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trans-Chloridotetrakis(4-methylpyridine-κ*N*)-(nitrosyl-κ*N*)ruthenium(II) bis(hexafluoridophosphate) acetone 0.75-solvate

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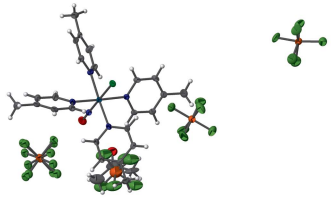
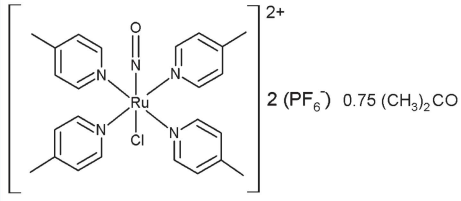
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[RuCl(NO)(C_6H_7N)_4](PF_6)_2\cdot 0.75(CH_3)_2CO$, comprises four ligands of 4-picoline in equatorial position around the central atom. Overall, the complex features an octahedral coordination environment around the central Ru^{II} atom, with the chlorido ligand *trans* to the nitrosyl. The bond length of the nitrosyl N═O ligand is 1.140 (5) Å, while the angle Ru—N═O is 179.0 (4)°. The asymmetric unit contains four PF_6^- counter-anions, two with occupancy of 0.25 and one with occupancy of 0.5. One PF_6^- anion is disordered over two sets of sites and one other is disordered with an acetone molecule that occupies the same site.

3D view



Chemical scheme



Structure description

Ruthenium nitrosyl complexes with substituted pyridine ligands possess unique photochromic properties such as Ru(NO) ⟷ Ru(ON) photoisomerization, which could allow for their use as high data storage optics and sensors (Schaniel *et al.*, 2007; García *et al.*, 2016). In addition, nitric oxide donors such as ruthenium(II) nitrosyl complexes are capable of releasing NO upon irradiation (De Candia *et al.*, 2010) and could find use as a means of inducing apoptosis in living beings (Kumar *et al.*, 2015), as antimicrobial agents (Schairer *et al.*, 2012) and as a way to help wounds heal (Childress *et al.*, 2008).

The asymmetric unit of the title salt (Fig. 1) is composed of a *trans*-$[Ru(C_6H_7N)_4Cl(NO)]^{2+}$ cation and two PF_6^- anions (the asymmetric unit contains four sites for PF_6^- anions with different occupancies). The Ru^{II} atom of the *trans*-$[Ru(C_6H_7N)_4Cl(NO)]^{2+}$ cation features a compressed octahedral coordination sphere with the four N atoms of the 4-picoline ligands in the equatorial positions, and chlorido

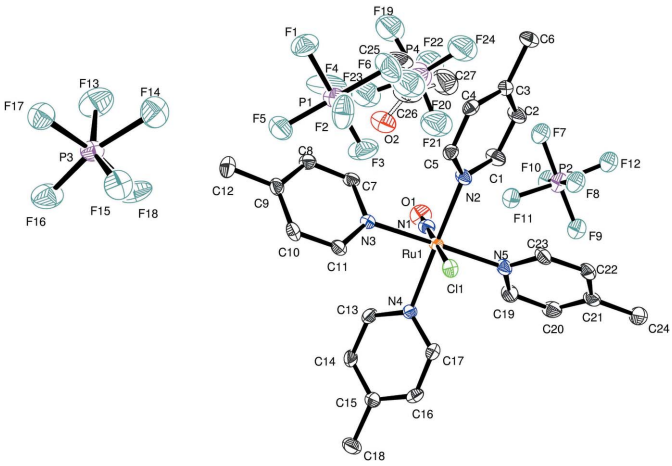


Figure 1
The structures of the molecular entities in the title salt with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. The acetone molecule (open bond) is disordered with one hexafluoridophosphate anion. Hydrogen atoms are omitted for clarity.

and nitrosyl ligands located at the *trans* axial sites. The N1═O1 bond length is 1.140 (5) Å, which is in the range of N═O groups in other examples of octahedral Ru^{II}–NO^{+} complexes, but shorter than the N═O bond of *trans*-$[Ru(py)_4(Cl)(NO)](PF_6)_2$ which is 1.146 (2) Å (Cormary *et al.*, 2009*a*,*b*), and longer than the N═O bond of *trans*-$[Ru(4\text{-}Clpy)_4(Cl)(NO)](PF_6)_2$ (Tassé *et al.*, 2016), which is 1.125 (5) Å. These differences are due to the substituents (electron donating or withdrawing) on the pyridine ligands. The Ru1—N1═O1 angle is essentially linear [179.0 (4)]°, which implies that the $\{Ru^{II}NO^{+}\}^6$ should be $\{Ru^{II}NO^{+}\}_6$ (McCleverty, 2004).

The Ru1—Cl1 bond length in the position *trans* to nitrosyl is 2.3163 (11) Å, which is shorter than that observed in *trans*-$[Ru(py)_4ClNO](PF_6)_2$ (2.3206 Å; Cormary *et al.*, 2012). The length of the Ru—Cl bond in other complexes without nitrosyl, as *trans*(Cl,pyz)-$[Ru(py)_4Cl(pyz)]PF_6$ and *trans*-(Cl,PhCN)-$[Ru(py)_4Cl(PhCN)]PF_6$ are 2.415 and 2.3931 Å, respectively (Coe *et al.*, 1995), reflecting the ability of nitrosyl as a π acceptor and the ability of chlorido ligand as a good σ donor. The Ru1—N1 distance is 1.757 (4) Å, in agreement with the Ru—N distances found in other ruthenium(II) nitrosyl complexes (Ferlay *et al.*, 2004), which is further supported by the stretching vibration of nitrosyl, which is 1895 cm^{-1} (Becker *et al.*, 2015; Sauaia & da Silva, 2003; Togano *et al.*, 1992).

