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Redetermination of *cis*-diacetonitrile-bis(2,2′-bipyridine)ruthenium(II) hexafluorophosphate

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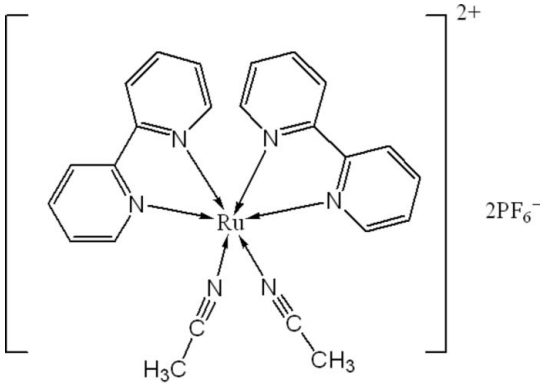
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.048; wR factor = 0.098; data-to-parameter ratio = 10.5.

The title compound, $[Ru(C_{10}H_8N_2)_2(CH_3CN)_2](PF_6)_2$, a six-coordinate ruthenium(II) complex, crystallizes in the monoclinic $C2/c$ space group showing different symmetry from the previously reported $P2_1/n$. A crystallographic twofold rotation axis passes through the Ru atom. The two C atoms and H atoms of one acetonitrile ligand are disordered over two positions, with site occupancy factors of *ca* 0.55 and 0.45. Three F atoms are disordered over two positions, with similar site occupancy factors.

Related literature

For the earlier report of this crystal structure, see: Heeg *et al.* (1985). For analogous complexes, see: Chattopadhyay *et al.* (2004); Cordes *et al.* (1992).



Experimental

Crystal data

$[Ru(C_{10}H_8N_2)_2(C_2H_3N)_2](PF_6)_2$
M_r = 785.49
Monoclinic, $C2/c$
a = 17.2499 (18) Å
b = 10.5008 (11) Å
c = 16.6600 (17) Å
β = 96.201 (2)°
V = 3000.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 291 (2) K
0.16 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.892, T_{max} = 0.931
7231 measured reflections
2641 independent reflections
1718 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.098
S = 0.99
2641 reflections
251 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—N3	2.012 (4)	C6—N2	1.340 (5)
Ru1—N1	2.016 (3)	C10—N2	1.319 (6)
Ru1—N2	2.045 (3)	C11—N3	1.251 (14)
C1—N1	1.358 (5)	C11′—N3	1.200 (15)
C5—N1	1.303 (5)		
N3—Ru1—N1	92.31 (17)	N1—Ru1—N2	79.13 (15)
N3—Ru1—N2	89.42 (15)		

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2089).

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supplementary materials

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Redetermination of *cis*-diacetonitrilebis(2,2'-bipyridine)ruthenium(II) hexafluorophosphate

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Comment

The structures of *cis*-bis(acetonitrile)bis(2,2'-bipyridine) ruthenium(II) diperchlorate (Chattopadhyay *et al.*, 2004), *trans*-bis(acetonitrile)bis(2,2'-bipyridine) ruthenium(II) diperchlorate (Cordes *et al.*, 1992), and the title complex (Heeg *et al.*, 1985) have been reported previously. We present herein the crystal structure of the title compound (I) again with the same unit cell as Heeg *et al.*'s within the experimental error, but it crystallizes in the monoclinic *C2/c* space group other than the earlier $P2_1/n$.

The atom-numbering scheme of compound (I) is shown in Fig.1, while selected bond distances and angles are given in Table 1. The Ru—N bond lengths and bond angles are comparable with those in literature. The presence of acetonitrile molecules in this Ru(II) complex can be verified by routine characterization. The main difference between our data and Heeg *et al.*'s is the assignment of the space group. Our results demonstrate the higher symmetry of molecule (*C2/c* instead of $P2_1/n$), and two carbon atoms of monodentate acetonitrile molecules are refined disorderly. We failed to solve this structure by assigning the reported $P2_1/n$ space group.

