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Crystal structure of *cis*(*S*),*trans*(*O*,N_{bpy})-(2,2′-bipyridyl-κ^2N,N')bis(dimethyl sulfoxide-κS)-[phenyl(pyridin-2-yl)methanone-κ^2N,O]-ruthenium(II) bis(trifluoromethanesulfonate)

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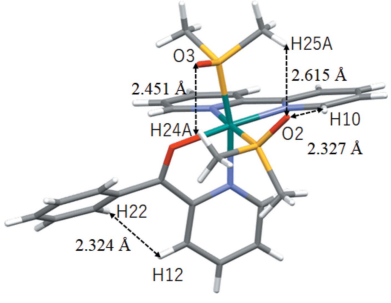
CCDC references: 2215310; 2215311

Supporting information: this article has supporting information at journals.iucr.org/e

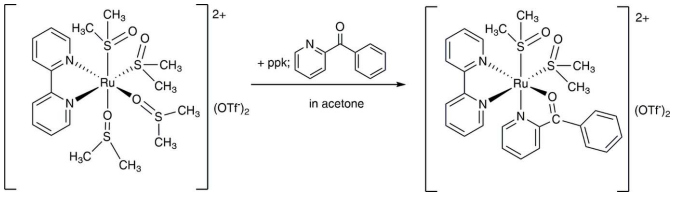
The molecular and crystal structures of the title complex, $[Ru(C_{10}H_8N_2)(C_{12}H_9NO)(C_2H_6OS)_2](CF_3O_3S)_2$ or *cis*(S),*trans*(O,N_{bpy})-[Ru(bpy)(ppk)(dmso-*S*)$_2$](OTf)$_2$ {bpy = 2,2′-bipyridine, ppk = phenyl-2-pyridyl ketone [IUPAC nomenclature: phenyl(pyridine-2-yl)methanone], dmso = dimethyl sulfoxide, and OTf^- = trifluoromethanesulfonate}, are reported. The Ru^{2+} ion has a distorted octahedral geometry with two bpy N atoms, the N and O atoms of ppk, and two S atoms of two *cis* dmso-*S* ligands. The carbonyl O atom of ppk is *trans* to bpy, and the N atom of pyridyl is *trans* to the dmso-*S* ligand [*trans*(O,N_{bpy}) geometry]. One of the trifluoromethanesulfonate anions is disordered over three positions, with occupancies of 0.4, 0.4, and 0.2, respectively, in the refined model. The original disordered and SQUEEZE [Spek (2015). *Acta Cryst.* C**71**, 9–18] models were found to be almost equivalent, indicating that both the SQUEEZE and the original disordered model are satisfactory.

1. Chemical context

Polypyridyl ruthenium(II) complexes have gained interest because of their unique photochemical and photophysical properties. Many homoleptic and bis-heteroleptic polypyridyl ruthenium(II) complexes have been synthesized, and their properties have been investigated (Gao *et al.*, 2008; Patra *et al.*, 2021). However, there are fewer studies on trisheteroleptic complexes, *i.e.* $[Ru(L1\text{-}L1)(L2\text{-}L2)(L3\text{-}L3)]^{2+}$, than on bis-heteroleptic complexes, *i.e.* $[Ru(L\text{-}L1)_2(L2\text{-}L2)]^{2+}$, (Spiccia *et al.*, 2004). The difference can be traced to the limited suitable precursors for the trisheteroleptic complexes, such as *cis*-$[Ru(L1\text{-}L1)(L2\text{-}L2)(X)_2]^{2+}$ (*X* = labile monodentate ligand) complexes. We have reported the synthesis, crystal structure, and substitution reaction of *trans*(*O*,*S*)-[Ru(bpy)(dmso-*S*)$_2$(dmso-*O*)$_2$](OTf)$_2$ (bpy = 2,2′-bipyridine, dmso = dimethyl sulfoxide, and OTf^- = trifluoromethanesulfonate), in which two dmso-*O* ligands were easily substituted by another bidentate ligand, *e.g.*, 1,10-phenanthroline (phen), to form *cis*-[Ru(bpy)(phen)(dmso-*S*)$_2$](OTf)$_2$ (Toyama *et al.*, 2018). To investigate the potential synthetic utility of *trans*(*O*,*S*)-[Ru(bpy)(dmso-*S*)$_2$(dmso-*O*)$_2$](OTf)$_2$ as a precursor, further complexes with different types of ligands must be synthesized. To this end, we became interested in unsymmetrical bidentate κ^2N,O-pyridyl ligands because of the selectivity and reactivity of the resulting geometrical isomers. We have previously reported the syntheses and structures of heteroleptic ruthenium(II) complexes with picolinate (pic^-) (Toyama *et al.*,



2017) and 2-picolinamide (H_2pia) (Toyama *et al.*, 2019), which are coordinated to the Ru^{2+} ion *via* a pyridyl N and a carbonic O^- or a carbonyl O atom. In our current work, phenyl-2-pyridyl ketone [ppk, IUPAC nomenclature : phenyl(pyridine-2-yl)methanone] has been chosen as a κ^2N,O-pyridyl ligand. Herein, we report the crystal structure of *cis*(*S*),-*trans*(*O*,N_{bpy})-[Ru(bpy)(ppk)(dmso-*S*)$_2$](OTf)$_2$. Notably, ppk is an analog of di-2-pyridyl ketone (dpk), which has three coordination modes: dpk–κ^2N,O, dpk–κ^2N,N', and dpk–OH-κ^3N,O,N' (Toyama *et al.*, 2007) and has attracted significant research attention. However, it is difficult to synthesize and control the stereoselectivity of complexes with dpk ligands. The ppk ligand is known to be analogous to the dpk ligand in the κ^2N,O coordination mode and hence has been used in our current synthesis to ease the complexity of syntheses with the dpk ligand.



2. Structural commentary

An *ORTEP* view of *cis*(*S*),*trans*(*O*,N_{bpy})-[Ru(bpy)(ppk)-(dmso-*S*)$_2$](OTf)$_2$ is shown in Fig. 1. The Ru^{2+} ion has a distorted octahedral geometry with two bpy N atoms, the N and O atoms of ppk, and the S atoms of the two dmso-*S* ligands, which are *cis* to each other. The O atom of the carbonyl group of the ppk ligand is *trans* to the bpy ligand, and the N atom of the pyridyl group is *trans* to the dmso-*S* ligand,

