Δ-Bis[(S)-2-(4-isopropyl-4,5-dihydrooxazol-2-yl)-phenolato-κ^2N,O^1](1,10-phenanthroline-κ^2N,N')-ruthenium(III) hexafluoridophosphate

Monsuru T. Kelani,* Alfred Muller and Koop Lammertsma

Department of Chemical Sciences, University of Johannesburg, Auckland Park, 2006, Johannesburg, South Africa. *Correspondence e-mail: mansieurkelani@gmail.com

The title compound, [Ru(C$_{12}$H$_{14}$NO$_2$)$_2$(C$_{12}$H$_8$N$_2$)]PF$_6$ crystallizes in the tetragonal Sohnke space group $P4_12_12$. The two bidentate chiral salicyloxazoline ligands and the phenanthroline co-ligand coordinate to the central Ru^{III} atom through N,O and N,N atom pairs to form bite angles of 89.76 (15) and 79.0 (2)°, respectively. The octahedral coordination of the bidentate ligands leads to a propeller-like shape, which induces metal-centered chirality onto the complex, with a right-handed (Δ) absolute configuration [the Flack parameter value is −0.003 (14)]. Both the complex cation and the disordered PF$_6$$^-$ counter-anion are located on twofold rotation axes. Apart from Coulombic forces, the crystal cohesion is ensured by non-classical C—H···O and C—H···F interactions.