The overall packing shows the presence of rows of cations with PF_6^- anions and acetone molecules inserted in between (Fig. 2). The investigation of the interactions in the crystal shows that C—H···F hydrogen bonds (Table 1) are dominant (Mohammed *et al.*, 2017; Cormary *et al.*, 2009*a*,*b*).

Synthesis and crystallization

According to literature reports (Cormary *et al.*, 2009*a*,*b*), four steps are required to synthesize *trans*-$[Ru(py)_4(Cl)(NO)](PF_6)_2$, where the pyridine acts as both a solvent and a ligand. However, in our case, we used ethanol as a solvent, and 4-picoline instead of pyridine, which afforded an orange solid in good yield (142 mg, 81.5%). ^{1}H NMR (400 MHz, acetone d_6, 298 K): δ (p.p.m.) 8.58 (8Hα, *d*, *J* = 6.4 Hz), 7.67 (8Hβ, *d*, *J* = 6.0 Hz), 2.61 (12*H*, *s*, CH_3). Crystals of the title complex were grown by slow diffusion of diethyl ether vapour into acetone solution over the course of one week.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F8	0.95	2.47	3.194 (12)	133
C1—H1···F11	0.95	2.48	3.405 (15)	165
C1—H1···F10′	0.95	2.3	3.243 (18)	173
C5—H5···F3	0.95	2.49	3.328 (6)	147
C7—H7···O2	0.95	2.45	3.320 (7)	153
C7—H7···F20	0.95	2.51	3.264 (18)	136
C13—H13···F22^{i}	0.95	2.54	3.16 (2)	123
C13—H13···F23^{i}	0.95	2.26	3.047 (18)	140
C14—H14···F19^{i}	0.95	2.4	2.995 (18)	120
C27—H27*A*···F7	0.98	2.41	3.297 (17)	150
C27—H27*B*···F7^{ii}	0.98	2.55	3.418 (17)	147

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The asymmetric unit contains four PF_6^- counter-anions, two with occupancy of 0.25 and one with occupancy of 0.5. One PF_6^- anion is disordered over two sets of sites and one other is disordered with an acetone molecule

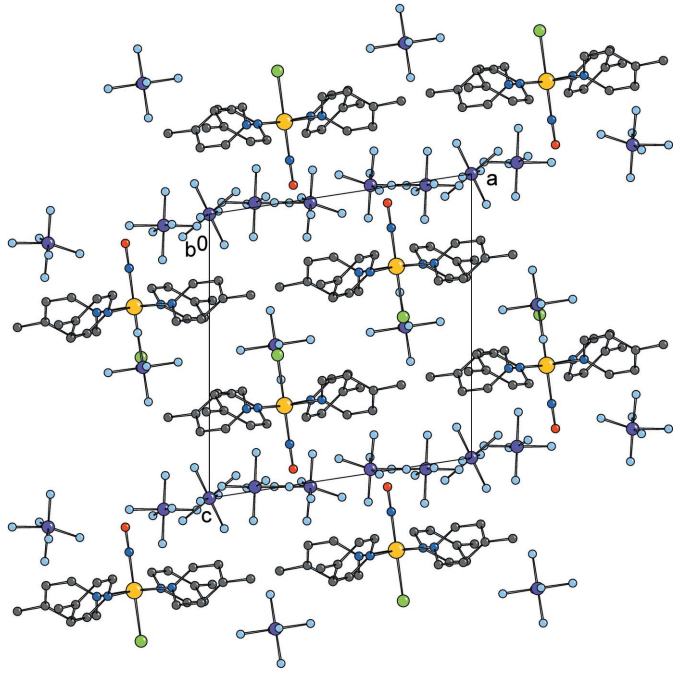


Figure 2
Crystal packing of *trans*-$[Ru(C_6H_7N)_4Cl(NO)](PF_6)_2{\cdot}0.75(CH_3)_2CO$ viewed along the *b* axis, showing cationic rows. Hydrogen atoms and solvent molecules are omitted for clarity.

that occupies the same site. Similarity restraints on bond lengths and angles as well as on displacement parameters were used to model those disorders.

Funding information

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[RuCl(NO)(C_6H_7N)_4](PF_6)_2\cdot 0.75C_3H_6O$
M_r	872.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	11.9904 (7), 12.0159 (8), 13.4432 (9)
α, β, γ (°)	107.065 (2), 98.270 (2), 90.388 (2)
V (Å^3)	1829.8 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.68
Crystal size (mm)	0.20 × 0.16 × 0.02
Data collection	
Diffractometer	Bruker Kappa APEXII Quazar
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.708, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	56033, 6707, 6081
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.149, 1.05
No. of reflections	6707
No. of parameters	635
No. of restraints	441
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.97, −1.45

Computer programs: *APEX2* and *SAINT* (Bruker, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015) and *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012).