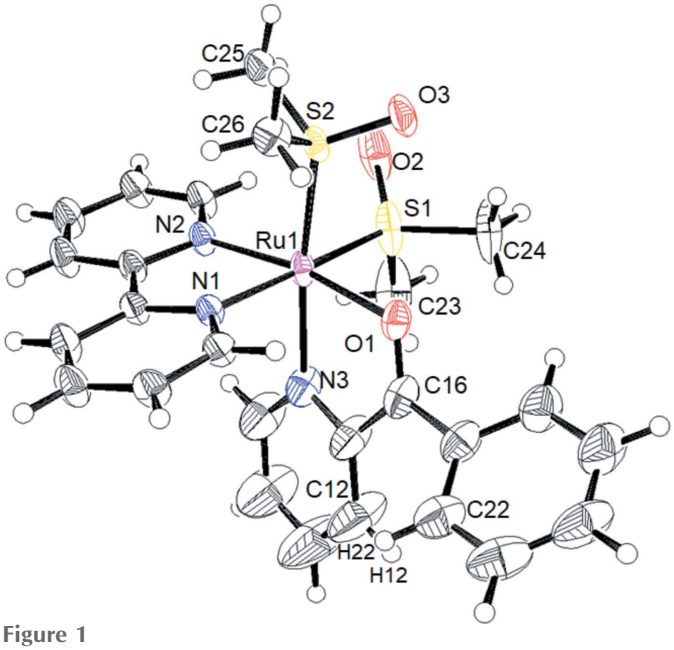


Figure 1
ORTEP view of the cation of the title complex, *cis*(*S*),*trans*(*O*,N_{bpy})-[Ru(bpy)(ppk)(dmso-*S*)$_2$](OTf)$_2$, showing 50% probability ellipsoids. Two OTf^- anions were omitted for clarity.

Table 1
Selected bond lengths and angles (Å, °).

Ru1—N1	2.0905 (16)	Ru1—N2	2.0705 (16)
Ru1—N3	2.105 (2)	Ru1—O1	2.0898 (14)
Ru1–S1	2.2845 (6)	Ru1—S2	2.2789 (6)
O1—C16	1.254 (3)		
N1—Ru1—N2	78.46 (6)	N3—Ru1—O1	77.20 (7)
S1—Ru1—S2	87.93 (3)		

i.e., the *trans*(*O*,N_{bpy})-isomer. Three isomers of [Ru(bpy)(ppk)(dmso)$_2$]$^{2+}$ are possible depending on the geometry of the two dmso ligands and the orientation of the ppk ligand: *trans*(dmso)-, *cis*(dmso),*trans*(*O*,N_{bpy})-, and *cis*(dmso),*trans*(*N*,N_{bpy})-isomers. The starting complex, *trans*(*O*,*S*)-[Ru(bpy)(dmso-*S*)$_2$(dmso-*O*)$_2$](OTf)$_2$ has two inert *cis* dmso-*S* ligands and two labile *cis* dmso-*O* ligands. The inert dmso-*S* ligands in the starting complex were retained during the reaction to afford an isomer with *cis*(dmso)-geometry, that is, the *cis*(S)-geometry. The bpy ligand is located in the equatorial plane. The dmso-*O* ligand at the axial site is more labile than that at the equatorial site (Toyama *et al.*, 2018). Hence, the pyridyl N atom of the ppk ligand attacks the labile axial dmso-*O* atom first, followed by the equatorial dmso-*O*, resulting in a *trans*(*O*,N_{bpy})-geometry.

Selected bond lengths and angles are listed in Table 1. For Ru—N(bpy), the Ru1—N1 bond *trans* to S1 [2.0905 (16) Å] is slightly longer than the Ru1—N2 bond *trans* to O1 [2.0705 (16) Å]. Both these bonds are slightly longer than the previously reported Ru—N bonds in [Ru(bpy)$_2$(N-O)]$^{2+}$ [N-O = pic$^-$ or H_2pia, which are the *N*,*O* bidentate ligands; 2.031–2.059 Å; Toyama *et al.*, 2017, 2019], but are similar to those in [Ru(bpy)(phen)(dmso-*S*)$_2$]$^{2+}$ (2.092 and 2.087 Å; Toyama *et al.*, 2018). These elongations are due to the electronic and steric effects of the two dmso ligands.

The H10 atom of pyridyl-N2 of bpy shows hydrogen-bonding interactions with the O2 atom of dmso-S1 [H10···O2 = 2.33 Å, Fig. 2]. The torsion angle N2—Ru1—S1—O2 is

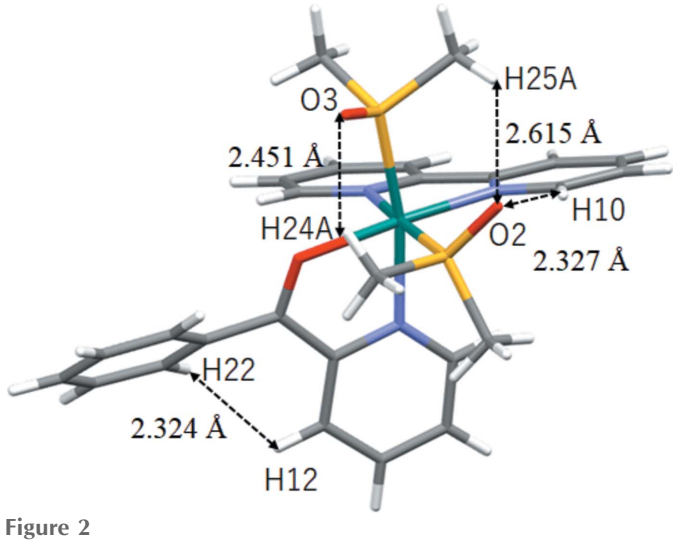


Figure 2
Capped stick model of the cation of the title complex. Three hydrogen-bonding interactions, O2···H10, O3···H24*A*, and O2···H25*A*, and a short H22(ph)···H12(py) contact in the ppk ligand are shown.

47.01 (6)°. The O2 atom of dmso-S1 orients toward the dmso-S2 ligand to reduce the steric hindrance with the pyridyl-N2 atom of the bpy ligand. The rotation of the dmso-S1 ligand is restricted by the pyridyl-N2 group of the bpy ligand. Moreover, hydrogen-bonding interactions can be observed between the neighboring methyl H atoms and the O atoms of the dmso-S1 and dmso-S2 ligands (H24*A*···O3 = 2.45 Å and H25*A*···O2 = 2.62 Å, Fig. 2). The rotation of the dmso-S2 ligand is also restricted by the dmso-S1 ligand. Hence, the two dmso-*S* ligands are *cis* to each other. A similar conformation in which the two dmso ligands are in the *cis* position has also been observed in $[Ru(bpy)(phen)(dmso\text{-}S)_2]^{2+}$ (Toyama *et al.*, 2018).

