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Bis(2-phenyl-4,6-di-2-pyridyl-1,3,5-triazine-κ^3N^4,N^5,N^6)ruthenium(II) bis(hexafluoridophosphate)

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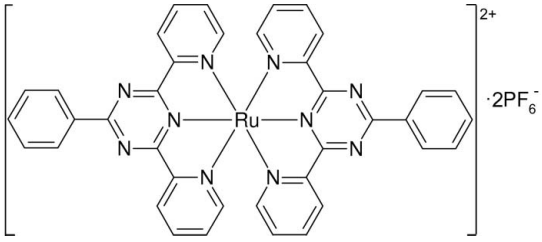
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.066; data-to-parameter ratio = 14.3.

The asymmetric unit of the title compound, $[Ru(C_{19}H_{13}N_5)_2](PF_6)_2$, consists of an Ru^{II} complex cation and two hexafluoridophosphate anions. The Ru^{II} atom is coordinated by three N atoms from the two outer pyridine and the central triazine rings of each of two tridentate ligands in a distorted octahedral environment. The ligands are approximately orthogonal to one another, with a dihedral angle of 88.34 (2)° between planes through the three six-membered rings of the two ligands. The pendant phenyl substituents are almost coplanar with the triazine rings to which they are bound, with dihedral angles of 5.41 (9) and 14.90 (10)°. This is reflected in the previously reported photophysical results with an increased lifetime of the triplet metal to ligand charge transfer (^{3}MLCT) excited state [Fang, Taylor, Hanan, Loiseau, Passalacqua, Campagna, Nierengarten & Van Dorsselaer (2002). *J. Am. Chem. Soc.* **124**, 7912–7913].

Related literature

For related synthetic details, see: Polson *et al.* (2002, 2004). For related structures, see: Polson *et al.* (2002). For general background on the photophysics of ruthenium polypyridyl complexes, see: Kalyanasundaram (1991); Barigelletti *et al.* (1995). For background on C—H···N interactions in α-diimines, see: Fitchett *et al.* (2005). For related literature, see: Beley *et al.* (1991); Fang *et al.* (2002).



Experimental

Crystal data

$[Ru(C_{19}H_{13}N_5)_2](PF_6)_2$
M_r = 1013.70
Monoclinic, $P2_1/n$
a = 9.0995 (3) Å
b = 32.5979 (11) Å
c = 13.1451 (5) Å
β = 91.774 (2)°
V = 3897.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 93 (2) K
0.30 × 0.13 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.822, T_{max} = 0.950
75901 measured reflections
8114 independent reflections
6511 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.066
S = 0.99
8114 reflections
568 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—N10	2.0982 (16)	Ru1—N50	2.0967 (16)
Ru1—N20	1.9773 (15)	Ru1—N60	1.9723 (15)
Ru1—N30	2.0990 (16)	Ru1—N70	2.0939 (17)
N10—Ru1—N30	154.76 (6)	N50—Ru1—N30	92.35 (6)
N60—Ru1—N20	179.28 (7)	N60—Ru1—N50	77.85 (6)
N70—Ru1—N50	155.22 (6)	N60—Ru1—N70	77.42 (6)
N20—Ru1—N70	103.31 (6)	N60—Ru1—N10	102.25 (6)
N20—Ru1—N50	101.42 (6)	N60—Ru1—N30	102.98 (6)
N20—Ru1—N10	77.77 (6)	N70—Ru1—N10	91.67 (6)
N20—Ru1—N30	77.00 (6)	N70—Ru1—N30	94.71 (6)
N50—Ru1—N10	91.99 (6)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C41—H41···N21	0.95	2.47	2.793 (3)	100
C45—H45···N22	0.95	2.52	2.826 (3)	99
C81—H81···N61	0.95	2.47	2.797 (2)	100
C85—H85···N62	0.95	2.50	2.823 (3)	100

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2423).

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supplementary materials

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Bis(2-phenyl-4,6-di-2-pyridyl-1,3,5-triazine-κ^3N^4,N^5,N^6)ruthenium(II) bis(hexafluoridophosphate)

M. I. J. Polson and G. S. Hanan

Comment

The structure of the title compound reveals the ruthenium(II) atom to be in a distorted octahedral environment, Table 1. The Ru—N bond lengths to the central triazine ring are significantly shortened when compared to those of the outer pyridine rings. The angles between the coordinating pyridine N atoms also deviate significantly from 180 ° indicating considerable distortion.