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full crystallographic data

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trans-Chloridotetrakis(4-methylpyridine-κN)(nitrosyl-κN)ruthenium(II) bis(hexafluoridophosphate) acetone 0.75-solvate

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trans-Chloridotetrakis(4-methylpyridine-κN)(nitrosyl-κN)ruthenium(II) bis(hexafluoridophosphate) acetone 0.75-solvate

Crystal data

$[RuCl(NO)(C_6H_7N)_4](PF_6)_2 \cdot 0.75C_3H_6O$
$M_r = 872.53$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 11.9904\ (7)$ Å
$b = 12.0159\ (8)$ Å
$c = 13.4432\ (9)$ Å
$\alpha = 107.065\ (2)°$
$\beta = 98.270\ (2)°$
$\gamma = 90.388\ (2)°$
$V = 1829.8\ (2)$ Å^3
$Z = 2$
$F(000) = 876.0$
$D_x = 1.584$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9786 reflections
$\theta = 2.4–30.8°$
$\mu = 0.68$ mm^{-1}
$T = 100$ K
Plate, orange
0.20 × 0.16 × 0.02 mm

Data collection

Bruker Kappa APEXII Quazar diffractometer
Radiation source: microfocus sealed tube
Multilayer optics monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2005)
$T_{min} = 0.708$, $T_{max} = 0.747$
56033 measured reflections
6707 independent reflections
6081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.7°$
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.149$
$S = 1.05$
6707 reflections
635 parameters
441 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0779P)^2 + 9.4314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.017$
$\Delta\rho_{max} = 1.97$ e Å^{-3}
$\Delta\rho_{min} = -1.45$ e Å^{-3}

Special details

Refinement. All H atoms were fixed geometrically and treated as riding with C—H = 0.95 Å (aromatic), 0.98 Å (methyl) and U_{iso}(H) =1.2U_{eq} (aromatic) or U_{iso}(H) =1.5U_{eq} (methyl).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.6304 (4)	0.8881 (4)	0.2326 (4)	0.0309 (11)	
H1	0.68539	0.869211	0.186822	0.037*	
C2	0.5718 (4)	0.9868 (4)	0.2372 (4)	0.0305 (11)	
H2	0.58711	1.035077	0.195609	0.037*	
C3	0.4900 (4)	1.0160 (4)	0.3028 (4)	0.0228 (9)	
C4	0.4713 (4)	0.9410 (4)	0.3609 (3)	0.0201 (9)	
H4	0.41542	0.956975	0.405965	0.024*	
C5	0.5332 (4)	0.8437 (4)	0.3534 (3)	0.0197 (9)	
H5	0.519163	0.793754	0.393985	0.024*	
C6	0.4249 (4)	1.1235 (4)	0.3076 (5)	0.0325 (11)	
H6A	0.47542	1.186481	0.304613	0.049*	
H6B	0.393169	1.14739	0.373452	0.049*	
H6C	0.363563	1.106626	0.247743	0.049*	
C7	0.4743 (4)	0.5714 (4)	0.2188 (3)	0.0206 (9)	
H7	0.474273	0.614333	0.169697	0.025*	
C8	0.3770 (4)	0.5116 (4)	0.2197 (4)	0.0222 (9)	
H8	0.31122	0.513874	0.171832	0.027*	
C9	0.3740 (4)	0.4475 (4)	0.2903 (4)	0.0211 (9)	
C10	0.4744 (4)	0.4457 (4)	0.3566 (4)	0.0224 (9)	
H10	0.476949	0.401414	0.404821	0.027*	
C11	0.5696 (4)	0.5074 (4)	0.3527 (3)	0.0195 (9)	
H11	0.63686	0.504821	0.398712	0.023*	
C12	0.2682 (4)	0.3837 (5)	0.2947 (4)	0.0330 (11)	
H12A	0.205913	0.43656	0.299461	0.05*	
H12B	0.278812	0.355418	0.356539	0.05*	
H12C	0.250384	0.317457	0.2308	0.05*	
C13	0.7807 (4)	0.4245 (4)	0.2301 (4)	0.0238 (10)	
H13	0.711679	0.413394	0.182935	0.029*	
C14	0.8425 (4)	0.3295 (4)	0.2337 (4)	0.0256 (10)	
H14	0.814992	0.254036	0.190147	0.031*	
C15	0.9449 (4)	0.3427 (4)	0.3005 (4)	0.0206 (9)	
C16	0.9802 (4)	0.4553 (4)	0.3614 (3)	0.0212 (9)	
H16	1.050219	0.468697	0.407369	0.025*	
C17	0.9153 (4)	0.5477 (4)	0.3561 (3)	0.0201 (9)	
H17	0.941325	0.623879	0.398905	0.024*	
C18	1.0115 (4)	0.2393 (4)	0.3056 (4)	0.0312 (11)	
H18A	0.95983	0.17214	0.295993	0.047*	
H18B	1.059468	0.256666	0.374287	0.047*	
H18C	1.058811	0.221271	0.249774	0.047*	
C19	0.9380 (4)	0.7351 (4)	0.2357 (4)	0.0267 (10)	
H19	0.927469	0.657448	0.190019	0.032*	