The Ru1—S1 bond length [2.2845 (8) Å] is similar to the corresponding bond length in the starting complex [2.2723 (5) Å; Toyama *et al.*, 2018]. However, the Ru1—S2 bond [2.2790 (6) Å] is longer than that of the starting complex [2.2063 (5) Å; Toyama *et al.*, 2018] because of the *trans* influence (π-backdonation) of the pyridyl-N3 group in ppk. In this complex, both dmso-*S* ligands are *trans* to the pyridine rings, implying that the Ru1—S1 and Ru1—S2 bond lengths are similar. Therefore, the *trans* influences of pyridyl groups of ppk and bpy are comparable. For the Ru-ppk moiety, the Ru1—N3 [2.105 (2) Å] and Ru1—O1 bond lengths [2.0898 (14) Å] are similar to the corresponding lengths in *trans*(Cl)-$[RuCl_2(dpk\text{-}\kappa^2N,O)(dmso\text{-}S)_2]$ [2.113 (2) and 2.089 (2) Å, respectively; Toyama *et al.*, 2007]. Moreover, the O1—C16 bond length [1.254 (3) Å] in the ketone group is comparable to the corresponding bond length in the Ru-dpk complex [1.243 (3) Å; Toyama *et al.*, 2007], indicating that the former is also a double bond, C═O. The dihedral angle between pyridyl-N3 and the phenyl group is 129.26 (13)°, and the *ortho* proton (H22) in the phenyl group is in contact with the 3-position proton (H12) in the pyridyl-N3 group (H12···H22 = 2.32 Å, Fig. 2).

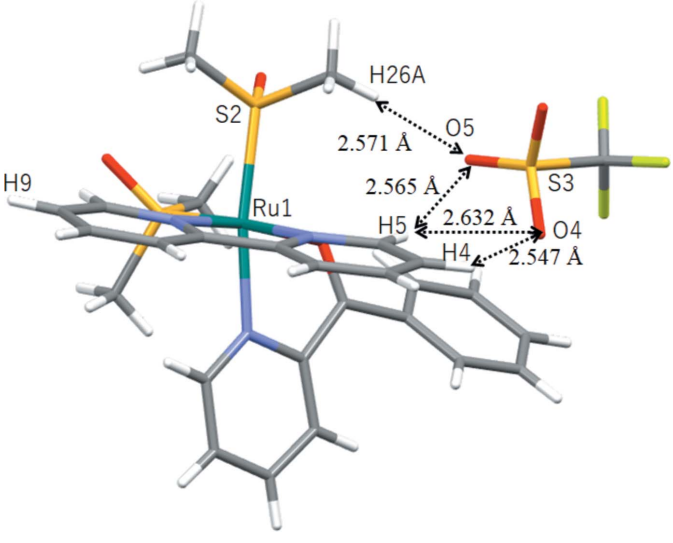


Figure 3
Capped stick models of a cation and an OTf-S3 ion in the title complex. Short contacts between the complex cation and the OTf-S3 anion are shown.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O5	0.95	2.56	3.436 (3)	152
C26—H26*A*···O5	0.98	2.57	3.543 (3)	171
C4—H4···O4	0.95	2.55	3.184 (3)	125
C5—H5···O4	0.95	2.63	3.236 (3)	122
C9—H9···O4^{i}	0.95	2.54	3.314 (3)	139
C25—H25*A*···F2^{i}	0.98	2.65	3.067 (2)	106
C25—H25*C*···O6^{ii}	0.98	2.49	3.404 (3)	156
C26—H26*B*···O6^{ii}	0.98	2.67	3.530 (3)	146
C25—H25*C*···O6^{ii}	0.98	2.49	3.404 (3)	1556
C26—H26*B*···O6^{ii}	0.98	2.67	3.530 (3)	146

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

One of the trifluoromethanesulfonate anions is disordered over three positions, referred to as *A*, *B*, and *C*, with occupancies of 0.4, 0.4, and 0.2, respectively, in the refined model. To confirm the validity of the application of SQUEEZE (Spek, 2015), a region of the disordered OTf^- anion was corrected using the SQUEEZE (Spek, 2015) routine in the *PLATON* program (Spek, 2020). The SQUEEZE model converged at $R1[F^2 > 2\sigma(F^2)] = 0.0315$, $wR(F^2) = 0.0712$, $GOF = 1.05$, mean s (C-C) = 0.0037 Å, and $r_{max} = 0.84$ eÅ^{-3}. The SQUEEZE model is an alternative to the original disordered model, with $R1[F^2 > 2s(F^2)] = 0.0348$, $wR(F^2) = 0.0806$, $GOF = 1.08$, mean σ(C—C) = 0.0041 Å, and $r_{max} = 0.86$ eÅ^{-3}. However, both the models are nearly equivalent, indicating that both the SQUEEZE and the original disordered model are satisfactory.

3. Supramolecular features

As shown in Fig. 3, the O5 atom of OTf-S3 forms hydrogen-bonding interactions (Table 2) with the H5 atom of the bpy ligand and the H26*A* atom of dmso-S2. As shown in Fig. 4, the O4 atom of OTf-S3 forms hydrogen-bonding interactions with the H4 and H5 atoms of bpy and H9 atom of bpy in a neighboring complex cation to form chains along the *b*-axis direction. Moreover, the F2 atom of OTf-S3 interacts with the H25*A* atom of dmso-S2 in the neighboring complex cation, and the rotation of the CF_3 moiety of OTf-S3 is restricted by hydrogen-bonding interactions in the chain. In addition, the O6 atom of OTf-S3 interacts with atoms H25*C* and H26*B* of

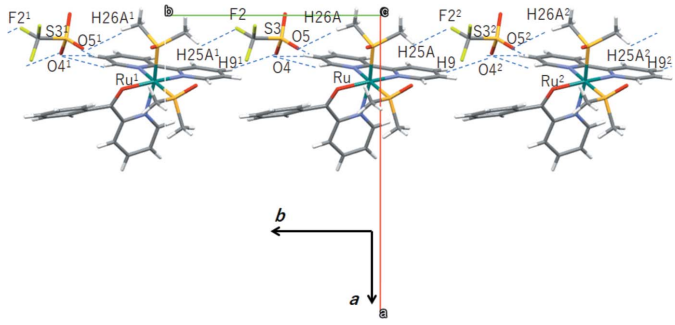


Figure 4
Hydrogen-bonded chain consisting of cations and an OTf-S3 ion in the crystal. [Symmetry codes: (1) $x, 1+y, z$; (2) $x, -1+y, z$; (3) $x, -2+y, z$]

Table 3
Experimental details.

	Disordered model	SQUEEZEd model
Crystal data		
Chemical formula	$[Ru(C_{10}H_8N_2)(C_{12}H_9NO)(C_2H_6OS)_2](CF_3O_3S)_2$	$[Ru(C_{10}H_8N_2)(C_{12}H_9NO)(C_2H_6OS)_2](CF_3O_3S)_2$
M_r	894.85	894.85
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	173	173
a, b, c (Å)	17.3772 (4), 12.2931 (2), 16.3443 (4)	17.3772 (4), 12.2931 (2), 16.3443 (4)
β (°)	98.895 (2)	98.895 (2)
V (Å^3)	3449.47 (13)	3449.47 (13)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.79	0.79
Crystal size (mm)	0.10 × 0.05 × 0.05	0.10 × 0.05 × 0.05
Data collection		
Diffractometer	Rigaku Mercury70	Rigaku Mercury70
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.921, 0.962	0.921, 0.962
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	42165, 9317, 8290	42165, 9317, 8290
R_{int}	0.019	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.711	0.711
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.081, 1.08	0.032, 0.071, 1.05
No. of reflections	9317	9317
No. of parameters	608	392
No. of restraints	29	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.87	0.84, −0.88

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2016), *CrysAlis PRO* (Rigaku OD, 2018), *SIR2014* (Burla *et al.*, 2015), *SHELXL2014/7* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *CrystalStructure* (Rigaku, 2019), and *publCIF* (Westrip, 2010).

dmso-S2 in a neighboring complex cation in another chain to cross-link two neighboring chains and form a ladder-like double-chain structure. Consequently, the OTf-S3 anions are located inside the double chains and properly accommodated between the bpy ligand in the cation and phenyl group of the ppk ligand in the other cation. In contrast, the OTf-S4 anions are located between the double chains but are disordered and not properly accommodated in the void between the double chains.