Experimental

The title complex (I) was obtained by refluxing equal molar ratio of $Ru(bpy)_2Cl_2·H_2O$ (0.02 g, 0.04 mmol) and a pre-synthesized schiff base, 4-[2-(pyridin-4-ylimino)-ethyl]-benzoic acid (0.01 g, 0.04 mmol) in 30 ml acetonitrile for 1 h. The mixture was cooled to room temperature and a 10 ml saturated NH_4PF_6 solution was added. Orange single-crystal of (I) suitable for the X-ray diffraction analysis was grown directly from the mother liquor as a by-product. Elemental analysis, calculated for $RuC_{24}H_{22}N_6P_2F_{12}$: C, 36.70; H, 2.82; N, 10.70%; found: C, 36.55; H, 2.99; N, 10.48%. IR (KBr): 3123, 3094, 3003, 2938, 1606, 1468, 1449, 1314, 1276, 1243, 1164, 1040, 833, 762, and 557 cm^{-1}. ^1H NMR (d_6-DMSO): δ (p.p.m.) 9.364 (2*H*), 8.778 (2*H*), 8.649 (2*H*), 8.353 (2*H*), 8.031 (2*H*), 7.931 (2*H*), 7.575 (2*H*), 7.373 (2*H*), 2.437 (6*H*).

Refinement

The non-hydrogen atoms were refined anisotropically, whereas the H atoms were placed in geometrically idealized positions (C—H = 0.93–0.96 Å) and refined as riding atoms, with $U_{iso}(H) = 1.5U_{eq}$(for methyl C) or $U_{iso}(H) = 1.2U_{eq}(C)$ for the other C atoms. F2, F3 and F6 atoms of hexafluorophosphate are refined over two sites with 0.557 (17):0.443 (17) site occupancy factors. Due to the disorder of acetonitrile molecules, the 'similar U^{ij}' restraints (SIMU) were used to restrain the U^{ij} components of neighboring atoms (N3—C11 and N3—C11', six for each). The effective standard deviations is set as 0.004 for N3—C11 and 0.003 for N3—C11', respectively.

Figures

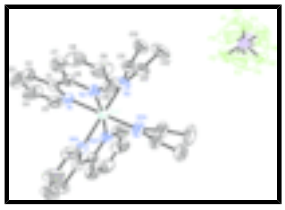


Fig. 1. A drawing of complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and the H atoms are omitted for clarity.

cis-diacetonitrilebis(2,2'-bipyridine)ruthenium(II) hexafluorophosphate

Crystal data

$[Ru(C_{10}H_8N_2)_2(C_2H_3N)_2](F_6P)_2$	F_{000} = 1560
M_r = 785.49	D_x = 1.739 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1829 reflections
a = 17.2499 (18) Å	θ = 2.3–19.1º
b = 10.5008 (11) Å	μ = 0.73 mm^{-1}
c = 16.6600 (17) Å	*T* = 291 (2) K
β = 96.201 (2)º	Block, orange
V = 3000.1 (5) Å^3	0.16 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2641 independent reflections
Radiation source: fine-focus sealed tube	1718 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 291(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −20→18
T_{min} = 0.892, T_{max} = 0.931	*k* = −9→12
7231 measured reflections	*l* = −19→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 1.566P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$