C20	1.0349 (4)	0.7994 (5)	0.2391 (4)	0.0303 (11)	
H20	1.09018	0.765519	0.196932	0.036*	
C21	1.0520 (4)	0.9135 (4)	0.3042 (4)	0.0277 (10)	
C22	0.9687 (4)	0.9581 (4)	0.3645 (4)	0.0274 (10)	
H22	0.976902	1.036021	0.409572	0.033*	
C23	0.8739 (4)	0.8894 (4)	0.3589 (4)	0.0247 (10)	
H23	0.818241	0.921006	0.401461	0.03*	
C24	1.1574 (4)	0.9848 (5)	0.3070 (5)	0.0374 (13)	
H24A	1.2224	0.935649	0.304872	0.056*	
H24B	1.169387	1.050279	0.371881	0.056*	
H24C	1.148621	1.014655	0.246002	0.056*	
N1	0.6939 (3)	0.6304 (3)	0.1466 (3)	0.0218 (8)	
N2	0.6131 (3)	0.8170 (3)	0.2904 (3)	0.0221 (8)	
N3	0.5707 (3)	0.5715 (3)	0.2856 (3)	0.0172 (7)	
N4	0.8151 (3)	0.5331 (3)	0.2917 (3)	0.0175 (7)	
N5	0.8578 (3)	0.7784 (3)	0.2947 (3)	0.0223 (8)	
O1	0.6796 (3)	0.6032 (3)	0.0569 (3)	0.0347 (8)	
F1	0.1192 (3)	0.7558 (3)	0.4962 (3)	0.0464 (8)	
F2	0.2736 (3)	0.7858 (3)	0.6215 (3)	0.0485 (9)	
F3	0.3860 (3)	0.7323 (4)	0.4967 (3)	0.0552 (10)	
F4	0.2325 (3)	0.7029 (4)	0.3722 (3)	0.0610 (12)	
F5	0.2396 (3)	0.6116 (3)	0.4982 (3)	0.0464 (8)	
F6	0.2656 (3)	0.8772 (3)	0.4964 (3)	0.0581 (10)	
F7	0.6950 (9)	0.9466 (11)	−0.0035 (9)	0.0340 (9)	0.27
F8	0.8214 (10)	0.9891 (10)	0.1350 (9)	0.0348 (9)	0.27
F9	0.9526 (10)	0.9017 (11)	0.0352 (9)	0.0334 (9)	0.27
F10	0.8320 (10)	0.8690 (10)	−0.1035 (9)	0.0338 (9)	0.27
F11	0.7843 (12)	0.8057 (13)	0.0314 (9)	0.0316 (10)	0.27
F12	0.8570 (10)	1.0561 (10)	0.0154 (10)	0.0338 (9)	0.27
F7′	0.7009 (11)	0.8999 (13)	−0.0515 (11)	0.0340 (9)	0.23
F8′	0.8494 (11)	1.0266 (12)	−0.0347 (11)	0.0334 (10)	0.23
F9′	0.9531 (12)	0.9422 (13)	0.0748 (11)	0.0335 (10)	0.23
F10′	0.7997 (14)	0.8134 (15)	0.0592 (10)	0.0303 (11)	0.23
F11′	0.7765 (12)	1.0179 (12)	0.1058 (10)	0.0341 (9)	0.23
F12′	0.8823 (12)	0.8345 (12)	−0.0761 (10)	0.0332 (10)	0.23
P1	0.25256 (11)	0.74423 (12)	0.49665 (11)	0.0304 (3)	
P2	0.8262 (2)	0.9222 (2)	0.0147 (2)	0.0315 (5)	0.5
P3	0.0096 (7)	0.4947 (8)	1.0065 (7)	0.0235 (11)	0.25
F13	−0.0554 (15)	0.5012 (18)	0.8912 (15)	0.055 (3)	0.25
F14	0.0159 (14)	0.6360 (14)	1.0186 (13)	0.043 (3)	0.25
F15	0.0819 (13)	0.5449 (11)	1.1104 (12)	0.037 (3)	0.25
F16	0.0327 (13)	0.3706 (15)	0.9944 (14)	0.044 (3)	0.25
F17	−0.1002 (13)	0.4859 (13)	1.0649 (11)	0.035 (3)	0.25
F18	0.1247 (11)	0.4940 (14)	0.9658 (13)	0.044 (3)	0.25
O2	0.4360 (6)	0.6354 (5)	−0.0073 (5)	0.0506 (13)	0.75
C25	0.3205 (8)	0.7753 (7)	0.0657 (7)	0.0543 (17)	0.75
H25A	0.246098	0.753724	0.022434	0.081*	0.75
H25B	0.330631	0.860441	0.092797	0.081*	0.75