4. Synthesis and crystallization

The title complex was prepared by the same procedure used for *cis*-[Ru(bpy)(phen)(dmso-*S*)$_2$](OTf)$_2$ (Toyama *et al.*, 2018). The reaction of *trans*(*O*,*S*)-[Ru(bpy)(dmso-*S*)$_2$(dmso-*O*)$_2$](OTf)$_2$ with ppk in acetone at room temperature afforded *cis*(*S*),*trans*(*O*,N_{bpy})-[Ru(bpy)(ppk)(dmso-*S*)$_2$](OTf)$_2$. Single crystals suitable for X-ray structural analysis were obtained by the vapor diffusion of diethyl ether into a mixed solution of DMSO and ethanol (1:3) of *cis*(*S*),*trans*(*O*,N_{bpy})-[Ru(bpy)(ppk)(dmso-*S*)$_2$](OTf)$_2$.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms attached to the carbon were included as riding contributions to the idealized positions [C—H = 0.95 Å (CH) or 0.98 Å (CH$_3$)]. The isotropic displacement parameters were fixed at U_{iso}(H) = 1.2U_{eq}(C) for CH, and 1.5U_{eq}(C) for CH$_3$. One of the trifluoromethanesulfonate anions is disordered over three positions (referred to as *A*, *B*, and *C*) with occupancies of 0.4, 0.4, and 0.2, respectively, in the refined model. Restraints (DFIX, DANG, and DELU) were used to correct the geometry and displacement parameters of the disordered OTf$^-$ ions. To confirm the validity of the disordered model, the SQUEEZE (Spek, 2015) routine in the *PLATON* program (Spek, 2020) was used to generate a modified dataset in which the contribution of the disordered OTf$^-$ anion to the structure amplitudes was discarded. The void volume of 511 Å^3 occupied by the disordered OTf$^-$ anion (14.8% of the unit-cell volume) contains 298 electrons, corresponding to approximately four OTf$^-$ anions (296 electrons).

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supporting information

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Crystal structure of *cis*(*S*),*trans*(*O*,N_{bpy})-(2,2′-bipyridyl-κ^2N,N')bis(dimethyl sulfoxide-κS)[phenyl(pyridin-2-yl)methanone-κ^2N,O]ruthenium(II) bis(trifluoromethanesulfonate)

Mari Toyama and Noriharu Nagao

Computing details

Data collection: *CrystalClear*-SM Expert (Rigaku, 2016) for disordered_model. For both structures, cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2019), *publCIF* (Westrip, 2010).

(2,2′-Bipyridyl-κ^2N,N')bis(dimethyl sulfoxide-κS)[phenyl(pyridin-2-yl)methanone-κ^2N,O]ruthenium(II) bis(trifluoromethanesulfonate) (disordered_model)

Crystal data

$[Ru(C_{10}H_8N_2)(C_{12}H_9NO)(C_2H_6OS)_2](CF_3O_3S)_2$
M_r = 894.85
Monoclinic, $P2_1/c$
a = 17.3772 (4) Å
b = 12.2931 (2) Å
c = 16.3443 (4) Å
β = 98.895 (2)°
V = 3449.47 (13) Å^3
Z = 4
$F(000)$ = 1808.00
D_x = 1.723 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 31997 reflections
θ = 2.2–30.5°
μ = 0.79 mm^{-1}
T = 173 K
Block, orange
0.10 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury70 diffractometer
Detector resolution: 14.629 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.921, T_{max} = 0.962
42165 measured reflections
9317 independent reflections
8290 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.019
θ_{max} = 30.4°, θ_{min} = 2.0°
h = −23→23
k = −16→16
l = −23→22

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.081
S = 1.08
9317 reflections
608 parameters
29 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 3.9158P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.86$ e Å^{-3}
	$\Delta\rho_{min} = -0.87$ e Å^{-3}

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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ru1	0.21892 (2)	0.05017 (2)	0.20103 (2)	0.02633 (5)	
S1	0.27377 (5)	−0.04295 (5)	0.10369 (4)	0.04978 (18)	
S2	0.10233 (3)	0.03559 (4)	0.11611 (3)	0.02870 (10)	
S3	0.07625 (4)	0.46067 (4)	0.18347 (3)	0.03402 (12)	
F1	0.03511 (10)	0.58328 (12)	0.05158 (8)	0.0487 (4)	
F2	0.04294 (10)	0.66781 (10)	0.16804 (9)	0.0480 (4)	
F3	0.14701 (9)	0.62211 (12)	0.12006 (9)	0.0489 (4)	
O1	0.24410 (9)	0.19932 (12)	0.14980 (9)	0.0332 (3)	
O2	0.23265 (16)	−0.14256 (15)	0.07013 (12)	0.0683 (7)	
O3	0.10620 (11)	0.06064 (13)	0.02803 (9)	0.0403 (4)	
O4	0.12551 (12)	0.48455 (14)	0.26074 (10)	0.0484 (4)	
O5	0.10877 (12)	0.38520 (13)	0.13067 (11)	0.0479 (4)	
O6	−0.00431 (11)	0.44379 (14)	0.19017 (12)	0.0484 (4)	
N2	0.19998 (10)	−0.08308 (13)	0.27279 (10)	0.0272 (3)	
N1	0.17314 (10)	0.12390 (12)	0.29825 (9)	0.0247 (3)	
N3	0.32656 (11)	0.09263 (17)	0.27151 (13)	0.0406 (4)	
C1	0.16540 (12)	0.05711 (15)	0.36240 (12)	0.0279 (4)	
C2	0.14501 (15)	0.09718 (18)	0.43554 (13)	0.0369 (5)	
H2	0.1394	0.0492	0.4798	0.044*	
C3	0.13286 (16)	0.20791 (18)	0.44327 (14)	0.0399 (5)	
H3	0.1196	0.2368	0.4932	0.048*	
C4	0.14022 (14)	0.27586 (17)	0.37750 (13)	0.0350 (5)	
H4	0.1316	0.3519	0.3813	0.042*	
C5	0.16033 (12)	0.23126 (15)	0.30602 (13)	0.0292 (4)	
H5	0.1653	0.2780	0.2608	0.035*	
C6	0.17955 (13)	−0.05890 (15)	0.34785 (12)	0.0282 (4)	
C7	0.17177 (15)	−0.13966 (17)	0.40547 (13)	0.0384 (5)	
H7	0.1584	−0.1210	0.4579	0.046*	
C8	0.18351 (16)	−0.24741 (18)	0.38621 (14)	0.0414 (5)	
H8	0.1792	−0.3032	0.4254	0.050*	
C9	0.20155 (15)	−0.27232 (17)	0.30936 (13)	0.0381 (5)	