2641 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
251 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Ru1	0.0000	0.97826 (5)	0.7500	0.0657 (2)	
C1	0.0270 (3)	1.1608 (4)	0.8777 (3)	0.0689 (12)	
C2	0.0579 (4)	1.2636 (5)	0.9204 (3)	0.1081 (19)	
H2	0.0346	1.2943	0.9644	0.130*	
C3	0.1238 (5)	1.3207 (6)	0.8976 (4)	0.147 (3)	
H3	0.1459	1.3898	0.9266	0.177*	
C4	0.1562 (4)	1.2770 (7)	0.8338 (4)	0.145 (3)	
H4	0.2005	1.3153	0.8174	0.174*	
C5	0.1225 (3)	1.1744 (6)	0.7932 (3)	0.0982 (17)	
H5	0.1456	1.1433	0.7492	0.118*	
C6	−0.0394 (3)	1.0877 (4)	0.8992 (3)	0.0652 (12)	
C7	−0.0783 (3)	1.1116 (5)	0.9658 (3)	0.0906 (15)	
H7	−0.0651	1.1818	0.9985	0.109*	
C8	−0.1358 (3)	1.0317 (7)	0.9831 (3)	0.1064 (19)	
H8	−0.1619	1.0462	1.0282	0.128*	
C9	−0.1549 (3)	0.9330 (7)	0.9356 (3)	0.120 (2)	
H9	−0.1944	0.8777	0.9470	0.144*	
C10	−0.1151 (3)	0.9134 (6)	0.8687 (3)	0.1113 (19)	
H10	−0.1285	0.8435	0.8357	0.134*	
C11	0.1279 (11)	0.7826 (11)	0.8336 (6)	0.115 (3)	0.546 (11)
C12	0.1854 (8)	0.6918 (10)	0.8694 (6)	0.109 (5)	0.546 (11)
H12A	0.2363	0.7293	0.8712	0.163*	0.546 (11)
H12B	0.1744	0.6717	0.9232	0.163*	0.546 (11)
H12C	0.1837	0.6154	0.8376	0.163*	0.546 (11)
C11'	0.0731 (12)	0.7344 (15)	0.8298 (8)	0.120 (2)	0.454 (11)
C12'	0.1042 (13)	0.6169 (14)	0.8608 (8)	0.141 (9)	0.454 (11)