Ruthenium complexes of this type have long been known to exhibit surprisingly short lived excited states. This is due to rapid deactivation of the excited state through a low lying metal centred state (Kalyanasundaram, 1991; Barigelletti *et al.*, 1995). By lowering the energy of the triplet metal to ligand charge transfer ^{3}MLCT state, this exchange can be slowed and the lifetime of the excited state is extended (Fang *et al.*, 2002). In the title compound (1) replacement of a the central pyridine ring with a triazine ring in complex with a 4-phenyl substituent allows the pendant phenyl ring to adopt an arrangement in which it is approximately co-planar with the rest of the ligand. This results from the removal of stericically conflicting C—H···H—C interactions and the addition of attractive intramolecular C—H···N interactions. Although the C—H···N angles are acute (approximately 100 °) they are typical of interactions in molecules of this kind (Fitchett *et al.*, 2005) with N···H lengths of 2.47 to 2.52 Å, Table 2. The greater overall planarity of the ligands extends the HOMO orbital (predominately π^* in nature) over more of the ligand surface, decreasing the energy of the ^{3}MLCT state (Beley *et al.*, 1991; Polson *et al.*, 2002).

Experimental

The complex was prepared as described by Polson *et al.* (2004). Crystals suitable for X-ray crystallography were prepared by the diffusion of diisopropyl ether into an acetonitrile solution of the complex over a week.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C).

Figures

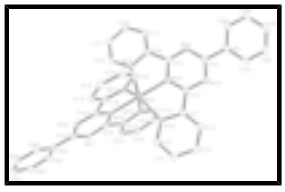


Fig. 1. The molecular structure of (1), showing displacement ellipsoids at the 50% probability level. All H atoms have been omitted for clarity.

Bis(2-phenyl-4,6-di-2-pyridyl-1,3,5-triazine- κ^3N^4,N^5,N^6)ruthenium(II) bis(hexafluoridophosphate)

Crystal data

$[Ru(C_{19}H_{13}N_5)_2](PF_6)_2$	F_{000} = 2024
M_r = 1013.70	D_x = 1.728 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7650 reflections
a = 9.0995 (3) Å	θ = 4.7–53.0º
b = 32.5979 (11) Å	μ = 0.59 mm^{-1}
c = 13.1451 (5) Å	T = 93 (2) K
β = 91.774 (2)º	Needle, red
V = 3897.3 (2) Å^3	0.30 × 0.13 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	8114 independent reflections
Radiation source: sealed tube	6511 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 93(2) K	θ_{max} = 26.6º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 2007)	h = −11→11
T_{min} = 0.822, T_{max} = 0.950	k = −40→40
75901 measured reflections	l = −16→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.066	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.5007P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
8114 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
568 parameters	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Ru1	0.511004 (17)	0.118305 (4)	0.711838 (12)	0.01108 (5)
N10	0.71581 (17)	0.12419 (5)	0.64422 (12)	0.0136 (4)
C10	0.8068 (2)	0.09472 (6)	0.61281 (16)	0.0179 (5)
H10	0.7805	0.0669	0.6231	0.021*
C11	0.9375 (2)	0.10327 (6)	0.56596 (17)	0.0232 (5)
H11	0.9978	0.0815	0.5433	0.028*
C12	0.9798 (2)	0.14335 (6)	0.55231 (17)	0.0240 (5)
H12	1.0700	0.1496	0.5212	0.029*
C13	0.8884 (2)	0.17461 (6)	0.58476 (16)	0.0192 (5)
H13	0.9150	0.2026	0.5765	0.023*
C14	0.7588 (2)	0.16422 (5)	0.62909 (15)	0.0141 (4)
N20	0.53678 (17)	0.17849 (5)	0.70707 (12)	0.0123 (3)
N21	0.67356 (18)	0.23500 (5)	0.65306 (13)	0.0158 (4)
N22	0.44719 (18)	0.24472 (5)	0.73807 (12)	0.0148 (4)
C20	0.6545 (2)	0.19520 (6)	0.66416 (15)	0.0137 (4)
C21	0.5662 (2)	0.25871 (6)	0.69099 (15)	0.0147 (4)
C22	0.4357 (2)	0.20427 (6)	0.74240 (15)	0.0132 (4)
N30	0.31752 (18)	0.14032 (5)	0.77547 (12)	0.0130 (3)
C30	0.2009 (2)	0.11839 (6)	0.80597 (16)	0.0177 (4)
H30	0.2042	0.0893	0.8016	0.021*
C31	0.0766 (2)	0.13690 (6)	0.84348 (17)	0.0220 (5)
H31	−0.0040	0.1205	0.8633	0.026*
C32	0.0698 (2)	0.17918 (6)	0.85204 (17)	0.0221 (5)
H32	−0.0141	0.1921	0.8790	0.027*
C33	0.1878 (2)	0.20221 (6)	0.82050 (15)	0.0180 (4)
H33	0.1858	0.2313	0.8247	0.022*
C34	0.3083 (2)	0.18235 (6)	0.78291 (15)	0.0133 (4)
C40	0.5820 (2)	0.30342 (6)	0.67733 (16)	0.0172 (4)
C41	0.6825 (2)	0.31883 (6)	0.60975 (17)	0.0223 (5)
H41	0.7451	0.3007	0.5747	0.027*
C42	0.6911 (3)	0.36089 (6)	0.59355 (18)	0.0268 (5)
H42	0.7585	0.3715	0.5464	0.032*
C43	0.6018 (3)	0.38746 (6)	0.64602 (18)	0.0263 (5)