H9	0.2082	−0.3459	0.2940	0.046*	
C10	0.20990 (14)	−0.18875 (16)	0.25483 (13)	0.0349 (5)	
H10	0.2233	−0.2066	0.2022	0.042*	
C11	0.35019 (15)	0.1962 (2)	0.2582 (2)	0.0520 (7)	
C12	0.41884 (19)	0.2382 (3)	0.3007 (3)	0.0886 (14)	
H12	0.4351	0.3099	0.2899	0.106*	
C13	0.4634 (2)	0.1735 (4)	0.3591 (4)	0.121 (2)	
H13	0.5106	0.2008	0.3891	0.145*	
C14	0.4398 (2)	0.0708 (4)	0.3737 (3)	0.0983 (16)	
H14	0.4704	0.0255	0.4131	0.118*	
C15	0.37045 (17)	0.0340 (3)	0.3300 (2)	0.0649 (9)	
H15	0.3530	−0.0366	0.3420	0.078*	
C16	0.29958 (14)	0.25231 (19)	0.18898 (16)	0.0400 (5)	
C17	0.31305 (14)	0.3652 (2)	0.16364 (17)	0.0436 (5)	
C18	0.30673 (18)	0.3877 (2)	0.07992 (19)	0.0540 (7)	
H18	0.2956	0.3310	0.0404	0.065*	
C19	0.3167 (2)	0.4937 (2)	0.0537 (2)	0.0652 (9)	
H19	0.3140	0.5086	−0.0037	0.078*	
C20	0.33044 (19)	0.5763 (2)	0.1095 (3)	0.0703 (10)	
H20	0.3362	0.6486	0.0909	0.084*	
C21	0.3360 (2)	0.5550 (3)	0.1929 (3)	0.0716 (10)	
H21	0.3453	0.6128	0.2318	0.086*	
C22	0.32810 (18)	0.4488 (2)	0.2206 (2)	0.0585 (7)	
H22	0.3330	0.4339	0.2782	0.070*	
C23	0.3719 (2)	−0.0815 (3)	0.1403 (2)	0.0880 (14)	
H23A	0.3733	−0.1297	0.1882	0.106*	
H23B	0.4030	−0.0163	0.1566	0.106*	
H23C	0.3933	−0.1195	0.0962	0.106*	
C24	0.2881 (2)	0.0413 (2)	0.01819 (18)	0.0623 (9)	
H24A	0.2379	0.0715	−0.0076	0.075*	
H24B	0.3104	−0.0022	−0.0226	0.075*	
H24C	0.3237	0.1008	0.0378	0.075*	
C25	0.05597 (16)	−0.09281 (17)	0.11911 (13)	0.0384 (5)	
H25A	0.0906	−0.1501	0.1043	0.046*	
H25B	0.0074	−0.0931	0.0796	0.046*	
H25C	0.0444	−0.1061	0.1751	0.046*	
C26	0.02969 (14)	0.12177 (18)	0.14662 (15)	0.0371 (5)	
H26A	0.0464	0.1978	0.1448	0.045*	
H26B	0.0219	0.1033	0.2031	0.045*	
H26C	−0.0193	0.1117	0.1088	0.045*	
C27	0.07521 (15)	0.58964 (17)	0.12770 (13)	0.0353 (5)	
S4A	0.48251 (10)	−0.24864 (15)	0.37611 (11)	0.0429 (4)	0.4
F4A	0.4352 (6)	−0.4487 (7)	0.3753 (8)	0.126 (5)	0.4
F5A	0.3693 (6)	−0.3243 (13)	0.4437 (10)	0.173 (8)	0.4
F6A	0.4788 (6)	−0.3941 (10)	0.4918 (6)	0.113 (5)	0.4
O7A	0.5571 (5)	−0.2950 (10)	0.3698 (7)	0.068 (2)	0.4
O8A	0.4295 (10)	−0.2279 (15)	0.2996 (9)	0.067 (4)	0.4
O9A	0.4780 (12)	−0.1661 (11)	0.4350 (7)	0.125 (6)	0.4

C28A	0.4392 (8)	−0.3598 (9)	0.4252 (8)	0.090 (4)	0.4
S4B	0.4632 (3)	−0.3128 (5)	0.3742 (4)	0.0781 (13)	0.2
F4B	0.5073 (15)	−0.1612 (13)	0.4572 (16)	0.125 (10)	0.2
F5B	0.3966 (12)	−0.214 (2)	0.4748 (17)	0.124 (10)	0.2
F6B	0.5118 (12)	−0.3220 (14)	0.5283 (8)	0.089 (5)	0.2
O7B	0.4210 (10)	−0.4114 (9)	0.3856 (10)	0.063 (5)	0.2
O8B	0.5444 (5)	−0.3400 (14)	0.380 (2)	0.098 (9)	0.2
O9B	0.441 (2)	−0.2190 (19)	0.323 (2)	0.094 (10)	0.2
C28B	0.4695 (12)	−0.2511 (13)	0.4737 (10)	0.131 (13)	0.2
S4C	0.41337 (10)	−0.26601 (16)	0.40330 (12)	0.0500 (4)	0.4
F4C	0.5126 (9)	−0.4124 (11)	0.3749 (7)	0.187 (6)	0.4
F5C	0.5622 (4)	−0.2694 (12)	0.4263 (10)	0.169 (6)	0.4
F6C	0.5134 (7)	−0.3747 (11)	0.5027 (8)	0.107 (4)	0.4
O7C	0.3645 (5)	−0.3697 (9)	0.3964 (6)	0.080 (3)	0.4
O8C	0.4107 (9)	−0.2271 (13)	0.3201 (8)	0.057 (3)	0.4
O9C	0.4163 (13)	−0.1813 (12)	0.4598 (8)	0.146 (9)	0.4
C28C	0.4981 (4)	−0.3400 (5)	0.4304 (4)	0.0430 (15)	0.4

