	117.9 (5)	H51B—C51—H51C	109.5
C20—C21—H21A	121	N52—C52—C53	179.4 (7)
C16—C21—H21A	121	C52—C53—H53A	109.5
N4—C22—C23	122.2 (3)	C52—C53—H53B	109.5
N4—C22—H22A	118.9	H53A—C53—H53B	109.5
C23—C22—H22A	118.9	C52—C53—H53C	109.5
C22—C23—C24	119.1 (4)	H53A—C53—H53C	109.5
C22—C23—H23A	120.5	H53B—C53—H53C	109.5
C24—C23—H23A	120.5		
N5—RU1—N1—C1	−0.2 (4)	RU1—N3—C11—C10	1.5 (4)
N2—RU1—N1—C1	−178.1 (4)	N2—C10—C11—N3	−2.3 (5)
N4—RU1—N1—C1	−78.7 (3)	C9—C10—C11—N3	174.0 (4)
N6—RU1—N1—C1	79.1 (3)	N2—C10—C11—C12	178.8 (4)
N3—RU1—N1—C1	−175.2 (3)	C9—C10—C11—C12	−4.8 (7)
N5—RU1—N1—C5	176.2 (3)	N3—C11—C12—C13	−1.1 (6)
N2—RU1—N1—C5	−1.6 (3)	C10—C11—C12—C13	177.8 (4)
N4—RU1—N1—C5	97.7 (3)	C11—C12—C13—C14	0.4 (7)
N6—RU1—N1—C5	−104.4 (3)	C12—C13—C14—C15	0.9 (7)
N3—RU1—N1—C5	1.3 (5)	C11—N3—C15—C14	0.9 (6)
N4—RU1—N2—C6	−81.4 (3)	RU1—N3—C15—C14	−179.1 (3)
N1—RU1—N2—C6	3.2 (3)	C13—C14—C15—N3	−1.6 (7)
N6—RU1—N2—C6	98.3 (3)	C9—C8—C16—C17	−138.5 (4)
N3—RU1—N2—C6	−175.7 (3)	C7—C8—C16—C17	40.2 (5)
N4—RU1—N2—C10	93.4 (3)	C9—C8—C16—C21	41.1 (5)
N1—RU1—N2—C10	177.9 (3)	C7—C8—C16—C21	−140.3 (4)
N6—RU1—N2—C10	−87.0 (3)	C21—C16—C17—C18	1.3 (5)

N3—RU1—N2—C10	−0.9 (3)	C8—C16—C17—C18	−179.2 (3)
N5—RU1—N3—C15	1.9 (4)	C16—C17—C18—C19	−0.2 (6)
N2—RU1—N3—C15	179.7 (4)	C16—C17—C18—BR1	−178.8 (3)
N4—RU1—N3—C15	82.1 (4)	C17—C18—C19—C20	−1.2 (5)
N1—RU1—N3—C15	176.7 (3)	BR1—C18—C19—C20	177.4 (3)
N6—RU1—N3—C15	−76.0 (4)	C18—C19—C20—C21	1.6 (6)
N5—RU1—N3—C11	−178.1 (3)	C18—C19—C20—BR2	−179.5 (3)
N2—RU1—N3—C11	−0.4 (3)	C19—C20—C21—C16	−0.6 (5)
N4—RU1—N3—C11	−97.9 (3)	BR2—C20—C21—C16	−179.5 (3)