H43	0.6081	0.4162	0.6349	0.032*
C44	0.5033 (2)	0.37218 (6)	0.71460 (18)	0.0237 (5)
H44	0.4433	0.3905	0.7513	0.028*
C45	0.4920 (2)	0.33042 (6)	0.72995 (17)	0.0207 (5)
H45	0.4232	0.3200	0.7763	0.025*
N50	0.40436 (17)	0.10703 (5)	0.57094 (12)	0.0124 (3)
C50	0.3662 (2)	0.13390 (6)	0.49749 (15)	0.0141 (4)
H50	0.3903	0.1620	0.5073	0.017*
C51	0.2932 (2)	0.12242 (6)	0.40811 (16)	0.0162 (4)
H51	0.2681	0.1424	0.3579	0.019*
C52	0.2572 (2)	0.08161 (6)	0.39243 (16)	0.0172 (4)
H52	0.2063	0.0732	0.3318	0.021*
C53	0.2965 (2)	0.05329 (6)	0.46646 (15)	0.0161 (4)
H53	0.2732	0.0251	0.4572	0.019*
C54	0.3700 (2)	0.06633 (5)	0.55407 (15)	0.0120 (4)
N60	0.48400 (17)	0.05829 (5)	0.71489 (12)	0.0129 (3)
N61	0.40078 (18)	−0.00188 (5)	0.63404 (12)	0.0143 (4)
N62	0.51801 (18)	−0.00465 (5)	0.79959 (13)	0.0147 (4)
C60	0.4180 (2)	0.03841 (6)	0.63663 (15)	0.0137 (4)
C61	0.4496 (2)	−0.02227 (6)	0.71801 (15)	0.0148 (4)
C62	0.5347 (2)	0.03559 (6)	0.79454 (15)	0.0143 (4)
N70	0.61068 (17)	0.10207 (5)	0.85180 (12)	0.0136 (4)
C70	0.6809 (2)	0.12700 (6)	0.91947 (15)	0.0158 (4)
H70	0.6798	0.1557	0.9076	0.019*
C71	0.7543 (2)	0.11210 (6)	1.00527 (16)	0.0187 (4)
H71	0.8037	0.1305	1.0508	0.022*
C72	0.7560 (2)	0.07045 (6)	1.02492 (16)	0.0197 (5)
H72	0.8068	0.0599	1.0835	0.024*
C73	0.6820 (2)	0.04436 (6)	0.95750 (16)	0.0173 (4)
H73	0.6803	0.0156	0.9695	0.021*
C74	0.6111 (2)	0.06077 (6)	0.87298 (15)	0.0145 (4)
C80	0.4271 (2)	−0.06706 (6)	0.71991 (15)	0.0155 (4)
C81	0.3459 (2)	−0.08622 (6)	0.64177 (16)	0.0194 (5)
H81	0.3037	−0.0703	0.5878	0.023*
C82	0.3265 (2)	−0.12824 (6)	0.64252 (18)	0.0236 (5)
H82	0.2722	−0.1411	0.5886	0.028*
C83	0.3860 (2)	−0.15176 (6)	0.72169 (18)	0.0237 (5)
H83	0.3720	−0.1806	0.7221	0.028*
C84	0.4651 (2)	−0.13302 (6)	0.79949 (17)	0.0227 (5)
H84	0.5049	−0.1490	0.8541	0.027*
C85	0.4873 (2)	−0.09084 (6)	0.79877 (16)	0.0197 (5)
H85	0.5435	−0.0782	0.8522	0.024*
P10	0.21119 (6)	0.252045 (16)	0.48554 (4)	0.02011 (13)
F10	0.18421 (15)	0.22740 (4)	0.58837 (10)	0.0386 (4)
F11	0.26219 (15)	0.29172 (4)	0.54874 (10)	0.0327 (3)
F12	0.04573 (14)	0.26820 (4)	0.48256 (10)	0.0362 (3)
F13	0.23965 (14)	0.27617 (3)	0.38108 (9)	0.0250 (3)
F14	0.16179 (15)	0.21244 (4)	0.42100 (10)	0.0339 (3)
F15	0.37791 (14)	0.23611 (4)	0.48793 (11)	0.0353 (3)