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.03761 (9)	0.02047 (7)	0.02264 (8)	0.00535 (6)	0.01015 (6)	0.00556 (6)
S1	0.0815 (5)	0.0380 (3)	0.0382 (3)	0.0272 (3)	0.0356 (3)	0.0154 (2)
S2	0.0468 (3)	0.0203 (2)	0.0192 (2)	−0.00074 (19)	0.00577 (19)	0.00434 (16)
S3	0.0545 (3)	0.0198 (2)	0.0293 (2)	0.0034 (2)	0.0115 (2)	0.00168 (18)
F1	0.0732 (10)	0.0421 (8)	0.0295 (7)	0.0040 (7)	0.0041 (7)	0.0053 (6)
F2	0.0813 (11)	0.0224 (6)	0.0434 (8)	0.0104 (6)	0.0190 (7)	0.0012 (5)
F3	0.0626 (9)	0.0412 (8)	0.0459 (8)	−0.0064 (7)	0.0174 (7)	0.0077 (6)
O1	0.0419 (8)	0.0264 (7)	0.0339 (8)	0.0030 (6)	0.0139 (6)	0.0078 (6)
O2	0.143 (2)	0.0320 (9)	0.0398 (10)	0.0161 (11)	0.0446 (12)	−0.0018 (8)
O3	0.0635 (11)	0.0365 (8)	0.0208 (7)	−0.0041 (8)	0.0063 (7)	0.0096 (6)
O4	0.0784 (13)	0.0313 (8)	0.0331 (8)	−0.0002 (8)	0.0009 (8)	0.0052 (7)
O5	0.0773 (13)	0.0265 (8)	0.0434 (9)	0.0104 (8)	0.0202 (9)	−0.0021 (7)
O6	0.0581 (11)	0.0397 (9)	0.0506 (10)	−0.0023 (8)	0.0190 (9)	0.0084 (8)
N2	0.0413 (9)	0.0198 (7)	0.0212 (7)	0.0039 (6)	0.0073 (7)	0.0035 (6)
N1	0.0340 (8)	0.0191 (7)	0.0211 (7)	0.0013 (6)	0.0047 (6)	0.0011 (6)
N3	0.0321 (9)	0.0406 (10)	0.0487 (11)	0.0054 (8)	0.0056 (8)	0.0151 (9)
C1	0.0415 (11)	0.0215 (8)	0.0209 (8)	0.0006 (8)	0.0052 (7)	0.0002 (7)
C2	0.0604 (14)	0.0281 (10)	0.0241 (9)	0.0014 (10)	0.0120 (9)	0.0001 (8)
C3	0.0633 (15)	0.0301 (11)	0.0283 (10)	0.0045 (10)	0.0132 (10)	−0.0059 (8)
C4	0.0491 (13)	0.0234 (9)	0.0324 (10)	0.0030 (9)	0.0065 (9)	−0.0042 (8)
C5	0.0383 (11)	0.0203 (8)	0.0290 (9)	0.0014 (8)	0.0049 (8)	0.0011 (7)
C6	0.0432 (11)	0.0211 (8)	0.0205 (8)	0.0017 (8)	0.0055 (8)	0.0016 (7)
C7	0.0678 (15)	0.0262 (10)	0.0227 (9)	0.0023 (10)	0.0117 (10)	0.0049 (8)
C8	0.0709 (16)	0.0246 (10)	0.0295 (10)	0.0003 (10)	0.0097 (11)	0.0090 (8)
C9	0.0637 (15)	0.0196 (9)	0.0304 (10)	0.0041 (9)	0.0057 (10)	0.0031 (8)
C10	0.0594 (14)	0.0221 (9)	0.0242 (9)	0.0069 (9)	0.0097 (9)	0.0011 (7)
C11	0.0337 (12)	0.0491 (15)	0.0728 (19)	−0.0020 (11)	0.0065 (12)	0.0237 (14)

C12	0.0450 (17)	0.077 (2)	0.134 (4)	−0.0191 (16)	−0.0167 (19)	0.049 (2)
C13	0.053 (2)	0.113 (4)	0.176 (5)	−0.028 (2)	−0.046 (3)	0.074 (4)
C14	0.054 (2)	0.093 (3)	0.133 (4)	−0.0064 (19)	−0.032 (2)	0.059 (3)
C15	0.0400 (14)	0.0660 (19)	0.084 (2)	0.0024 (13)	−0.0056 (14)	0.0409 (17)
C16	0.0376 (12)	0.0347 (11)	0.0505 (13)	0.0034 (9)	0.0153 (10)	0.0105 (10)
C17	0.0386 (12)	0.0330 (11)	0.0601 (15)	0.0006 (9)	0.0103 (11)	0.0093 (11)
C18	0.0654 (18)	0.0359 (13)	0.0605 (17)	−0.0002 (12)	0.0093 (14)	0.0126 (12)
C19	0.073 (2)	0.0428 (15)	0.077 (2)	−0.0031 (14)	0.0023 (17)	0.0248 (15)
C20	0.0601 (18)	0.0333 (14)	0.110 (3)	−0.0073 (12)	−0.0098 (18)	0.0211 (16)
C21	0.0611 (19)	0.0404 (15)	0.109 (3)	−0.0063 (14)	0.0001 (19)	−0.0076 (17)
C22	0.0545 (16)	0.0459 (15)	0.074 (2)	−0.0077 (13)	0.0051 (14)	0.0002 (14)
C23	0.095 (3)	0.097 (3)	0.086 (2)	0.068 (2)	0.058 (2)	0.051 (2)
C24	0.093 (2)	0.0563 (17)	0.0492 (15)	0.0332 (16)	0.0482 (16)	0.0272 (13)
C25	0.0630 (15)	0.0239 (9)	0.0275 (10)	−0.0093 (10)	0.0048 (10)	0.0036 (8)
C26	0.0410 (12)	0.0303 (10)	0.0391 (12)	0.0040 (9)	0.0037 (9)	0.0028 (9)
C27	0.0539 (13)	0.0249 (9)	0.0286 (10)	0.0024 (9)	0.0113 (9)	0.0023 (8)
S4A	0.0488 (9)	0.0355 (8)	0.0449 (9)	−0.0039 (7)	0.0086 (7)	0.0100 (7)
F4A	0.099 (7)	0.060 (5)	0.195 (11)	−0.037 (5)	−0.055 (6)	0.042 (5)
F5A	0.079 (7)	0.223 (16)	0.242 (15)	0.054 (8)	0.105 (9)	0.159 (13)
F6A	0.143 (9)	0.109 (8)	0.101 (6)	0.056 (7)	0.071 (6)	0.088 (7)
O7A	0.051 (4)	0.067 (5)	0.093 (5)	0.011 (4)	0.035 (4)	0.026 (5)
O8A	0.069 (9)	0.059 (5)	0.061 (7)	−0.015 (5)	−0.033 (6)	0.024 (6)
O9A	0.184 (15)	0.118 (11)	0.075 (6)	0.094 (10)	0.029 (8)	0.025 (6)
C28A	0.119 (11)	0.071 (7)	0.087 (8)	0.036 (7)	0.040 (7)	0.053 (7)
S4B	0.076 (3)	0.077 (4)	0.086 (4)	0.011 (3)	0.026 (3)	0.008 (3)
F4B	0.15 (2)	0.053 (9)	0.18 (2)	−0.068 (13)	0.049 (15)	−0.023 (10)
F5B	0.099 (11)	0.112 (17)	0.18 (2)	0.006 (11)	0.095 (13)	−0.061 (15)
F6B	0.113 (11)	0.103 (12)	0.048 (6)	0.000 (11)	0.003 (7)	0.028 (7)
O7B	0.092 (13)	0.052 (10)	0.050 (7)	0.021 (9)	0.028 (8)	0.007 (6)
O8B	0.064 (11)	0.043 (9)	0.21 (3)	0.022 (8)	0.080 (15)	0.022 (14)
O9B	0.085 (16)	0.080 (14)	0.094 (18)	0.043 (12)	−0.057 (14)	0.007 (12)
C28B	0.23 (4)	0.074 (16)	0.083 (16)	−0.07 (2)	0.00 (2)	0.005 (14)
S4C	0.0421 (8)	0.0549 (10)	0.0551 (10)	0.0193 (7)	0.0142 (7)	0.0171 (8)
F4C	0.246 (15)	0.152 (9)	0.185 (10)	0.155 (11)	0.099 (11)	0.035 (10)
F5C	0.041 (3)	0.233 (17)	0.234 (15)	−0.027 (6)	0.024 (6)	0.112 (12)
F6C	0.079 (6)	0.085 (7)	0.150 (10)	0.029 (6)	−0.006 (6)	0.013 (6)
O7C	0.043 (4)	0.100 (7)	0.098 (6)	−0.026 (4)	0.014 (4)	0.045 (5)
O8C	0.080 (8)	0.041 (4)	0.051 (6)	−0.002 (5)	0.007 (4)	0.021 (4)
O9C	0.25 (2)	0.092 (10)	0.085 (8)	0.089 (14)	−0.019 (11)	0.008 (6)
C28C	0.039 (3)	0.050 (4)	0.040 (3)	0.032 (3)	0.004 (3)	0.022 (3)