N1—RU1—N3—C11	−3.3 (5)	C17—C16—C21—C20	−0.9 (5)
N6—RU1—N3—C11	104.0 (3)	C8—C16—C21—C20	179.5 (3)
N5—RU1—N4—C22	179.8 (3)	C26—N4—C22—C23	−3.0 (5)
N2—RU1—N4—C22	−2.2 (3)	RU1—N4—C22—C23	169.1 (3)
N1—RU1—N4—C22	−80.5 (3)	N4—C22—C23—C24	1.0 (6)
N6—RU1—N4—C22	178.7 (3)	C22—C23—C24—C25	0.9 (6)
N3—RU1—N4—C22	77.3 (3)	C23—C24—C25—C26	−0.8 (5)
N5—RU1—N4—C26	−7.7 (2)	C22—N4—C26—C25	3.1 (5)
N2—RU1—N4—C26	170.2 (2)	RU1—N4—C26—C25	−170.0 (3)
N1—RU1—N4—C26	91.9 (2)	C22—N4—C26—C27	−176.9 (3)
N6—RU1—N4—C26	−8.9 (5)	RU1—N4—C26—C27	10.0 (4)
N3—RU1—N4—C26	−110.3 (2)	C24—C25—C26—N4	−1.3 (5)
N4—RU1—N5—C27	4.3 (3)	C24—C25—C26—C27	178.8 (3)
N1—RU1—N5—C27	−80.2 (3)	C31—N5—C27—C28	3.0 (5)
N6—RU1—N5—C27	−176.2 (3)	RU1—N5—C27—C28	−178.8 (3)
N3—RU1—N5—C27	97.8 (3)	C31—N5—C27—C26	−178.4 (3)
N4—RU1—N5—C31	−177.5 (3)	RU1—N5—C27—C26	−0.2 (4)
N1—RU1—N5—C31	98.0 (3)	N4—C26—C27—N5	−6.6 (4)
N6—RU1—N5—C31	2.1 (3)	C25—C26—C27—N5	173.3 (3)
N3—RU1—N5—C31	−84.0 (3)	N4—C26—C27—C28	171.9 (3)
N5—RU1—N6—C36	−177.3 (3)	C25—C26—C27—C28	−8.2 (6)
N2—RU1—N6—C36	4.7 (3)	N5—C27—C28—C29	−0.4 (5)
N4—RU1—N6—C36	−176.2 (3)	C26—C27—C28—C29	−178.8 (3)
N1—RU1—N6—C36	85.2 (3)	C27—C28—C29—C30	−1.7 (5)
N3—RU1—N6—C36	−73.4 (3)	C27—C28—C29—C37	176.8 (3)
N5—RU1—N6—C32	−2.0 (2)	C28—C29—C30—C31	1.3 (5)
N2—RU1—N6—C32	−179.9 (2)	C37—C29—C30—C31	−177.3 (3)
N4—RU1—N6—C32	−0.8 (4)	C27—N5—C31—C30	−3.4 (5)
N1—RU1—N6—C32	−99.5 (2)	RU1—N5—C31—C30	178.4 (3)
N3—RU1—N6—C32	101.9 (2)	C27—N5—C31—C32	176.4 (3)
C5—N1—C1—C2	2.6 (6)	RU1—N5—C31—C32	−1.8 (4)
RU1—N1—C1—C2	178.8 (3)	C29—C30—C31—N5	1.2 (5)
N1—C1—C2—C3	−1.0 (7)	C29—C30—C31—C32	−178.6 (4)