P20	0.01052 (6)	0.008488 (16)	0.76644 (5)	0.02301 (14)
F20	−0.05493 (16)	−0.01201 (4)	0.86490 (11)	0.0395 (4)
F21	−0.04478 (14)	0.05249 (3)	0.80299 (10)	0.0278 (3)
F22	−0.14343 (15)	0.00207 (4)	0.70590 (11)	0.0369 (4)
F23	0.07743 (16)	0.02936 (4)	0.66771 (11)	0.0399 (4)
F24	0.06484 (16)	−0.03543 (4)	0.72907 (12)	0.0396 (4)
F25	0.16550 (15)	0.01533 (4)	0.82574 (13)	0.0452 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01126 (9)	0.00884 (8)	0.01317 (9)	−0.00001 (6)	0.00056 (6)	−0.00003 (6)
N10	0.0122 (9)	0.0126 (8)	0.0159 (9)	0.0005 (6)	−0.0007 (7)	0.0005 (7)
C10	0.0173 (11)	0.0149 (10)	0.0214 (12)	0.0028 (8)	−0.0001 (9)	0.0018 (8)
C11	0.0189 (12)	0.0222 (11)	0.0288 (13)	0.0087 (9)	0.0053 (10)	0.0020 (9)
C12	0.0129 (11)	0.0274 (12)	0.0320 (14)	0.0020 (9)	0.0074 (10)	0.0044 (10)
C13	0.0155 (11)	0.0182 (10)	0.0240 (12)	−0.0028 (8)	0.0010 (9)	0.0028 (9)
C14	0.0149 (11)	0.0135 (9)	0.0135 (11)	−0.0004 (8)	−0.0032 (8)	−0.0011 (8)
N20	0.0124 (9)	0.0125 (8)	0.0120 (9)	−0.0001 (6)	−0.0015 (7)	−0.0014 (6)
N21	0.0170 (9)	0.0124 (8)	0.0178 (10)	−0.0018 (7)	−0.0025 (7)	−0.0012 (7)
N22	0.0182 (9)	0.0106 (8)	0.0153 (9)	0.0016 (7)	−0.0031 (7)	−0.0012 (7)
C20	0.0127 (10)	0.0152 (10)	0.0130 (11)	−0.0019 (8)	−0.0031 (8)	−0.0006 (8)
C21	0.0166 (11)	0.0133 (9)	0.0140 (11)	−0.0020 (8)	−0.0047 (8)	−0.0014 (8)
C22	0.0112 (10)	0.0144 (9)	0.0136 (11)	0.0006 (8)	−0.0033 (8)	−0.0012 (8)
N30	0.0139 (9)	0.0137 (8)	0.0114 (9)	−0.0001 (7)	−0.0002 (7)	−0.0005 (6)
C30	0.0181 (11)	0.0163 (10)	0.0189 (11)	−0.0040 (8)	0.0010 (9)	−0.0006 (8)
C31	0.0174 (12)	0.0256 (11)	0.0234 (13)	−0.0048 (9)	0.0069 (9)	−0.0032 (9)
C32	0.0176 (11)	0.0258 (11)	0.0233 (13)	0.0045 (9)	0.0055 (9)	−0.0038 (9)
C33	0.0198 (11)	0.0168 (10)	0.0174 (11)	0.0017 (8)	0.0010 (9)	−0.0008 (8)
C34	0.0149 (10)	0.0131 (9)	0.0116 (10)	−0.0011 (8)	−0.0022 (8)	0.0004 (8)
C40	0.0189 (11)	0.0118 (9)	0.0203 (12)	−0.0021 (8)	−0.0091 (9)	0.0007 (8)
C41	0.0276 (13)	0.0157 (10)	0.0233 (13)	−0.0021 (9)	−0.0030 (10)	−0.0006 (9)
C42	0.0321 (14)	0.0194 (11)	0.0283 (14)	−0.0084 (10)	−0.0078 (11)	0.0061 (9)
C43	0.0321 (14)	0.0129 (10)	0.0329 (14)	−0.0011 (9)	−0.0184 (11)	0.0019 (9)
C44	0.0225 (12)	0.0155 (10)	0.0326 (14)	0.0019 (9)	−0.0093 (10)	−0.0031 (9)
C45	0.0195 (12)	0.0162 (10)	0.0260 (13)	−0.0004 (8)	−0.0067 (9)	−0.0020 (9)
N50	0.0096 (8)	0.0120 (8)	0.0156 (9)	0.0008 (6)	0.0028 (7)	−0.0017 (6)
C50	0.0124 (10)	0.0136 (9)	0.0164 (11)	0.0022 (8)	0.0038 (8)	0.0010 (8)
C51	0.0140 (10)	0.0165 (10)	0.0182 (11)	0.0045 (8)	0.0019 (8)	0.0029 (8)
C52	0.0164 (11)	0.0210 (10)	0.0143 (11)	0.0026 (8)	0.0006 (9)	−0.0026 (8)
C53	0.0138 (10)	0.0142 (9)	0.0202 (12)	0.0006 (8)	0.0016 (9)	−0.0032 (8)
C54	0.0087 (10)	0.0133 (9)	0.0142 (11)	0.0018 (7)	0.0041 (8)	−0.0002 (8)
N60	0.0119 (9)	0.0139 (8)	0.0128 (9)	0.0010 (6)	0.0019 (7)	0.0000 (7)
N61	0.0152 (9)	0.0123 (8)	0.0154 (9)	0.0002 (7)	0.0028 (7)	0.0004 (7)
N62	0.0139 (9)	0.0123 (8)	0.0180 (10)	−0.0002 (6)	0.0026 (7)	0.0007 (7)
C60	0.0100 (10)	0.0145 (9)	0.0168 (11)	−0.0007 (8)	0.0033 (8)	−0.0020 (8)
C61	0.0127 (10)	0.0142 (9)	0.0177 (11)	0.0010 (8)	0.0047 (8)	0.0004 (8)
C62	0.0114 (10)	0.0148 (9)	0.0171 (11)	0.0019 (8)	0.0032 (8)	0.0028 (8)