3D view

Chemical scheme
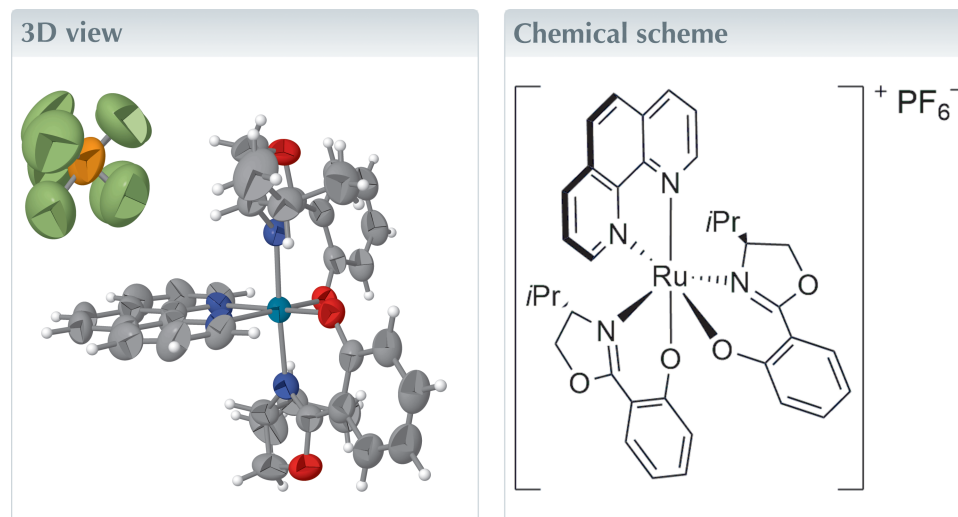
Structure description

The syntheses of optically pure metal complexes are usually costly and sophisticated, especially with the use of traditional methods for the resolution of racemic mixtures. A straightforward alternative strategy, therefore, requires the coordination of pure chiral auxiliary ligands tailored for the selective synthesis of diastereomers, which are easily converted to the corresponding enantiomerically pure complexes (Knof & von Zelewsky, 1999). Hayoz and co-workers were the first to report the diastereoselective synthesis of optically pure ruthenium polypyridyl complexes in the quest for generating compounds with metal-centered chirality, so-called chiral-at-metal complexes (Hayoz *et al.*, 1993). Such metal-centered chirality refers to the type of chirality induced at a central metal atom as a result of an helical octahedral coordination around a metal in bis-chelate or tris-chelate systems. In this context, optically pure salicyloxazoline is often used as an auxiliary ligand to implement and control the absolute configuration at central metal atoms during ligand exchange. In this case, the absolute configurations at the central metal could either be right-handed or left-handed twist systems, which are symbolized by
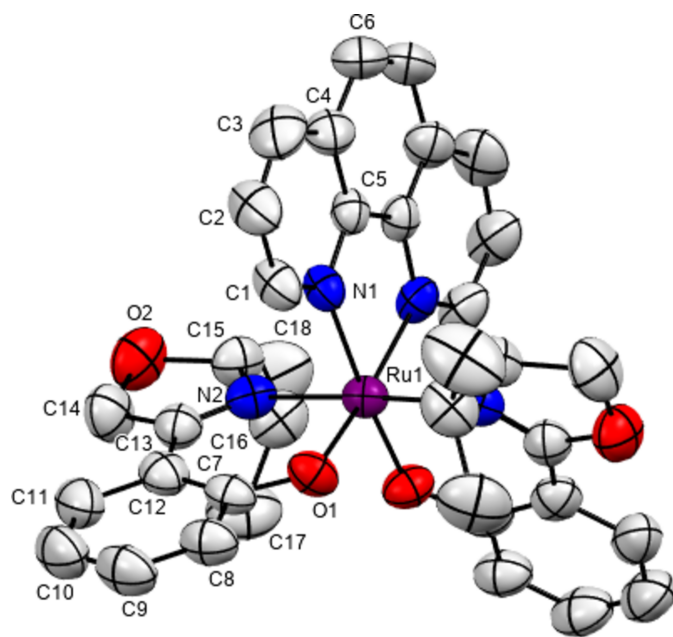
Table 1
Hydrogen-bond geometry (Å, °).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C1—H1$\cdots$O1[i]	0.95	2.59	3.102 (6)	114
C16—H16$\cdots$O1[i]	1.00	2.53	3.224 (6)	126
C17—H17$A\cdots$F3[ii]	0.98	2.52	3.464 (11)	162
C18—H18$A\cdots$F2	0.98	2.48	3.357 (12)	149

Symmetry codes: (i) $y, x, -z + 1$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{7}{4}$.

Δ and Λ stereochemical descriptors, respectively (Gong *et al.*, 2010). The salicyloxazoline ligand is often used in this manner because of its reversible coordination upon acid protonation of its phenolate group while leaving the stereochemistry of the metal complex intact (Gong *et al.*, 2009, 2010, 2013).

The complex cation of the title salt constitutes of two optically pure bidentate salicyloxazoline ligands and a phenanthroline co-ligand arranged within an octahedral coordination sphere around the central Ru^{III} atom, which is located about a twofold rotation axis bisecting the phenanthroline ligand (Fig. 1). This right-handed twist of the ligands leads to a Δ stereochemical configuration of the complex; the correctness of the absolute configuration is indicated by a Flack parameter (Parsons *et al.*, 2013) value of −0.003 (14). The bite angles, 89.76 (15)°, for the salicyloxazoline ligands are comparable with reported values, *e.g.* 86.68° (Brunner *et al.*, 1998), 88.29° (Davenport *et al.*, 2004), 86.88° (Kelani *et al.*, 2024), or 90.00 (Gong *et al.*, 2010) while that for the phenanthroline ligand, 79.0 (2)°, is almost similar to that of 80.12° (Gong *et al.*, 2010). The bond lengths of the Ru^{III} atom with the ligating atoms of 1.974 (3), 2.079 (4) and 2.072 (4) Å to O1, N1(phenanthroline) and N2(salicyloxazoline) atoms, respectively, also agree well with reported values. The crystal packing
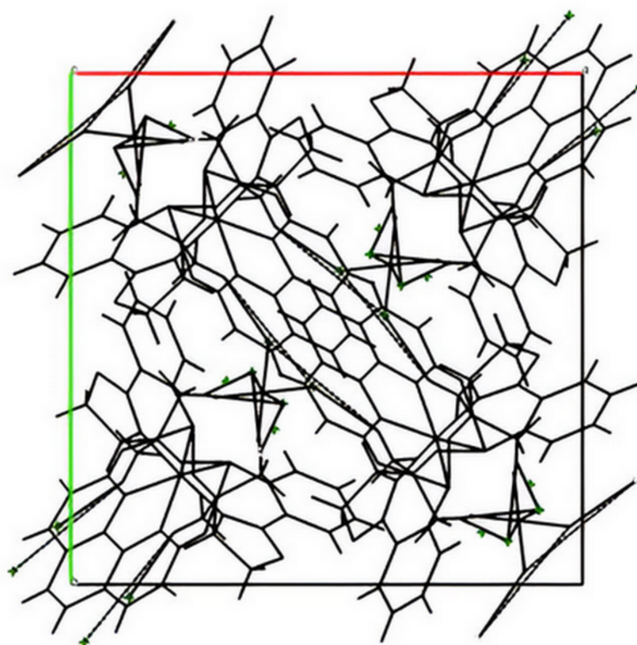
(Fig. 2) includes the disordered PF$_6^-$ counter-anion (located about a twofold rotation axis). Non-classical intermolecular interactions featuring C—H$\cdots$O and C—H$\cdots$F contacts (Table 1) are present.