H25C	0.326049	0.74244	0.124747	0.081*	0.75
C26	0.4079 (9)	0.7297 (10)	0.0018 (8)	0.0626 (17)	0.75
C27	0.4482 (11)	0.8030 (10)	−0.0534 (10)	0.072 (2)	0.75
H27A	0.516295	0.848073	−0.011498	0.107*	0.75
H27B	0.389859	0.856427	−0.065322	0.107*	0.75
H27C	0.46595	0.754874	−0.121279	0.107*	0.75
P4	0.3853 (8)	0.7754 (8)	0.0142 (8)	0.0695 (16)	0.25
F19	0.2485 (12)	0.7786 (15)	−0.0055 (14)	0.073 (3)	0.25
F20	0.3720 (17)	0.7832 (16)	0.1335 (11)	0.078 (3)	0.25
F21	0.5042 (14)	0.7665 (17)	0.0707 (15)	0.081 (3)	0.25
F22	0.3936 (17)	0.7839 (17)	−0.0996 (13)	0.075 (3)	0.25
F23	0.3516 (18)	0.6382 (13)	−0.0083 (15)	0.073 (3)	0.25
F24	0.3869 (17)	0.9163 (12)	0.0572 (15)	0.079 (3)	0.25
Ru1	0.71356 (3)	0.67328 (3)	0.28492 (3)	0.01662 (13)	
Cl1	0.73954 (9)	0.73137 (9)	0.46724 (8)	0.0205 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.029 (3)	0.031 (3)	0.046 (3)	0.011 (2)	0.022 (2)	0.025 (2)
C2	0.029 (3)	0.028 (3)	0.047 (3)	0.008 (2)	0.018 (2)	0.025 (2)
C3	0.018 (2)	0.019 (2)	0.032 (2)	0.0013 (17)	0.0030 (18)	0.0085 (19)
C4	0.016 (2)	0.024 (2)	0.019 (2)	0.0009 (17)	0.0035 (16)	0.0033 (17)
C5	0.017 (2)	0.022 (2)	0.021 (2)	−0.0001 (17)	0.0038 (17)	0.0080 (17)
C6	0.027 (3)	0.023 (2)	0.050 (3)	0.009 (2)	0.008 (2)	0.014 (2)
C7	0.021 (2)	0.023 (2)	0.022 (2)	0.0048 (17)	0.0031 (17)	0.0119 (18)
C8	0.021 (2)	0.023 (2)	0.023 (2)	0.0028 (18)	0.0007 (18)	0.0078 (18)
C9	0.024 (2)	0.014 (2)	0.024 (2)	−0.0010 (17)	0.0038 (18)	0.0034 (17)
C10	0.032 (2)	0.015 (2)	0.020 (2)	−0.0028 (18)	0.0015 (18)	0.0067 (17)
C11	0.025 (2)	0.015 (2)	0.018 (2)	0.0014 (17)	−0.0010 (17)	0.0053 (16)
C12	0.028 (3)	0.031 (3)	0.043 (3)	−0.008 (2)	0.003 (2)	0.015 (2)
C13	0.016 (2)	0.021 (2)	0.029 (2)	−0.0004 (17)	−0.0018 (18)	0.0022 (19)
C14	0.021 (2)	0.015 (2)	0.037 (3)	−0.0017 (17)	0.0027 (19)	0.0030 (19)
C15	0.017 (2)	0.024 (2)	0.026 (2)	0.0038 (17)	0.0099 (17)	0.0128 (18)
C16	0.014 (2)	0.030 (2)	0.021 (2)	0.0014 (18)	0.0020 (16)	0.0093 (19)
C17	0.017 (2)	0.021 (2)	0.021 (2)	−0.0024 (17)	0.0028 (17)	0.0042 (17)
C18	0.029 (3)	0.028 (3)	0.044 (3)	0.009 (2)	0.009 (2)	0.019 (2)
C19	0.025 (2)	0.024 (2)	0.034 (3)	0.0040 (19)	0.012 (2)	0.010 (2)
C20	0.023 (2)	0.036 (3)	0.041 (3)	0.008 (2)	0.013 (2)	0.021 (2)
C21	0.024 (2)	0.027 (2)	0.041 (3)	0.0039 (19)	0.005 (2)	0.024 (2)
C22	0.028 (2)	0.022 (2)	0.039 (3)	0.0017 (19)	0.005 (2)	0.019 (2)
C23	0.027 (2)	0.019 (2)	0.033 (3)	0.0049 (18)	0.010 (2)	0.0129 (19)
C24	0.024 (3)	0.036 (3)	0.060 (4)	−0.001 (2)	0.006 (2)	0.027 (3)
N1	0.0195 (19)	0.025 (2)	0.026 (2)	0.0052 (15)	0.0081 (15)	0.0129 (16)
N2	0.0233 (19)	0.0204 (19)	0.028 (2)	0.0043 (15)	0.0112 (16)	0.0126 (16)
N3	0.0185 (18)	0.0170 (17)	0.0171 (17)	0.0026 (14)	0.0031 (14)	0.0062 (14)
N4	0.0172 (17)	0.0154 (17)	0.0184 (18)	0.0016 (14)	0.0013 (14)	0.0031 (14)
N5	0.0224 (19)	0.0203 (19)	0.029 (2)	0.0023 (15)	0.0092 (16)	0.0120 (16)