N70	0.0125 (9)	0.0119 (8)	0.0166 (9)	−0.0002 (7)	0.0021 (7)	−0.0002 (7)
C70	0.0156 (11)	0.0142 (10)	0.0177 (11)	−0.0022 (8)	0.0016 (9)	−0.0021 (8)
C71	0.0185 (11)	0.0209 (11)	0.0165 (11)	−0.0018 (9)	−0.0016 (9)	−0.0021 (8)
C72	0.0212 (12)	0.0219 (10)	0.0160 (12)	0.0020 (9)	−0.0003 (9)	0.0026 (9)
C73	0.0180 (11)	0.0146 (10)	0.0194 (12)	−0.0006 (8)	0.0024 (9)	0.0024 (8)
C74	0.0140 (10)	0.0142 (9)	0.0154 (11)	0.0001 (8)	0.0040 (8)	0.0005 (8)
C80	0.0138 (11)	0.0124 (9)	0.0208 (12)	0.0015 (8)	0.0069 (9)	0.0002 (8)
C81	0.0175 (11)	0.0166 (10)	0.0242 (12)	0.0018 (8)	0.0020 (9)	0.0008 (9)
C82	0.0228 (12)	0.0163 (10)	0.0318 (14)	−0.0018 (9)	0.0008 (10)	−0.0053 (9)
C83	0.0224 (12)	0.0108 (10)	0.0382 (15)	−0.0009 (9)	0.0062 (10)	0.0008 (9)
C84	0.0247 (13)	0.0158 (10)	0.0280 (14)	0.0038 (9)	0.0044 (10)	0.0068 (9)
C85	0.0194 (11)	0.0171 (10)	0.0228 (13)	−0.0001 (9)	0.0034 (9)	0.0005 (9)
P10	0.0221 (3)	0.0165 (3)	0.0213 (3)	−0.0062 (2)	−0.0066 (2)	0.0052 (2)
F10	0.0444 (9)	0.0439 (8)	0.0267 (8)	−0.0221 (7)	−0.0129 (7)	0.0191 (6)
F11	0.0482 (9)	0.0203 (6)	0.0289 (8)	−0.0060 (6)	−0.0121 (7)	−0.0017 (6)
F12	0.0238 (8)	0.0526 (9)	0.0321 (8)	0.0031 (6)	−0.0023 (6)	0.0042 (7)
F13	0.0325 (8)	0.0205 (6)	0.0221 (7)	−0.0048 (5)	−0.0007 (6)	0.0061 (5)
F14	0.0488 (9)	0.0168 (6)	0.0350 (8)	−0.0108 (6)	−0.0161 (7)	0.0028 (6)
F15	0.0278 (8)	0.0266 (7)	0.0510 (9)	0.0031 (6)	−0.0085 (7)	0.0075 (6)
P20	0.0197 (3)	0.0132 (3)	0.0362 (4)	0.0013 (2)	0.0028 (3)	0.0045 (2)
F20	0.0471 (9)	0.0261 (7)	0.0462 (9)	0.0023 (6)	0.0159 (7)	0.0127 (6)
F21	0.0287 (7)	0.0152 (6)	0.0396 (8)	−0.0012 (5)	0.0023 (6)	−0.0028 (5)
F22	0.0330 (8)	0.0214 (7)	0.0556 (10)	−0.0009 (6)	−0.0114 (7)	−0.0082 (6)
F23	0.0446 (9)	0.0280 (7)	0.0483 (10)	0.0128 (6)	0.0215 (7)	0.0156 (7)
F24	0.0415 (9)	0.0165 (6)	0.0616 (10)	0.0101 (6)	0.0152 (7)	0.0042 (6)
F25	0.0277 (8)	0.0321 (8)	0.0746 (12)	−0.0004 (6)	−0.0156 (8)	0.0129 (8)