Synthesis and crystallization

Dichlorido-bis(1,10-phenanthroline)ruthenium(II) (50.0 mg, 0.09 mmol, 1 eq) was added to (*S*)-isopropyl-2-(2-hydroxyphenyl)oxazoline (38.5 mg, 0.2 mmol, 2 eq) in ethanol in the presence of K$_2$CO$_3$ (26.0 mg, 0.2 mmol, 2 eq). The reaction mixture was refluxed for 6 h under continuous stirring after which it was cooled to room temperature and then concentrated *in vacuo* under reduced pressure. The crude product was purified by column chromatography with silica gel using a solvent system of CH$_2$Cl$_2$:CH$_3$OH:CH$_3$CN = 9.7:0.2:0.1 *v:v:v*) to obtain a purple crystalline compound. Yield, 31 mg (46%, 0.04 mmol).

Refinement

Details of the data collection, solution and refinement are given in Table 2. The disordered PF$_6^-$ anion was treated as equally disordered around the twofold rotation axis and was kept stable with SADI, SIMU and DELU restraints in *SHELXL* (Sheldrick, 2015*b*). The highest remaining maximum and minimum electron density are 1.32 and 0.76 Å away from F1*A* and Ru1, respectively.

Figure 1
The molecular structure of the title compound drawn with displacement ellipsoids at the 50% probability level; hydrogen atoms and the PF$_6^-$ counter-anion were removed for clarity. Non-labelled atoms are generated by a twofold rotation axis (symmetry operation: $y, x, -z$).

Figure 2
Crystal packing arrangement of the title compound in a view along the *c* axis. Non-classical hydrogen-bonding interactions are indicated by dotted lines.

Acknowledgements

References

Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Brunner, H., Nuber, B. & Prommesberger, M. (1998). *Tetrahedron Asymmetry*, **9**, 3223–3229.

Davenport, A. J., Davies, D. L., Fawcett, J. & Russell, D. R. (2004). *Dalton Trans.* **9**, 1481–1492.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Gong, L., Mulcahy, S. P., Devarajan, D., Harms, K., Frenking, G. & Meggers, E. (2010). *Inorg. Chem.* **49**, 7692–7699.

Gong, L., Mulcahy, S. P., Harms, K. & Meggers, E. (2009). *J. Am. Chem. Soc.* **131**, 9602–9603.

Gong, L., Wenzel, M. & Meggers, E. (2013). *Acc. Chem. Res.* **46**, 2635–2644.

Hayoz, P., von Zelewsky, A. & Stoeckli-Evans, H. (1993). *J. Am. Chem. Soc.* **115**, 5111–5114.

Kelani, M. T., Muller, A. & Lammertsma, K. (2024). *IUCrData*, **9**, x240720.