O1	0.041 (2)	0.044 (2)	0.0202 (19)	0.0019 (17)	0.0056 (15)	0.0116 (16)
F1	0.0316 (17)	0.053 (2)	0.054 (2)	0.0105 (15)	0.0143 (15)	0.0123 (17)
F2	0.060 (2)	0.051 (2)	0.0327 (18)	−0.0212 (17)	0.0054 (16)	0.0112 (15)
F3	0.0299 (18)	0.082 (3)	0.073 (3)	0.0146 (17)	0.0175 (17)	0.048 (2)
F4	0.068 (3)	0.089 (3)	0.0325 (18)	0.048 (2)	0.0165 (17)	0.0241 (19)
F5	0.049 (2)	0.0329 (17)	0.055 (2)	0.0018 (15)	−0.0028 (16)	0.0152 (15)
F6	0.071 (3)	0.045 (2)	0.080 (3)	0.0111 (18)	0.037 (2)	0.039 (2)
F7	0.0338 (17)	0.0376 (18)	0.0283 (17)	−0.0025 (15)	0.0035 (16)	0.0068 (15)
F8	0.0351 (17)	0.0380 (18)	0.0277 (18)	−0.0029 (16)	0.0015 (16)	0.0059 (16)
F9	0.0347 (17)	0.0374 (18)	0.0272 (18)	−0.0027 (16)	0.0038 (16)	0.0090 (16)
F10	0.0348 (16)	0.0385 (17)	0.0269 (16)	−0.0036 (14)	0.0046 (15)	0.0078 (15)
F11	0.0341 (17)	0.0341 (17)	0.0267 (18)	−0.0038 (15)	0.0025 (16)	0.0104 (16)
F12	0.0345 (17)	0.0371 (18)	0.0277 (18)	−0.0026 (15)	0.0032 (16)	0.0073 (16)
F7′	0.0343 (16)	0.0379 (17)	0.0278 (17)	−0.0031 (14)	0.0026 (15)	0.0077 (15)
F8′	0.0345 (17)	0.0377 (18)	0.0270 (18)	−0.0025 (16)	0.0037 (16)	0.0089 (16)
F9′	0.0348 (17)	0.0372 (18)	0.0268 (18)	−0.0027 (16)	0.0023 (16)	0.0081 (16)
F10′	0.0338 (19)	0.0328 (19)	0.025 (2)	−0.0036 (17)	0.0028 (18)	0.0111 (18)
F11′	0.0343 (16)	0.0375 (17)	0.0279 (17)	−0.0030 (15)	0.0034 (15)	0.0066 (15)
F12′	0.0342 (17)	0.0377 (18)	0.0269 (17)	−0.0034 (16)	0.0054 (16)	0.0083 (16)
P1	0.0291 (7)	0.0357 (7)	0.0323 (7)	0.0069 (5)	0.0102 (5)	0.0167 (6)
P2	0.0325 (12)	0.0361 (12)	0.0257 (12)	−0.0032 (9)	0.0039 (10)	0.0092 (10)
P3	0.0237 (14)	0.0231 (13)	0.0212 (13)	0.0048 (9)	0.0046 (10)	0.0021 (9)
F13	0.044 (7)	0.072 (8)	0.045 (5)	0.002 (6)	−0.003 (5)	0.017 (6)
F14	0.048 (6)	0.030 (4)	0.042 (5)	−0.001 (5)	0.007 (5)	−0.006 (4)
F15	0.043 (5)	0.017 (5)	0.033 (4)	0.000 (4)	0.000 (4)	−0.017 (4)
F16	0.037 (6)	0.036 (4)	0.049 (6)	0.011 (5)	0.004 (5)	0.000 (4)
F17	0.034 (3)	0.036 (3)	0.034 (3)	0.0025 (19)	0.008 (2)	0.0086 (19)
F18	0.023 (5)	0.062 (6)	0.047 (5)	0.017 (4)	0.012 (4)	0.014 (5)
O2	0.056 (3)	0.046 (3)	0.054 (3)	0.015 (2)	0.013 (3)	0.019 (2)
C25	0.058 (3)	0.041 (3)	0.050 (3)	0.016 (3)	−0.030 (3)	0.011 (3)
C26	0.066 (3)	0.059 (3)	0.054 (3)	0.018 (3)	−0.015 (3)	0.015 (3)
C27	0.083 (4)	0.056 (4)	0.068 (4)	0.003 (4)	−0.017 (4)	0.019 (3)
P4	0.0704 (18)	0.0676 (18)	0.0678 (17)	0.0055 (10)	0.0040 (10)	0.0192 (10)
F19	0.084 (5)	0.058 (6)	0.064 (6)	0.004 (5)	−0.023 (5)	0.014 (5)
F20	0.093 (5)	0.063 (5)	0.064 (4)	0.014 (5)	−0.019 (4)	0.011 (4)
F21	0.087 (4)	0.067 (4)	0.073 (4)	0.014 (4)	−0.019 (4)	0.009 (4)
F22	0.080 (6)	0.063 (5)	0.070 (5)	0.003 (5)	−0.018 (5)	0.014 (4)
F23	0.082 (5)	0.059 (4)	0.065 (5)	0.010 (4)	−0.012 (5)	0.011 (4)
F24	0.084 (6)	0.057 (4)	0.077 (5)	0.008 (4)	−0.029 (5)	0.009 (4)
Ru1	0.0176 (2)	0.0165 (2)	0.0185 (2)	0.00384 (13)	0.00650 (13)	0.00763 (14)
Cl1	0.0243 (5)	0.0185 (5)	0.0186 (5)	−0.0003 (4)	0.0055 (4)	0.0041 (4)

Geometric parameters (Å, º)