Geometric parameters (Å, °)

Ru1—N10	2.0982 (16)	C50—H50	0.9500
Ru1—N20	1.9773 (15)	C51—C52	1.384 (3)
Ru1—N30	2.0990 (16)	C51—H51	0.9500
Ru1—N50	2.0967 (16)	C52—C53	1.380 (3)
Ru1—N60	1.9723 (15)	C52—H52	0.9500
Ru1—N70	2.0939 (17)	C53—C54	1.381 (3)
N10—C10	1.342 (2)	C53—H53	0.9500
N10—C14	1.378 (2)	C54—C60	1.472 (3)
C10—C11	1.385 (3)	N60—C60	1.342 (2)
C10—H10	0.9500	N60—C62	1.351 (2)
C11—C12	1.375 (3)	N61—C60	1.323 (2)
C11—H11	0.9500	N61—C61	1.352 (2)
C12—C13	1.390 (3)	N62—C62	1.323 (2)
C12—H12	0.9500	N62—C61	1.351 (3)
C13—C14	1.374 (3)	C61—C80	1.475 (3)
C13—H13	0.9500	C62—C74	1.475 (3)
C14—C20	1.470 (3)	N70—C70	1.351 (2)
N20—C22	1.340 (2)	N70—C74	1.375 (2)
N20—C20	1.341 (2)	C70—C71	1.381 (3)
N21—C20	1.318 (2)	C70—H70	0.9500

N21—C21	1.353 (3)	C71—C72	1.382 (3)
N22—C22	1.324 (2)	C71—H71	0.9500
N22—C21	1.344 (3)	C72—C73	1.388 (3)
C21—C40	1.476 (3)	C72—H72	0.9500
C22—C34	1.475 (3)	C73—C74	1.376 (3)
N30—C30	1.351 (2)	C73—H73	0.9500
N30—C34	1.376 (2)	C80—C85	1.393 (3)
C30—C31	1.386 (3)	C80—C81	1.394 (3)
C30—H30	0.9500	C81—C82	1.381 (3)
C31—C32	1.384 (3)	C81—H81	0.9500
C31—H31	0.9500	C82—C83	1.389 (3)
C32—C33	1.385 (3)	C82—H82	0.9500
C32—H32	0.9500	C83—C84	1.376 (3)
C33—C34	1.378 (3)	C83—H83	0.9500
C33—H33	0.9500	C84—C85	1.390 (3)
C40—C41	1.388 (3)	C84—H84	0.9500
C40—C45	1.400 (3)	C85—H85	0.9500
C41—C42	1.390 (3)	P10—F12	1.5943 (14)
C41—H41	0.9500	P10—F10	1.5980 (13)
C42—C43	1.386 (3)	P10—F11	1.5981 (13)
C42—H42	0.9500	P10—F14	1.6015 (13)
C43—C44	1.383 (3)	P10—F15	1.6029 (14)
C43—H43	0.9500	P10—F13	1.6104 (13)
C44—C45	1.380 (3)	P20—F20	1.5887 (14)
C44—H44	0.9500	P20—F24	1.5970 (13)
C45—H45	0.9500	P20—F21	1.5988 (13)
N50—C50	1.341 (2)	P20—F23	1.6022 (14)
N50—C54	1.380 (2)	P20—F22	1.6033 (15)
C50—C51	1.383 (3)	P20—F25	1.6056 (15)
N10—Ru1—N30	154.76 (6)	C52—C51—H51	120.3
N60—Ru1—N20	179.28 (7)	C53—C52—C51	118.88 (19)
N70—Ru1—N50	155.22 (6)	C53—C52—H52	120.6
N20—Ru1—N70	103.31 (6)	C51—C52—H52	120.6
N20—Ru1—N50	101.42 (6)	C52—C53—C54	119.35 (18)
N20—Ru1—N10	77.77 (6)	C52—C53—H53	120.3
N20—Ru1—N30	77.00 (6)	C54—C53—H53	120.3
N50—Ru1—N10	91.99 (6)	N50—C54—C53	122.12 (18)
N50—Ru1—N30	92.35 (6)	N50—C54—C60	114.54 (17)
N60—Ru1—N50	77.85 (6)	C53—C54—C60	123.34 (17)
N60—Ru1—N70	77.42 (6)	C60—N60—C62	117.61 (16)
N60—Ru1—N10	102.25 (6)	C60—N60—Ru1	121.10 (13)
N60—Ru1—N30	102.98 (6)	C62—N60—Ru1	121.27 (13)
N70—Ru1—N10	91.67 (6)	C60—N61—C61	115.55 (17)
N70—Ru1—N30	94.71 (6)	C62—N62—C61	115.62 (17)
C10—N10—C14	116.93 (17)	N61—C60—N60	123.30 (18)
C10—N10—Ru1	129.03 (13)	N61—C60—C54	124.22 (18)
C14—N10—Ru1	114.03 (12)	N60—C60—C54	112.47 (16)
N10—C10—C11	122.65 (18)	N62—C61—N61	124.81 (17)
N10—C10—H10	118.7	N62—C61—C80	117.91 (18)