C1—C2—C3—C4	−0.7 (7)	C36—N6—C32—C33	−2.0 (5)
C2—C3—C4—C5	0.7 (6)	RU1—N6—C32—C33	−177.8 (3)
C1—N1—C5—C4	−2.5 (6)	C36—N6—C32—C31	177.5 (3)
RU1—N1—C5—C4	−179.3 (3)	RU1—N6—C32—C31	1.6 (4)
C1—N1—C5—C6	176.9 (3)	N5—C31—C32—N6	0.0 (4)
RU1—N1—C5—C6	0.1 (4)	C30—C31—C32—N6	179.8 (3)
C3—C4—C5—N1	0.9 (6)	N5—C31—C32—C33	179.5 (3)

C3—C4—C5—C6	−178.5 (4)	C30—C31—C32—C33	−0.8 (6)
C10—N2—C6—C7	−0.9 (6)	N6—C32—C33—C34	1.9 (5)
RU1—N2—C6—C7	173.8 (3)	C31—C32—C33—C34	−177.5 (3)
C10—N2—C6—C5	−178.6 (3)	C32—C33—C34—C35	−0.3 (6)
RU1—N2—C6—C5	−4.0 (4)	C33—C34—C35—C36	−1.2 (5)
N1—C5—C6—N2	2.4 (5)	C32—N6—C36—C35	0.5 (5)
C4—C5—C6—N2	−178.2 (4)	RU1—N6—C36—C35	175.7 (3)
N1—C5—C6—C7	−175.2 (4)	C34—C35—C36—N6	1.1 (5)
C4—C5—C6—C7	4.2 (6)	C28—C29—C37—C42	−139.9 (4)
N2—C6—C7—C8	0.6 (6)	C30—C29—C37—C42	38.6 (5)
C5—C6—C7—C8	178.0 (4)	C28—C29—C37—C38	40.8 (5)
C6—C7—C8—C9	0.5 (6)	C30—C29—C37—C38	−140.6 (4)
C6—C7—C8—C16	−178.2 (4)	C42—C37—C38—C39	−0.8 (5)
C7—C8—C9—C10	−1.3 (6)	C29—C37—C38—C39	178.4 (3)
C16—C8—C9—C10	177.4 (4)	C37—C38—C39—C40	0.3 (6)
C6—N2—C10—C9	0.0 (6)	C37—C38—C39—BR3	−177.1 (3)
RU1—N2—C10—C9	−174.6 (3)	C38—C39—C40—C41	0.3 (6)
C6—N2—C10—C11	176.6 (3)	BR3—C39—C40—C41	177.7 (3)
RU1—N2—C10—C11	2.0 (4)	C39—C40—C41—C42	−0.5 (6)
C8—C9—C10—N2	1.1 (6)	C39—C40—C41—BR4	−179.2 (3)
C8—C9—C10—C11	−175.0 (4)	C40—C41—C42—C37	0.0 (6)
C15—N3—C11—C12	0.4 (6)	BR4—C41—C42—C37	178.8 (3)
RU1—N3—C11—C12	−179.6 (3)	C38—C37—C42—C41	0.7 (5)
C15—N3—C11—C10	−178.5 (4)	C29—C37—C42—C41	−178.6 (3)

Fig. 1

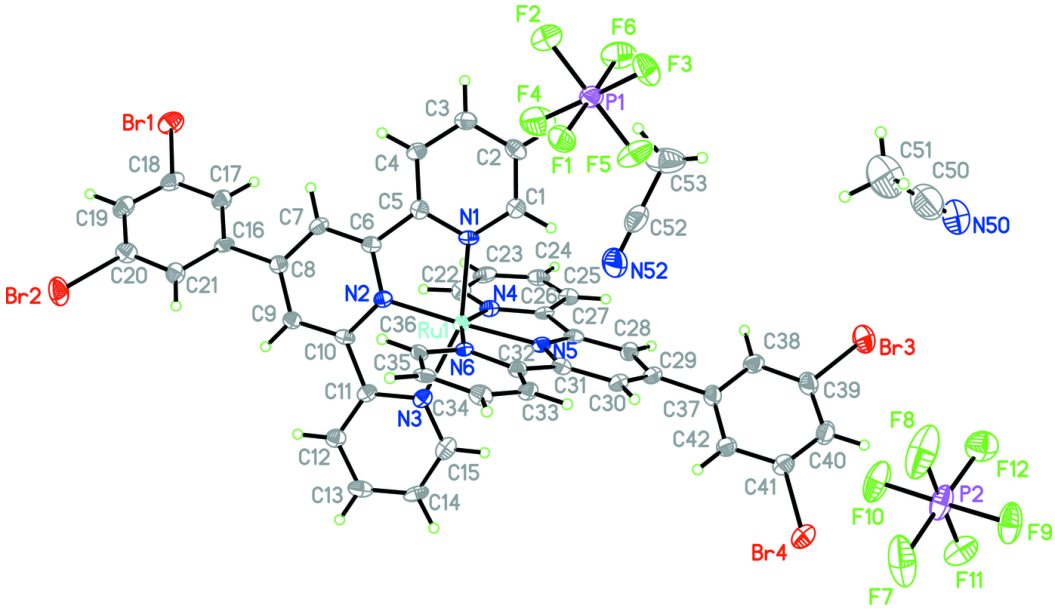
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Fig. 2