Knof, U. & von Zelewsky, A. (1999). *Angew. Chem. Int. Ed.* **38**, 302–322.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ru(C_{12}H_{14}NO_2)_2(C_{12}H_8N_2)]PF_6$
M_r	834.73
Crystal system, space group	Tetragonal, $P4_12_12$
Temperature (K)	173
a, c (Å)	15.3094 (13), 15.315 (2)
V (Å^3)	3589.5 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.56
Crystal size (mm)	$0.46 \times 0.43 \times 0.42$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.638, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53896, 4516, 3564
R_{int}	0.067
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.107, 1.04
No. of reflections	4516
No. of parameters	245
No. of restraints	26
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.41
Absolute structure	Flack x determined using 1296 quotients [$(I^+)-(I^-)$]/[$(I^+)+(I^-)$] (Parsons *et al.*, 2013)
Absolute structure parameter	−0.003 (14)

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 2012).

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

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Crystal data

$[Ru(C_{12}H_{14}NO_2)_2(C_{12}H_8N_2)]PF_6$	$D_x = 1.545$ Mg m^{-3}
$M_r = 834.73$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Tetragonal, $P4_12_12$	Cell parameters from 8341 reflections
$a = 15.3094$ (13) Å	$\theta = 2.3–20.4°$
$c = 15.315$ (2) Å	$\mu = 0.56$ mm^{-1}
$V = 3589.5$ (8) Å^3	$T = 173$ K
$Z = 4$	Cuboid, purple
$F(000) = 1700$	$0.46 \times 0.43 \times 0.42$ mm

Data collection

Bruker APEXII CCD diffractometer	53896 measured reflections
Radiation source: sealed-tube	4516 independent reflections
Triumph monochromator	3564 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.067$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$\theta_{max} = 28.4°$, $\theta_{min} = 1.9°$
$T_{min} = 0.638$, $T_{max} = 0.746$	$h = -20 \rightarrow 20$
	$k = -20 \rightarrow 20$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.7144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
4516 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
245 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
26 restraints	Absolute structure: Flack x determined using 1296 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	Absolute structure parameter: −0.003 (14)

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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2882 (4)	0.4278 (4)	0.6429 (3)	0.0615 (13)	
H1	0.237967	0.400278	0.666771	0.074*	
C2	0.3215 (4)	0.5005 (4)	0.6832 (4)	0.0760 (18)	
H2	0.294934	0.521584	0.735125	0.091*	
C3	0.3917 (5)	0.5426 (4)	0.6499 (4)	0.0828 (19)	
H3	0.412522	0.594417	0.676826	0.099*	
C4	0.4345 (4)	0.5090 (4)	0.5742 (4)	0.0615 (13)	
C5	0.3979 (3)	0.4353 (3)	0.5381 (3)	0.0463 (10)	
C6	0.5100 (4)	0.5455 (4)	0.5356 (4)	0.0723 (16)	
H6	0.535851	0.595990	0.560765	0.087*	
C7	0.3015 (3)	0.1129 (3)	0.4108 (3)	0.0539 (12)	
C8	0.2786 (4)	0.0607 (4)	0.3381 (3)	0.0678 (14)	
H8	0.238849	0.082913	0.295931	0.081*	
C9	0.3130 (5)	−0.0217 (4)	0.3273 (4)	0.0815 (19)	
H9	0.295857	−0.055716	0.278301	0.098*	
C10	0.3710 (5)	−0.0552 (4)	0.3853 (5)	0.0852 (19)	
H10	0.393287	−0.112595	0.377536	0.102*	
C11	0.3975 (4)	−0.0054 (4)	0.4556 (5)	0.0759 (17)	
H11	0.439237	−0.028411	0.495301	0.091*	
C12	0.3633 (4)	0.0795 (3)	0.4695 (3)	0.0592 (12)	
C13	0.3904 (3)	0.1261 (4)	0.5476 (3)	0.0553 (12)	
C14	0.4704 (4)	0.1478 (5)	0.6678 (4)	0.0838 (19)	
H14A	0.529714	0.171713	0.658200	0.101*	
H14B	0.468526	0.119533	0.725909	0.101*	
C15	0.4011 (3)	0.2208 (4)	0.6615 (3)	0.0618 (13)	
H15	0.430056	0.279348	0.662139	0.074*	
C16	0.3308 (4)	0.2163 (4)	0.7321 (3)	0.0730 (15)	
H16	0.285475	0.260943	0.717068	0.088*	
C17	0.2847 (5)	0.1280 (5)	0.7371 (4)	0.102 (2)	
H17A	0.240548	0.129560	0.783417	0.152*	
H17B	0.256291	0.115575	0.681064	0.152*	
H17C	0.327529	0.082258	0.749904	0.152*	
C18	0.3698 (6)	0.2424 (7)	0.8209 (4)	0.122 (3)	
H18A	0.398851	0.299210	0.815570	0.183*	
H18B	0.323026	0.246367	0.864392	0.183*	
H18C	0.412379	0.198299	0.839249	0.183*	
N1	0.3248 (2)	0.3946 (3)	0.5709 (2)	0.0483 (9)	
N2	0.3638 (3)	0.2026 (3)	0.5728 (2)	0.0523 (9)	
O1	0.2614 (2)	0.1896 (2)	0.4175 (2)	0.0570 (9)	