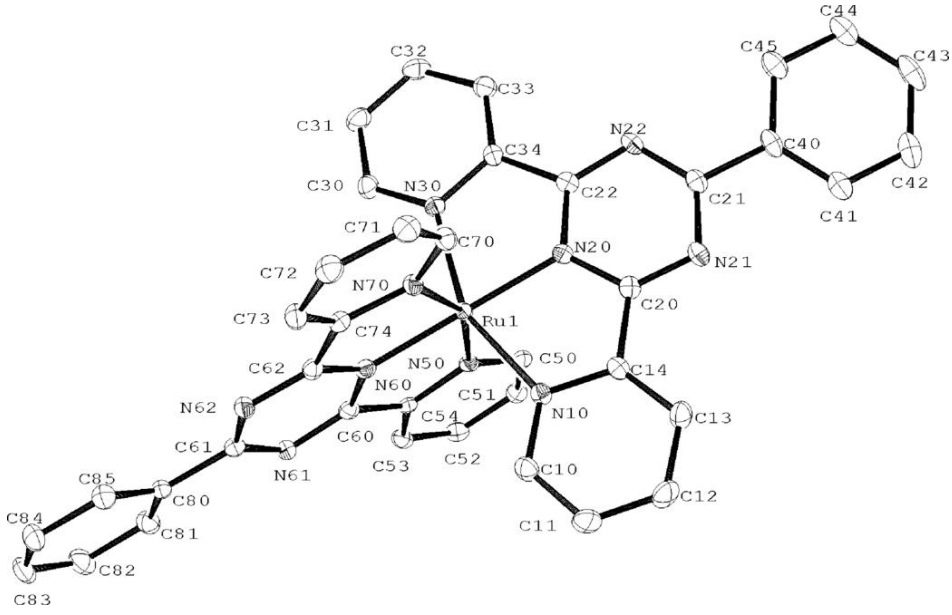
C11—C10—H10	118.7	N61—C61—C80	117.28 (18)
C12—C11—C10	119.80 (19)	N62—C62—N60	123.03 (18)
C12—C11—H11	120.1	N62—C62—C74	124.68 (18)
C10—C11—H11	120.1	N60—C62—C74	112.28 (16)
C11—C12—C13	118.93 (19)	C70—N70—C74	117.23 (17)
C11—C12—H12	120.5	C70—N70—Ru1	127.56 (13)
C13—C12—H12	120.5	C74—N70—Ru1	115.09 (13)
C14—C13—C12	118.61 (19)	N70—C70—C71	122.21 (18)
C14—C13—H13	120.7	N70—C70—H70	118.9
C12—C13—H13	120.7	C71—C70—H70	118.9
C13—C14—N10	123.06 (18)	C70—C71—C72	120.02 (19)
C13—C14—C20	122.33 (17)	C70—C71—H71	120.0
N10—C14—C20	114.62 (17)	C72—C71—H71	120.0
C22—N20—C20	117.20 (16)	C71—C72—C73	118.71 (19)
C22—N20—Ru1	121.87 (13)	C71—C72—H72	120.6
C20—N20—Ru1	120.87 (12)	C73—C72—H72	120.6
C20—N21—C21	114.99 (17)	C74—C73—C72	118.93 (18)
C22—N22—C21	115.08 (16)	C74—C73—H73	120.5
N21—C20—N20	123.77 (18)	C72—C73—H73	120.5
N21—C20—C14	123.59 (18)	C73—C74—N70	122.87 (18)
N20—C20—C14	112.63 (16)	C73—C74—C62	123.19 (17)
N22—C21—N21	125.27 (17)	N70—C74—C62	113.88 (17)
N22—C21—C40	118.31 (17)	C85—C80—C81	119.08 (18)
N21—C21—C40	116.42 (18)	C85—C80—C61	120.80 (19)
N22—C22—N20	123.61 (18)	C81—C80—C61	120.12 (18)
N22—C22—C34	124.21 (17)	C82—C81—C80	120.3 (2)
N20—C22—C34	112.13 (16)	C82—C81—H81	119.9
C30—N30—C34	117.11 (16)	C80—C81—H81	119.9
C30—N30—Ru1	127.86 (13)	C81—C82—C83	120.4 (2)
C34—N30—Ru1	114.98 (12)	C81—C82—H82	119.8
N30—C30—C31	122.18 (18)	C83—C82—H82	119.8
N30—C30—H30	118.9	C84—C83—C82	119.66 (19)
C31—C30—H30	118.9	C84—C83—H83	120.2
C32—C31—C30	120.11 (19)	C82—C83—H83	120.2
C32—C31—H31	119.9	C83—C84—C85	120.5 (2)
C30—C31—H31	119.9	C83—C84—H84	119.8
C33—C32—C31	118.56 (19)	C85—C84—H84	119.8
C33—C32—H32	120.7	C84—C85—C80	120.1 (2)
C31—C32—H32	120.7	C84—C85—H85	119.9
C34—C33—C32	119.07 (18)	C80—C85—H85	119.9
C34—C33—H33	120.5	F12—P10—F10	90.99 (8)
C32—C33—H33	120.5	F12—P10—F11	90.25 (8)
N30—C34—C33	122.95 (17)	F10—P10—F11	90.97 (7)
N30—C34—C22	114.00 (16)	F12—P10—F14	90.22 (8)
C33—C34—C22	122.99 (17)	F10—P10—F14	89.70 (7)
C41—C40—C45	119.70 (18)	F11—P10—F14	179.17 (9)
C41—C40—C21	120.25 (18)	F12—P10—F15	179.52 (9)
C45—C40—C21	120.01 (19)	F10—P10—F15	89.46 (8)
C40—C41—C42	119.8 (2)	F11—P10—F15	89.57 (7)