Geometric parameters (Å, º)

Ru1—N2	2.0705 (16)	C14—C15	1.378 (5)
Ru1—O1	2.0898 (14)	C14—H14	0.9500
Ru1—N1	2.0905 (16)	C15—H15	0.9500
Ru1—N3	2.105 (2)	C16—C17	1.477 (3)
Ru1—S2	2.2789 (6)	C17—C18	1.384 (4)

Ru1—S1	2.2845 (6)	C17—C22	1.384 (4)
S1—O2	1.480 (2)	C18—C19	1.391 (4)
S1—C23	1.781 (4)	C18—H18	0.9500
S1—C24	1.787 (2)	C19—C20	1.360 (5)
S2—O3	1.4839 (15)	C19—H19	0.9500
S2—C25	1.776 (2)	C20—C21	1.377 (5)
S2—C26	1.777 (2)	C20—H20	0.9500
S3—O6	1.436 (2)	C21—C22	1.396 (4)
S3—O5	1.4407 (17)	C21—H21	0.9500
S3—O4	1.4421 (18)	C22—H22	0.9500
S3—C27	1.827 (2)	C23—H23A	0.9800
F1—C27	1.331 (3)	C23—H23B	0.9800
F2—C27	1.337 (2)	C23—H23C	0.9800
F3—C27	1.334 (3)	C24—H24A	0.9800
O1—C16	1.254 (3)	C24—H24B	0.9800
N2—C10	1.349 (2)	C24—H24C	0.9800
N2—C6	1.362 (2)	C25—H25A	0.9800
N1—C5	1.348 (2)	C25—H25B	0.9800
N1—C1	1.355 (2)	C25—H25C	0.9800
N3—C15	1.338 (3)	C26—H26A	0.9800
N3—C11	1.366 (3)	C26—H26B	0.9800
C1—C2	1.389 (3)	C26—H26C	0.9800
C1—C6	1.473 (3)	S4A—O9A	1.409 (12)
C2—C3	1.386 (3)	S4A—O7A	1.435 (8)
C2—H2	0.9500	S4A—O8A	1.456 (11)
C3—C4	1.383 (3)	S4A—C28A	1.806 (10)
C3—H3	0.9500	F4A—C28A	1.359 (13)
C4—C5	1.383 (3)	F5A—C28A	1.367 (11)
C4—H4	0.9500	F6A—C28A	1.267 (15)
C5—H5	0.9500	S4B—O8B	1.438 (5)
C6—C7	1.389 (3)	S4B—O9B	1.439 (5)
C7—C8	1.384 (3)	S4B—O7B	1.444 (5)
C7—H7	0.9500	S4B—C28B	1.784 (16)
C8—C9	1.375 (3)	F4B—C28B	1.335 (16)
C8—H8	0.9500	F5B—C28B	1.350 (18)
C9—C10	1.382 (3)	F6B—C28B	1.375 (16)
C9—H9	0.9500	S4C—O9C	1.387 (13)
C10—H10	0.9500	S4C—O8C	1.435 (11)
C11—C12	1.384 (4)	S4C—O7C	1.526 (9)
C11—C16	1.490 (4)	S4C—C28C	1.730 (6)
C12—C13	1.384 (5)	F4C—C28C	1.323 (11)
C12—H12	0.9500	F5C—C28C	1.421 (11)
C13—C14	1.359 (6)	F6C—C28C	1.245 (11)
C13—H13	0.9500		

N2—Ru1—O1	169.28 (6)	O1—C16—C17	119.2 (2)
N2—Ru1—N1	78.46 (6)	O1—C16—C11	117.7 (2)
O1—Ru1—N1	92.98 (6)	C17—C16—C11	123.2 (2)