O2	0.4479 (3)	0.0854 (3)	0.5994 (3)	0.0767 (11)	
F1A	0.6349 (16)	0.2780 (8)	0.7374 (14)	0.203 (8)	0.5
F1B	0.6026 (17)	0.3041 (13)	0.8114 (17)	0.250 (11)	0.5
F2	0.5257 (5)	0.3866 (6)	0.7660 (8)	0.247 (5)	
F3	0.6459 (7)	0.4151 (7)	0.8395 (6)	0.241 (4)	
P1	0.6246 (2)	0.3754 (2)	0.750000	0.1405 (16)	
Ru1	0.28566 (2)	0.28566 (2)	0.500000	0.04461 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.049 (3)	0.084 (4)	0.051 (2)	0.001 (3)	0.006 (2)	−0.025 (2)
C2	0.064 (3)	0.093 (4)	0.072 (3)	0.001 (3)	0.007 (3)	−0.046 (3)
C3	0.096 (5)	0.072 (4)	0.080 (4)	0.000 (3)	−0.015 (4)	−0.036 (3)
C4	0.060 (3)	0.062 (3)	0.063 (3)	−0.004 (2)	−0.009 (3)	−0.013 (3)
C5	0.046 (2)	0.048 (2)	0.046 (2)	0.0082 (19)	−0.0020 (19)	−0.0070 (19)
C6	0.067 (4)	0.060 (3)	0.090 (4)	−0.017 (3)	−0.005 (3)	−0.006 (3)
C7	0.063 (3)	0.050 (3)	0.049 (2)	−0.013 (2)	0.009 (2)	−0.0008 (19)
C8	0.076 (4)	0.068 (3)	0.060 (3)	−0.015 (3)	0.009 (3)	−0.015 (3)
C9	0.098 (5)	0.065 (4)	0.081 (4)	−0.015 (3)	0.020 (4)	−0.025 (3)
C10	0.091 (5)	0.059 (4)	0.106 (5)	−0.001 (3)	0.021 (4)	−0.018 (4)
C11	0.069 (4)	0.060 (3)	0.099 (4)	0.001 (3)	0.020 (3)	−0.003 (3)
C12	0.063 (3)	0.056 (3)	0.060 (3)	−0.006 (2)	0.013 (2)	0.005 (2)
C13	0.055 (3)	0.057 (3)	0.054 (3)	−0.001 (2)	0.004 (2)	0.004 (2)
C14	0.078 (4)	0.108 (5)	0.066 (3)	0.011 (4)	−0.018 (3)	0.017 (4)
C15	0.063 (3)	0.073 (3)	0.049 (2)	−0.003 (3)	−0.012 (2)	0.005 (3)
C16	0.076 (3)	0.098 (4)	0.044 (3)	−0.001 (4)	−0.003 (2)	0.001 (3)
C17	0.110 (5)	0.124 (6)	0.071 (4)	−0.029 (5)	0.013 (4)	0.019 (4)
C18	0.125 (6)	0.195 (10)	0.047 (3)	−0.025 (6)	−0.005 (4)	−0.020 (4)
N1	0.042 (2)	0.061 (2)	0.0424 (18)	0.0039 (17)	−0.0001 (16)	−0.0117 (17)
N2	0.054 (2)	0.064 (3)	0.0390 (16)	−0.0075 (19)	−0.0008 (16)	0.0044 (19)
O1	0.071 (2)	0.0503 (19)	0.0500 (17)	−0.0074 (16)	−0.0063 (16)	−0.0046 (14)
O2	0.082 (3)	0.072 (3)	0.075 (3)	0.009 (2)	−0.015 (2)	0.012 (2)
F1A	0.29 (2)	0.091 (7)	0.225 (17)	0.020 (10)	−0.067 (18)	−0.003 (11)
F1B	0.24 (2)	0.145 (16)	0.36 (3)	−0.025 (16)	0.01 (2)	0.080 (16)
F2	0.149 (6)	0.235 (9)	0.357 (14)	−0.025 (6)	−0.022 (8)	−0.047 (11)
F3	0.268 (10)	0.262 (11)	0.194 (8)	−0.019 (9)	−0.078 (8)	−0.046 (8)
P1	0.1223 (17)	0.1223 (17)	0.177 (4)	−0.025 (2)	−0.051 (2)	−0.051 (2)
Ru1	0.04954 (19)	0.04954 (19)	0.0347 (2)	−0.0046 (2)	0.00213 (16)	−0.00213 (16)