C40—C41—H41	120.1	F14—P10—F15	89.95 (8)
C42—C41—H41	120.1	F12—P10—F13	89.68 (7)
C43—C42—C41	120.2 (2)	F10—P10—F13	178.99 (8)
C43—C42—H42	119.9	F11—P10—F13	89.79 (7)
C41—C42—H42	119.9	F14—P10—F13	89.53 (7)
C44—C43—C42	120.07 (19)	F15—P10—F13	89.87 (7)
C44—C43—H43	120.0	F20—P20—F24	90.05 (7)
C42—C43—H43	120.0	F20—P20—F21	90.18 (7)
C45—C44—C43	120.2 (2)	F24—P20—F21	179.50 (9)
C45—C44—H44	119.9	F20—P20—F23	179.55 (10)
C43—C44—H44	119.9	F24—P20—F23	90.15 (7)
C44—C45—C40	120.0 (2)	F21—P20—F23	89.63 (7)
C44—C45—H45	120.0	F20—P20—F22	90.33 (8)
C40—C45—H45	120.0	F24—P20—F22	90.25 (8)
C50—N50—C54	117.38 (17)	F21—P20—F22	89.31 (7)
C50—N50—Ru1	128.60 (13)	F23—P20—F22	90.08 (8)
C54—N50—Ru1	114.01 (13)	F20—P20—F25	90.50 (9)
N50—C50—C51	122.80 (18)	F24—P20—F25	89.90 (8)
N50—C50—H50	118.6	F21—P20—F25	90.54 (7)
C51—C50—H50	118.6	F23—P20—F25	89.10 (9)
C50—C51—C52	119.45 (19)	F22—P20—F25	179.16 (9)
C50—C51—H51	120.3		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C41—H41···N21	0.95	2.47	2.793 (3)	100
C45—H45···N22	0.95	2.52	2.826 (3)	99
C81—H81···N61	0.95	2.47	2.797 (2)	100
C85—H85···N62	0.95	2.50	2.823 (3)	100

Fig. 1


C44
C45
C43
C32
C33
C31
N22
C34
C40
C30
N30
C22
C21
C42
C41
C71
C70
N20
N21
C72
N70
C20
C73
C74
Ru1
C62
N50
C50
C14
N60
C51
N62
C54
N10
C13
C61
C60
C53
C52
C10
N61
C85
C80
C12
C84
C81
C11
C82
C83