H12D	0.0652	0.5539	0.8676	0.212*	0.454 (11)
H12E	0.1392	0.5854	0.8244	0.212*	0.454 (11)
H12F	0.1330	0.6351	0.9122	0.212*	0.454 (11)
F1	0.6154 (3)	0.8889 (5)	0.6588 (3)	0.220 (3)	
F2	0.7125 (6)	1.035 (2)	0.5688 (7)	0.183 (7)	0.559 (18)
F3	0.7302 (9)	0.9507 (18)	0.6692 (13)	0.203 (8)	0.559 (18)
F4	0.6351 (8)	1.0821 (9)	0.6847 (6)	0.384 (7)	
F5	0.5853 (3)	1.0436 (9)	0.5748 (5)	0.288 (4)	
F6	0.7016 (15)	0.887 (2)	0.587 (2)	0.326 (13)	0.559 (18)
F2'	0.6890 (14)	1.1222 (15)	0.5882 (13)	0.180 (9)	0.441 (18)
F3'	0.7146 (12)	1.006 (3)	0.7012 (8)	0.187 (11)	0.441 (18)
F6'	0.6389 (14)	0.9189 (12)	0.5469 (6)	0.168 (8)	0.441 (18)
N1	0.0599 (2)	1.1177 (3)	0.8125 (2)	0.0642 (9)	
N2	−0.0591 (2)	0.9896 (3)	0.8497 (2)	0.0687 (10)	
N3	0.0682 (3)	0.8417 (4)	0.8050 (2)	0.1189 (17)	
P1	0.65715 (12)	0.9967 (2)	0.62417 (10)	0.1139 (6)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.0907 (4)	0.0551 (3)	0.0515 (3)	0.000	0.0074 (3)	0.000
C1	0.085 (4)	0.057 (3)	0.061 (3)	0.000 (3)	−0.008 (3)	0.000 (2)
C2	0.166 (6)	0.082 (4)	0.074 (4)	−0.031 (4)	0.005 (4)	−0.012 (3)
C3	0.218 (8)	0.130 (6)	0.089 (5)	−0.103 (6)	−0.004 (5)	−0.003 (4)
C4	0.155 (6)	0.197 (8)	0.078 (5)	−0.096 (6)	−0.013 (5)	0.013 (5)
C5	0.084 (4)	0.144 (5)	0.064 (3)	−0.033 (4)	−0.006 (3)	0.009 (3)
C6	0.075 (3)	0.064 (3)	0.056 (3)	0.011 (3)	0.003 (2)	0.005 (2)
C7	0.107 (4)	0.096 (4)	0.071 (4)	0.021 (4)	0.015 (3)	−0.005 (3)
C8	0.088 (4)	0.159 (6)	0.075 (4)	0.011 (4)	0.021 (3)	0.016 (4)
C9	0.094 (4)	0.193 (7)	0.074 (4)	−0.050 (5)	0.012 (4)	0.019 (4)
C10	0.135 (5)	0.132 (5)	0.069 (4)	−0.059 (4)	0.016 (4)	−0.002 (3)
C11	0.205 (7)	0.081 (5)	0.061 (4)	0.052 (4)	0.028 (5)	0.010 (4)
C12	0.146 (12)	0.082 (8)	0.099 (8)	0.034 (8)	0.013 (7)	0.020 (6)
C11'	0.213 (6)	0.087 (4)	0.063 (4)	0.059 (4)	0.028 (4)	0.012 (3)
C12'	0.22 (2)	0.096 (11)	0.115 (11)	0.073 (13)	0.047 (12)	0.043 (9)
F1	0.222 (5)	0.218 (5)	0.208 (5)	−0.120 (4)	−0.027 (4)	0.087 (4)
F2	0.142 (7)	0.30 (2)	0.126 (7)	0.003 (13)	0.080 (6)	0.050 (12)
F3	0.191 (11)	0.197 (13)	0.198 (16)	0.025 (9)	−0.082 (11)	0.049 (11)
F4	0.569 (16)	0.342 (11)	0.225 (8)	0.239 (12)	−0.031 (10)	−0.106 (8)
F5	0.146 (4)	0.454 (12)	0.262 (7)	0.016 (6)	0.007 (5)	0.195 (8)
F6	0.228 (19)	0.34 (2)	0.42 (3)	0.023 (18)	0.09 (2)	−0.14 (2)
F2'	0.217 (19)	0.117 (10)	0.193 (15)	−0.078 (10)	−0.044 (12)	0.073 (9)
F3'	0.181 (15)	0.29 (2)	0.084 (7)	−0.153 (17)	0.000 (8)	−0.019 (9)
F6'	0.26 (2)	0.150 (9)	0.084 (7)	0.009 (11)	−0.018 (8)	−0.029 (6)
N1	0.068 (3)	0.069 (2)	0.054 (2)	−0.006 (2)	−0.0019 (19)	0.0053 (18)
N2	0.081 (3)	0.072 (3)	0.053 (2)	−0.017 (2)	0.0063 (19)	0.0030 (19)
N3	0.213 (5)	0.085 (3)	0.061 (2)	0.061 (3)	0.027 (3)	0.012 (2)
P1	0.1182 (15)	0.1435 (18)	0.0797 (11)	−0.0289 (14)	0.0096 (12)	0.0056 (12)

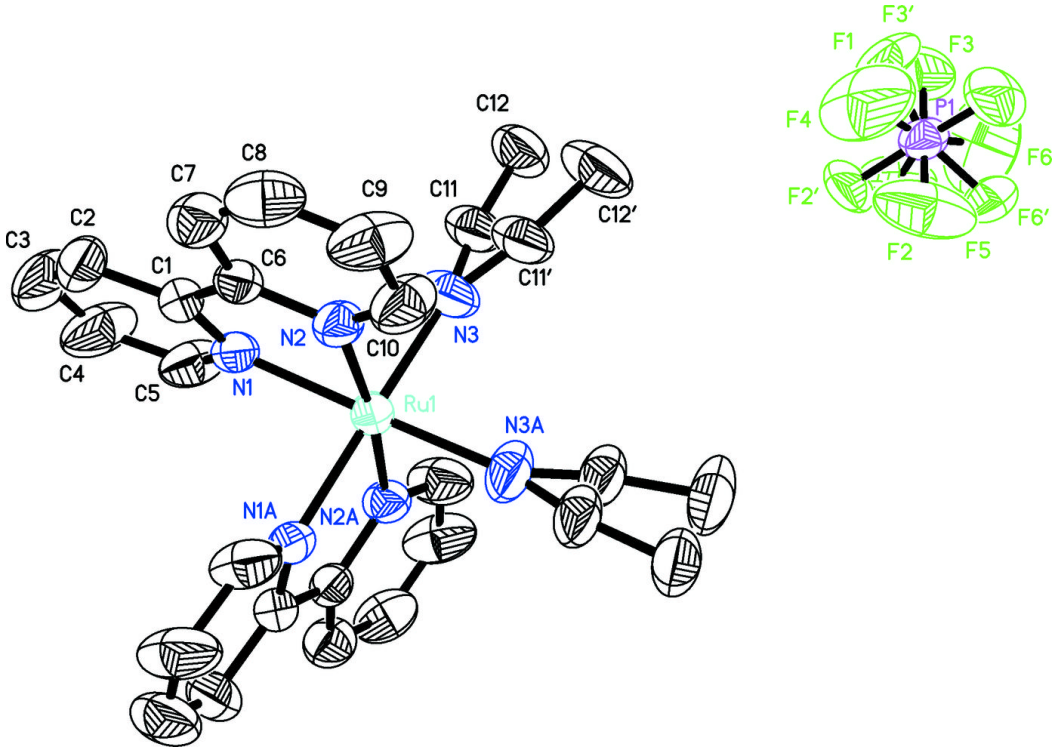
Geometric parameters (Å, °)