Geometric parameters (Å, º)

C1—N1	1.337 (5)	C13—N2	1.299 (7)
C1—C2	1.370 (8)	C13—O2	1.338 (6)
C1—H1	0.9500	C14—O2	1.458 (7)
C2—C3	1.353 (9)	C14—C15	1.544 (8)
C2—H2	0.9500	C14—H14A	0.9900
C3—C4	1.426 (8)	C14—H14B	0.9900

C3—H3	0.9500	C15—N2	1.499 (6)
C4—C5	1.375 (7)	C15—C16	1.528 (7)
C4—C6	1.414 (8)	C15—H15	1.0000
C5—N1	1.376 (6)	C16—C17	1.527 (10)
C5—C5ⁱ	1.421 (8)	C16—C18	1.538 (8)
C6—C6ⁱ	1.335 (12)	C16—H16	1.0000
C6—H6	0.9500	C17—H17A	0.9800
C7—O1	1.329 (6)	C17—H17B	0.9800
C7—C12	1.402 (7)	C17—H17C	0.9800
C7—C8	1.414 (7)	C18—H18A	0.9800
C8—C9	1.377 (9)	C18—H18B	0.9800
C8—H8	0.9500	C18—H18C	0.9800
C9—C10	1.356 (10)	N1—Ru1	2.079 (4)
C9—H9	0.9500	N2—Ru1	2.072 (4)
C10—C11	1.380 (9)	O1—Ru1	1.974 (3)
C10—H10	0.9500	F1A—P1	1.512 (12)
C11—C12	1.418 (8)	F1B—P1	1.479 (14)
C11—H11	0.9500	F2—P1	1.544 (8)
C12—C13	1.453 (7)	F3—P1	1.535 (8)
N1—C1—C2	121.6 (5)	H17A—C17—H17B	109.5
N1—C1—H1	119.2	C16—C17—H17C	109.5
C2—C1—H1	119.2	H17A—C17—H17C	109.5
C3—C2—C1	120.8 (5)	H17B—C17—H17C	109.5
C3—C2—H2	119.6	C16—C18—H18A	109.5
C1—C2—H2	119.6	C16—C18—H18B	109.5
C2—C3—C4	120.0 (5)	H18A—C18—H18B	109.5
C2—C3—H3	120.0	C16—C18—H18C	109.5
C4—C3—H3	120.0	H18A—C18—H18C	109.5
C5—C4—C6	119.3 (5)	H18B—C18—H18C	109.5
C5—C4—C3	115.8 (5)	C1—N1—C5	118.0 (4)
C6—C4—C3	124.9 (5)	C1—N1—Ru1	127.9 (4)
C4—C5—N1	123.8 (4)	C5—N1—Ru1	114.1 (3)
C4—C5—C5ⁱ	119.8 (3)	C13—N2—C15	108.5 (4)
N1—C5—C5ⁱ	116.4 (2)	C13—N2—Ru1	125.1 (3)
C6ⁱ—C6—C4	120.9 (3)	C15—N2—Ru1	126.4 (4)
C6ⁱ—C6—H6	119.5	C7—O1—Ru1	128.4 (3)
C4—C6—H6	119.5	C13—O2—C14	106.1 (4)
O1—C7—C12	125.7 (4)	F1B—P1—F1Bⁱⁱ	138 (2)
O1—C7—C8	116.5 (5)	F1B—P1—F1Aⁱⁱ	93.8 (14)
C12—C7—C8	117.8 (5)	F1Bⁱⁱ—P1—F1Aⁱⁱ	51.5 (10)
C9—C8—C7	121.1 (6)	F1A—P1—F1Aⁱⁱ	79.1 (18)
C9—C8—H8	119.4	F1B—P1—F3	76.9 (11)
C7—C8—H8	119.4	F1Bⁱⁱ—P1—F3	108.7 (11)
C10—C9—C8	121.2 (6)	F1A—P1—F3	118.9 (9)
C10—C9—H9	119.4	F1Aⁱⁱ—P1—F3	73.6 (8)
C8—C9—H9	119.4	F1B—P1—F3ⁱⁱ	108.7 (11)
C9—C10—C11	119.6 (6)	F1Bⁱⁱ—P1—F3ⁱⁱ	76.9 (11)