C1—N2	1.344 (6)	C23—N5	1.354 (6)
C1—C2	1.373 (7)	C23—H23	0.95
C1—H1	0.95	C24—H24A	0.98
C2—C3	1.391 (7)	C24—H24B	0.98

C2—H2	0.95	C24—H24C	0.98
C3—C4	1.391 (6)	N1—O1	1.140 (5)
C3—C6	1.504 (6)	N1—Ru1	1.757 (4)
C4—C5	1.375 (6)	N2—Ru1	2.102 (4)
C4—H4	0.95	N3—Ru1	2.101 (4)
C5—N2	1.348 (6)	N4—Ru1	2.101 (4)
C5—H5	0.95	N5—Ru1	2.101 (4)
C6—H6A	0.98	F1—P1	1.605 (3)
C6—H6B	0.98	F2—P1	1.585 (3)
C6—H6C	0.98	F3—P1	1.607 (3)
C7—N3	1.358 (6)	F4—P1	1.580 (4)
C7—C8	1.369 (6)	F5—P1	1.606 (3)
C7—H7	0.95	F6—P1	1.605 (4)
C8—C9	1.391 (6)	F7—P2	1.600 (12)
C8—H8	0.95	F8—P2	1.590 (11)
C9—C10	1.395 (6)	F9—P2	1.535 (12)
C9—C12	1.495 (6)	F10—P2	1.541 (11)
C10—C11	1.372 (6)	F11—P2	1.572 (16)
C10—H10	0.95	F12—P2	1.645 (12)
C11—N3	1.348 (6)	F7′—P2	1.610 (13)
C11—H11	0.95	F8′—P2	1.621 (14)
C12—H12A	0.98	F9′—P2	1.597 (14)
C12—H12B	0.98	F10′—P2	1.635 (17)
C12—H12C	0.98	F11′—P2	1.603 (13)
C13—N4	1.349 (6)	F12′—P2	1.595 (13)
C13—C14	1.374 (7)	P3—F16	1.484 (19)
C13—H13	0.95	P3—F15	1.489 (16)
C14—C15	1.391 (7)	P3—F18	1.555 (17)
C14—H14	0.95	P3—F17	1.644 (18)
C15—C16	1.387 (7)	P3—F13	1.655 (19)
C15—C18	1.495 (6)	P3—F14	1.658 (19)
C16—C17	1.373 (6)	O2—C26	1.161 (12)
C16—H16	0.95	C25—C26	1.459 (16)
C17—N4	1.353 (6)	C25—H25A	0.98
C17—H17	0.95	C25—H25B	0.98
C18—H18A	0.98	C25—H25C	0.98
C18—H18B	0.98	C26—C27	1.428 (17)
C18—H18C	0.98	C27—H27A	0.98
C19—N5	1.345 (6)	C27—H27B	0.98
C19—C20	1.379 (7)	C27—H27C	0.98
C19—H19	0.95	P4—F21	1.535 (13)
C20—C21	1.389 (7)	P4—F22	1.580 (14)
C20—H20	0.95	P4—F20	1.610 (14)
C21—C22	1.388 (7)	P4—F24	1.620 (13)
C21—C24	1.511 (7)	P4—F23	1.624 (14)
C22—C23	1.380 (7)	P4—F19	1.626 (14)
C22—H22	0.95	Ru1—Cl1	2.3163 (11)

N2—C1—C2	122.7 (4)	F2—P1—F6	89.9 (2)
N2—C1—H1	118.7	F1—P1—F6	90.2 (2)
C2—C1—H1	118.7	F4—P1—F5	90.6 (2)
C1—C2—C3	120.0 (4)	F2—P1—F5	89.52 (19)
C1—C2—H2	120	F1—P1—F5	89.8 (2)
C3—C2—H2	120	F6—P1—F5	179.4 (2)
C2—C3—C4	117.0 (4)	F4—P1—F3	89.9 (2)
C2—C3—C6	120.3 (4)	F2—P1—F3	89.7 (2)
C4—C3—C6	122.7 (4)	F1—P1—F3	179.8 (3)
C5—C4—C3	120.3 (4)	F6—P1—F3	89.9 (2)
C5—C4—H4	119.8	F5—P1—F3	90.1 (2)
C3—C4—H4	119.8	F9—P2—F10	87.3 (6)
N2—C5—C4	122.1 (4)	F9—P2—F11	95.7 (7)
N2—C5—H5	119	F10—P2—F11	95.3 (6)
C4—C5—H5	119	F9—P2—F8	93.5 (6)
C3—C6—H6A	109.5	F10—P2—F8	174.5 (7)
C3—C6—H6B	109.5	F11—P2—F8	90.0 (6)
H6A—C6—H6B	109.5	F12′—P2—F9′	82.8 (7)
C3—C6—H6C	109.5	F9—P2—F7	178.3 (7)
H6A—C6—H6C	109.5	F10—P2—F7	94.2 (6)
H6B—C6—H6C	109.5	F11—P2—F7	84.9 (7)
N3—C7—C8	122.4 (4)	F8—P2—F7	85.0 (6)
N3—C7—H7	118.8	F12′—P2—F11′	175.7 (7)
C8—C7—H7	118.8	F9′—P2—F11′	94.7 (7)
C7—C8—C9	120.4 (4)	F12′—P2—F7′	94.5 (7)
C7—C8—H8	119.8	F9′—P2—F7′	177.0 (8)
C9—C8—H8	119.8	F11′—P2—F7′	87.9 (7)
C8—C9—C10	116.7 (4)	F12′—P2—F8′	89.3 (7)
C8—C9—C12	121.4 (4)	F9′—P2—F8′	89.2 (7)
C10—C9—C12	121.9 (4)	F11′—P2—F8′	87.0 (7)
C11—C10—C9	120.6 (4)	F7′—P2—F8′	89.6 (7)
C11—C10—H10	119.7	F12′—P2—F10′	89.1 (8)
C9—C10—H10	119.7	F9′—P2—F10′	92.8 (7)
N3—C11—C10	122.1 (4)	F11′—P2—F10′	94.6 (8)
N3—C11—H11	118.9	F7′—P2—F10′	88.3 (7)
C10—C11—H11	118.9	F8′—P2—F10′	177.3 (7)
C9—C12—H12A	109.5	F9—P2—F12	89.9 (6)
C9—C12—H12B	109.5	F10—P2—F12	94.1 (6)
H12A—C12—H12B	109.5	F11—P2—F12	169.2 (7)
C9—C12—H12C	109.5	F8—P2—F12	80.4 (6)
H12A—C12—H12C	109.5	F7—P2—F12	89.2 (6)
H12B—C12—H12C	109.5	F16—P3—F15	97.2 (10)
N4—C13—C14	121.9 (4)	F16—P3—F18	82.2 (10)
N4—C13—H13	119	F15—P3—F18	82.2 (10)
C14—C13—H13	119	F16—P3—F17	91.7 (10)
C13—C14—C15	120.7 (4)	F15—P3—F17	90.8 (10)
C13—C14—H14	119.7	F18—P3—F17	170.0 (8)
C15—C14—H14	119.7	F16—P3—F13	107.0 (11)