Ru1—N3^{i}	2.012 (4)	C9—C10	1.387 (7)
Ru1—N3	2.012 (4)	C9—H9	0.9300
Ru1—N1	2.016 (3)	C10—N2	1.319 (6)
Ru1—N1^{i}	2.016 (3)	C10—H10	0.9300
Ru1—N2	2.045 (3)	C11—N3	1.251 (14)
Ru1—N2^{i}	2.045 (3)	C11—C12	1.456 (13)
C1—N1	1.358 (5)	C12—H12A	0.9599
C1—C2	1.369 (6)	C12—H12B	0.9601
C1—C6	1.455 (6)	C12—H12C	0.9600
C2—C3	1.375 (8)	C11'—N3	1.200 (15)
C2—H2	0.9300	C11'—C12'	1.421 (15)
C3—C4	1.335 (9)	C12'—H12D	0.9600
C3—H3	0.9300	C12'—H12E	0.9600
C4—C5	1.368 (7)	C12'—H12F	0.9601
C4—H4	0.9300	F1—P1	1.490 (4)
C5—N1	1.303 (5)	F2—P1	1.455 (10)
C5—H5	0.9300	F3—P1	1.477 (12)
C6—N2	1.340 (5)	F4—P1	1.432 (7)
C6—C7	1.381 (6)	F5—P1	1.495 (5)
C7—C8	1.354 (7)	F6—P1	1.549 (17)
C7—H7	0.9300	F2'—P1	1.571 (11)
C8—C9	1.323 (8)	F3'—P1	1.538 (15)
C8—H8	0.9300	F6'—P1	1.529 (10)
N3^{i}—Ru1—N3	89.1 (3)	H12A—C12—H12F	145.9
N3^{i}—Ru1—N1	174.27 (17)	H12C—C12—H12F	86.5
N3—Ru1—N1	92.31 (17)	H12E—C12—H12F	65.8
N3^{i}—Ru1—N1^{i}	92.31 (17)	N3—C11'—C12'	161.9 (19)
N3—Ru1—N1^{i}	174.27 (17)	C11'—C12'—H12C	104.0
N1—Ru1—N1^{i}	86.83 (19)	C11'—C12'—H12D	113.5
N3^{i}—Ru1—N2	95.34 (16)	H12C—C12'—H12D	135.4
N3—Ru1—N2	89.42 (15)	C11'—C12'—H12E	108.0
N1—Ru1—N2	79.13 (15)	H12D—C12'—H12E	109.5
N1^{i}—Ru1—N2	95.98 (15)	C11'—C12'—H12F	106.9
N3^{i}—Ru1—N2^{i}	89.42 (15)	H12C—C12'—H12F	80.2
N3—Ru1—N2^{i}	95.34 (16)	H12D—C12'—H12F	109.5
N1—Ru1—N2^{i}	95.98 (15)	H12E—C12'—H12F	109.5
N1^{i}—Ru1—N2^{i}	79.13 (15)	C5—N1—C1	118.4 (4)
N2—Ru1—N2^{i}	173.3 (2)	C5—N1—Ru1	126.7 (4)
N1—C1—C2	120.4 (5)	C1—N1—Ru1	114.8 (3)
N1—C1—C6	115.5 (4)	C10—N2—C6	117.6 (4)
C2—C1—C6	124.1 (5)	C10—N2—Ru1	127.0 (3)
C1—C2—C3	119.2 (6)	C6—N2—Ru1	115.4 (3)
C1—C2—H2	120.4	C11'—N3—C11	51.6 (9)