C9—C10—H10	120.2	F1A—P1—F3^{ii}	73.6 (8)
C11—C10—H10	120.2	F1A^{ii}—P1—F3^{ii}	118.9 (9)
C10—C11—C12	121.0 (7)	F3—P1—F3^{ii}	165.1 (9)
C10—C11—H11	119.5	F1B—P1—F2	75.9 (10)
C12—C11—H11	119.5	F1B^{ii}—P1—F2	143.1 (12)
C7—C12—C11	119.1 (5)	F1A—P1—F2	103.4 (10)
C7—C12—C13	122.9 (5)	F1A^{ii}—P1—F2	163.5 (9)
C11—C12—C13	117.9 (5)	F3—P1—F2	91.3 (7)
N2—C13—O2	116.7 (4)	F3^{ii}—P1—F2	77.1 (5)
N2—C13—C12	126.7 (5)	F1B—P1—F2^{ii}	143.1 (12)
O2—C13—C12	116.6 (5)	F1B^{ii}—P1—F2^{ii}	75.9 (10)
O2—C14—C15	105.4 (4)	F1A—P1—F2^{ii}	163.5 (9)
O2—C14—H14A	110.7	F1A^{ii}—P1—F2^{ii}	103.4 (10)
C15—C14—H14A	110.7	F3—P1—F2^{ii}	77.1 (5)
O2—C14—H14B	110.7	F3^{ii}—P1—F2^{ii}	91.3 (7)
C15—C14—H14B	110.7	F2—P1—F2^{ii}	78.9 (8)
H14A—C14—H14B	108.8	O1—Ru1—O1^{i}	97.4 (2)
N2—C15—C16	111.3 (4)	O1—Ru1—N2	89.76 (15)
N2—C15—C14	100.6 (4)	O1^{i}—Ru1—N2	88.30 (15)
C16—C15—C14	114.1 (5)	O1—Ru1—N2^{i}	88.30 (15)
N2—C15—H15	110.2	O1^{i}—Ru1—N2^{i}	89.77 (15)
C16—C15—H15	110.2	N2—Ru1—N2^{i}	177.1 (2)
C14—C15—H15	110.2	O1—Ru1—N1	170.53 (15)
C17—C16—C15	113.6 (5)	O1^{i}—Ru1—N1	91.80 (15)
C17—C16—C18	111.4 (5)	N2—Ru1—N1	92.57 (16)
C15—C16—C18	109.9 (5)	N2^{i}—Ru1—N1	89.70 (15)
C17—C16—H16	107.2	O1—Ru1—N1^{i}	91.80 (15)
C15—C16—H16	107.2	O1^{i}—Ru1—N1^{i}	170.53 (15)
C18—C16—H16	107.2	N2—Ru1—N1^{i}	89.70 (15)
C16—C17—H17A	109.5	N2^{i}—Ru1—N1^{i}	92.56 (16)
C16—C17—H17B	109.5	N1—Ru1—N1^{i}	79.0 (2)
N1—C1—C2—C3	1.6 (10)	O2—C14—C15—N2	−15.9 (6)
C1—C2—C3—C4	−2.9 (11)	O2—C14—C15—C16	103.4 (5)
C2—C3—C4—C5	2.0 (9)	N2—C15—C16—C17	58.9 (7)
C2—C3—C4—C6	−177.6 (7)	C14—C15—C16—C17	−54.2 (7)
C6—C4—C5—N1	179.7 (5)	N2—C15—C16—C18	−175.5 (6)
C3—C4—C5—N1	0.1 (8)	C14—C15—C16—C18	71.4 (8)
C6—C4—C5—C5^{i}	−1.3 (9)	C2—C1—N1—C5	0.5 (8)
C3—C4—C5—C5^{i}	179.1 (6)	C2—C1—N1—Ru1	179.8 (5)
C5—C4—C6—C6^{i}	0.8 (11)	C4—C5—N1—C1	−1.3 (7)
C3—C4—C6—C6^{i}	−179.6 (7)	C5^{i}—C5—N1—C1	179.6 (5)
O1—C7—C8—C9	−176.8 (5)	C4—C5—N1—Ru1	179.2 (4)
C12—C7—C8—C9	2.8 (8)	C5^{i}—C5—N1—Ru1	0.2 (6)
C7—C8—C9—C10	−1.0 (10)	O2—C13—N2—C15	−5.2 (6)
C8—C9—C10—C11	−1.2 (10)	C12—C13—N2—C15	173.8 (5)
C9—C10—C11—C12	1.6 (10)	O2—C13—N2—Ru1	173.3 (3)
O1—C7—C12—C11	177.1 (5)	C12—C13—N2—Ru1	−7.7 (7)