C16—C15—C14	116.6 (4)	F15—P3—F13	153.1 (10)
C16—C15—C18	122.6 (4)	F18—P3—F13	89.5 (10)
C14—C15—C18	120.8 (4)	F17—P3—F13	99.9 (9)
C17—C16—C15	120.8 (4)	F16—P3—F14	166.5 (10)
C17—C16—H16	119.6	F15—P3—F14	77.2 (9)
C15—C16—H16	119.6	F18—P3—F14	84.9 (10)
N4—C17—C16	121.8 (4)	F17—P3—F14	100.5 (9)
N4—C17—H17	119.1	F13—P3—F14	76.6 (10)
C16—C17—H17	119.1	C26—C25—H25A	109.5
C15—C18—H18A	109.5	C26—C25—H25B	109.5
C15—C18—H18B	109.5	H25A—C25—H25B	109.5
H18A—C18—H18B	109.5	C26—C25—H25C	109.5
C15—C18—H18C	109.5	H25A—C25—H25C	109.5
H18A—C18—H18C	109.5	H25B—C25—H25C	109.5
H18B—C18—H18C	109.5	O2—C26—C27	123.4 (12)
N5—C19—C20	122.3 (5)	O2—C26—C25	119.9 (11)
N5—C19—H19	118.9	C27—C26—C25	116.5 (10)
C20—C19—H19	118.9	C26—C27—H27A	109.5
C19—C20—C21	120.1 (5)	C26—C27—H27B	109.5
C19—C20—H20	119.9	H27A—C27—H27B	109.5
C21—C20—H20	119.9	C26—C27—H27C	109.5
C22—C21—C20	117.4 (4)	H27A—C27—H27C	109.5
C22—C21—C24	122.4 (5)	H27B—C27—H27C	109.5
C20—C21—C24	120.3 (5)	F21—P4—F22	109.3 (13)
C23—C22—C21	120.1 (5)	F21—P4—F20	73.6 (12)
C23—C22—H22	119.9	F22—P4—F20	172.8 (12)
C21—C22—H22	119.9	F21—P4—F24	94.8 (11)
N5—C23—C22	122.0 (4)	F22—P4—F24	89.3 (11)
N5—C23—H23	119	F20—P4—F24	83.8 (11)
C22—C23—H23	119	F21—P4—F23	93.5 (11)
C21—C24—H24A	109.5	F22—P4—F23	102.7 (11)
C21—C24—H24B	109.5	F20—P4—F23	83.6 (11)
H24A—C24—H24B	109.5	F24—P4—F23	162.2 (14)
C21—C24—H24C	109.5	F21—P4—F19	158.8 (13)
H24A—C24—H24C	109.5	F22—P4—F19	91.9 (11)
H24B—C24—H24C	109.5	F20—P4—F19	85.5 (11)
O1—N1—Ru1	179.0 (4)	F24—P4—F19	86.5 (10)
C1—N2—C5	117.9 (4)	F23—P4—F19	80.2 (10)
C1—N2—Ru1	119.9 (3)	N1—Ru1—N3	91.79 (16)
C5—N2—Ru1	122.1 (3)	N1—Ru1—N4	92.55 (15)
C11—N3—C7	117.8 (4)	N3—Ru1—N4	89.70 (14)
C11—N3—Ru1	122.3 (3)	N1—Ru1—N5	91.84 (16)
C7—N3—Ru1	119.9 (3)	N3—Ru1—N5	176.37 (14)
C13—N4—C17	118.1 (4)	N4—Ru1—N5	90.17 (14)
C13—N4—Ru1	119.6 (3)	N1—Ru1—N2	91.71 (16)
C17—N4—Ru1	122.2 (3)	N3—Ru1—N2	89.97 (14)
C19—N5—C23	118.1 (4)	N4—Ru1—N2	175.74 (14)
C19—N5—Ru1	119.5 (3)	N5—Ru1—N2	89.90 (15)

C23—N5—Ru1	122.4 (3)	N1—Ru1—Cl1	179.52 (13)
F4—P1—F2	179.6 (2)	N3—Ru1—Cl1	88.51 (10)
F4—P1—F1	89.9 (2)	N4—Ru1—Cl1	87.83 (10)
F2—P1—F1	90.4 (2)	N5—Ru1—Cl1	87.86 (11)
F4—P1—F6	90.0 (2)	N2—Ru1—Cl1	87.92 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F8	0.95	2.47	3.194 (12)	133
C1—H1···F11	0.95	2.48	3.405 (15)	165
C1—H1···F10′	0.95	2.3	3.243 (18)	173
C5—H5···F3	0.95	2.49	3.328 (6)	147
C7—H7···O2	0.95	2.45	3.320 (7)	153
C7—H7···F20	0.95	2.51	3.264 (18)	136
C13—H13···F22^{i}	0.95	2.54	3.16 (2)	123
C13—H13···F23^{i}	0.95	2.26	3.047 (18)	140
C14—H14···F19^{i}	0.95	2.4	2.995 (18)	120
C27—H27*A*···F7	0.98	2.41	3.297 (17)	150
C27—H27*B*···F7^{ii}	0.98	2.55	3.418 (17)	147

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