C3—C2—H2	120.4	C11'—N3—Ru1	147.3 (12)
C4—C3—C2	120.0 (6)	C11—N3—Ru1	160.7 (9)
C4—C3—H3	120.0	F4—P1—F2	121.0 (11)
C2—C3—H3	120.0	F4—P1—F3	97.1 (10)
C3—C4—C5	118.2 (6)	F2—P1—F3	80.2 (10)
C3—C4—H4	120.9	F4—P1—F1	91.5 (6)
C5—C4—H4	120.9	F2—P1—F1	146.6 (10)
N1—C5—C4	123.8 (6)	F3—P1—F1	88.7 (6)
N1—C5—H5	118.1	F4—P1—F5	85.0 (6)
C4—C5—H5	118.1	F2—P1—F5	97.0 (6)
N2—C6—C7	121.4 (5)	F3—P1—F5	177.1 (9)
N2—C6—C1	114.1 (4)	F1—P1—F5	93.2 (3)
C7—C6—C1	124.4 (5)	F4—P1—F6'	151.9 (10)
C8—C7—C6	119.3 (5)	F2—P1—F6'	72.8 (13)
C8—C7—H7	120.4	F3—P1—F6'	109.9 (15)
C6—C7—H7	120.4	F1—P1—F6'	81.8 (6)
C9—C8—C7	120.0 (6)	F5—P1—F6'	68.3 (8)
C9—C8—H8	120.0	F4—P1—F3'	64.3 (9)
C7—C8—H8	120.0	F2—P1—F3'	95.9 (8)
C8—C9—C10	118.9 (6)	F1—P1—F3'	91.2 (7)
C8—C9—H9	120.5	F5—P1—F3'	149.1 (12)
C10—C9—H9	120.5	F6'—P1—F3'	142.6 (15)
N2—C10—C9	122.8 (5)	F4—P1—F6	158.4 (15)
N2—C10—H10	118.6	F2—P1—F6	64.1 (9)
C9—C10—H10	118.6	F3—P1—F6	62.0 (18)
N3—C11—C12	167.6 (14)	F1—P1—F6	82.8 (9)
C11—C12—H12A	109.0	F5—P1—F6	116.1 (15)
C11—C12—H12B	109.4	F6'—P1—F6	47.9 (10)
H12A—C12—H12B	109.5	F3'—P1—F6	94.8 (19)
C11—C12—H12C	110.0	F4—P1—F2'	82.7 (11)
H12A—C12—H12C	109.5	F3—P1—F2'	98.8 (9)
H12B—C12—H12C	109.5	F1—P1—F2'	171.1 (11)
C11—C12—H12E	89.0	F5—P1—F2'	79.5 (7)
H12A—C12—H12E	138.1	F6'—P1—F2'	100.1 (11)
H12B—C12—H12E	98.8	F3'—P1—F2'	92.4 (9)
C11—C12—H12F	92.2	F6—P1—F2'	105.0 (12)

Symmetry codes: (i) $-x$, y, $-z+3/2$.

Fig. 1


F3′
F1
F3
F4
P1
F6
F2′
F6′
F2
F5
C12
C8
C7
C9
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C12′
C2
C3
C1
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C11′
N2
C10
N3
C4
C5
N1
Ru1
N3A
N1A
N2A