C8—C7—C12—C11	−2.4 (7)	C16—C15—N2—C13	−108.2 (5)
O1—C7—C12—C13	1.0 (8)	C14—C15—N2—C13	13.0 (6)
C8—C7—C12—C13	−178.5 (5)	C16—C15—N2—Ru1	73.3 (6)
C10—C11—C12—C7	0.3 (8)	C14—C15—N2—Ru1	−165.4 (4)
C10—C11—C12—C13	176.5 (5)	C12—C7—O1—Ru1	8.7 (7)
C7—C12—C13—N2	−1.2 (8)	C8—C7—O1—Ru1	−171.7 (3)
C11—C12—C13—N2	−177.3 (5)	N2—C13—O2—C14	−5.9 (6)
C7—C12—C13—O2	177.9 (5)	C12—C13—O2—C14	175.0 (5)
C11—C12—C13—O2	1.7 (7)	C15—C14—O2—C13	13.9 (6)

Symmetry codes: (i) $y, x, -z+1$; (ii) $-y+1, -x+1, -z+3/2$.

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C1—H1⋯O1[i]	0.95	2.59	3.102 (6)	114
C16—H16⋯O1[i]	1.00	2.53	3.224 (6)	126
C17—H17*A*⋯F3[iii]	0.98	2.52	3.464 (11)	162
C18—H18*A*⋯F2	0.98	2.48	3.357 (12)	149

Symmetry codes: (i) $y, x, -z+1$; (iii) $x-1/2, -y+1/2, -z+7/4$.