N2—Ru1—N3	95.27 (7)	C18—C17—C22	119.6 (3)
O1—Ru1—N3	77.20 (7)	C18—C17—C16	118.3 (2)
N1—Ru1—N3	83.51 (7)	C22—C17—C16	122.0 (3)
N2—Ru1—S2	94.50 (5)	C17—C18—C19	119.8 (3)
O1—Ru1—S2	92.67 (5)	C17—C18—H18	120.1
N1—Ru1—S2	95.17 (5)	C19—C18—H18	120.1
N3—Ru1—S2	169.66 (5)	C20—C19—C18	120.7 (3)
N2—Ru1—S1	96.77 (5)	C20—C19—H19	119.7
O1—Ru1—S1	91.43 (4)	C18—C19—H19	119.7
N1—Ru1—S1	174.49 (5)	C19—C20—C21	120.0 (3)
N3—Ru1—S1	94.26 (6)	C19—C20—H20	120.0
S2—Ru1—S1	87.93 (3)	C21—C20—H20	120.0
O2—S1—C23	106.67 (18)	C20—C21—C22	120.2 (3)
O2—S1—C24	107.89 (15)	C20—C21—H21	119.9
C23—S1—C24	100.07 (16)	C22—C21—H21	119.9
O2—S1—Ru1	116.32 (9)	C17—C22—C21	119.6 (3)
C23—S1—Ru1	112.34 (14)	C17—C22—H22	120.2
C24—S1—Ru1	112.18 (9)	C21—C22—H22	120.2
O3—S2—C25	107.45 (10)	S1—C23—H23A	109.5
O3—S2—C26	106.81 (11)	S1—C23—H23B	109.5
C25—S2—C26	100.20 (12)	H23A—C23—H23B	109.5
O3—S2—Ru1	113.90 (8)	S1—C23—H23C	109.5
C25—S2—Ru1	114.67 (8)	H23A—C23—H23C	109.5
C26—S2—Ru1	112.67 (8)	H23B—C23—H23C	109.5
O6—S3—O5	115.46 (12)	S1—C24—H24A	109.5
O6—S3—O4	114.59 (12)	S1—C24—H24B	109.5
O5—S3—O4	114.90 (12)	H24A—C24—H24B	109.5
O6—S3—C27	103.23 (11)	S1—C24—H24C	109.5
O5—S3—C27	103.57 (10)	H24A—C24—H24C	109.5
O4—S3—C27	102.65 (10)	H24B—C24—H24C	109.5
C16—O1—Ru1	116.30 (14)	S2—C25—H25A	109.5
C10—N2—C6	117.79 (16)	S2—C25—H25B	109.5
C10—N2—Ru1	127.01 (13)	H25A—C25—H25B	109.5
C6—N2—Ru1	115.09 (13)	S2—C25—H25C	109.5
C5—N1—C1	118.88 (17)	H25A—C25—H25C	109.5
C5—N1—Ru1	125.73 (13)	H25B—C25—H25C	109.5
C1—N1—Ru1	114.87 (12)	S2—C26—H26A	109.5
C15—N3—C11	117.6 (2)	S2—C26—H26B	109.5
C15—N3—Ru1	128.15 (19)	H26A—C26—H26B	109.5
C11—N3—Ru1	114.06 (16)	S2—C26—H26C	109.5
N1—C1—C2	121.35 (18)	H26A—C26—H26C	109.5
N1—C1—C6	115.02 (16)	H26B—C26—H26C	109.5
C2—C1—C6	123.63 (18)	F1—C27—F3	106.99 (18)
C3—C2—C1	119.3 (2)	F1—C27—F2	107.71 (19)
C3—C2—H2	120.3	F3—C27—F2	107.51 (18)
C1—C2—H2	120.3	F1—C27—S3	112.25 (15)
C4—C3—C2	119.3 (2)	F3—C27—S3	111.65 (16)
C4—C3—H3	120.4	F2—C27—S3	110.50 (14)

C2—C3—H3	120.4	O9A—S4A—O7A	118.8 (9)
C3—C4—C5	118.88 (19)	O9A—S4A—O8A	111.5 (10)
C3—C4—H4	120.6	O7A—S4A—O8A	117.8 (9)
C5—C4—H4	120.6	O9A—S4A—C28A	99.8 (8)
N1—C5—C4	122.32 (19)	O7A—S4A—C28A	100.1 (5)
N1—C5—H5	118.8	O8A—S4A—C28A	105.2 (8)
C4—C5—H5	118.8	F6A—C28A—F4A	102.6 (10)
N2—C6—C7	121.39 (18)	F6A—C28A—F5A	107.5 (10)
N2—C6—C1	115.48 (16)	F4A—C28A—F5A	115.1 (15)
C7—C6—C1	123.12 (18)	F6A—C28A—S4A	115.1 (11)
C8—C7—C6	119.78 (19)	F4A—C28A—S4A	109.1 (8)
C8—C7—H7	120.1	F5A—C28A—S4A	107.6 (7)
C6—C7—H7	120.1	O8B—S4B—O9B	113.5 (17)
C9—C8—C7	118.90 (19)	O8B—S4B—O7B	108.0 (11)
C9—C8—H8	120.6	O9B—S4B—O7B	130.5 (15)
C7—C8—H8	120.6	O8B—S4B—C28B	96.7 (14)
C8—C9—C10	119.0 (2)	O9B—S4B—C28B	99.2 (19)
C8—C9—H9	120.5	O7B—S4B—C28B	101.5 (9)
C10—C9—H9	120.5	F4B—C28B—F5B	102 (2)
N2—C10—C9	123.08 (19)	F4B—C28B—F6B	115 (2)
N2—C10—H10	118.5	F5B—C28B—F6B	128 (2)
C9—C10—H10	118.5	F4B—C28B—S4B	97.4 (14)
N3—C11—C12	121.7 (3)	F5B—C28B—S4B	103.3 (14)
N3—C11—C16	113.3 (2)	F6B—C28B—S4B	105.8 (12)
C12—C11—C16	124.7 (3)	O9C—S4C—O8C	111.9 (9)
C11—C12—C13	118.5 (3)	O9C—S4C—O7C	129.7 (10)
C11—C12—H12	120.7	O8C—S4C—O7C	105.8 (8)
C13—C12—H12	120.7	O9C—S4C—C28C	106.4 (7)
C14—C13—C12	120.2 (4)	O8C—S4C—C28C	108.6 (7)
C14—C13—H13	119.9	O7C—S4C—C28C	91.3 (5)
C12—C13—H13	119.9	F6C—C28C—F4C	112.7 (9)
C13—C14—C15	118.5 (3)	F6C—C28C—F5C	101.6 (10)
C13—C14—H14	120.7	F4C—C28C—F5C	98.4 (10)
C15—C14—H14	120.7	F6C—C28C—S4C	118.1 (7)
N3—C15—C14	123.3 (3)	F4C—C28C—S4C	115.0 (7)
N3—C15—H15	118.3	F5C—C28C—S4C	108.0 (6)
C14—C15—H15	118.3		

C5—N1—C1—C2	−0.3 (3)	C11—C16—C17—C22	−46.8 (4)
Ru1—N1—C1—C2	171.93 (17)	C22—C17—C18—C19	1.0 (4)
C5—N1—C1—C6	179.25 (19)	C16—C17—C18—C19	178.1 (3)
Ru1—N1—C1—C6	−8.5 (2)	C17—C18—C19—C20	−1.9 (5)
N1—C1—C2—C3	−0.5 (4)	C18—C19—C20—C21	1.3 (5)
C6—C1—C2—C3	−180.0 (2)	C19—C20—C21—C22	0.3 (5)
C1—C2—C3—C4	0.9 (4)	C18—C17—C22—C21	0.6 (4)
C2—C3—C4—C5	−0.7 (4)	C16—C17—C22—C21	−176.4 (3)
C1—N1—C5—C4	0.6 (3)	C20—C21—C22—C17	−1.3 (5)
Ru1—N1—C5—C4	−170.71 (16)	O6—S3—C27—F1	−63.67 (19)

C3—C4—C5—N1	−0.1 (3)	O5—S3—C27—F1	57.06 (19)
C10—N2—C6—C7	2.2 (3)	O4—S3—C27—F1	176.93 (17)
Ru1—N2—C6—C7	−174.22 (18)	O6—S3—C27—F3	176.19 (15)
C10—N2—C6—C1	−176.9 (2)	O5—S3—C27—F3	−63.08 (18)
Ru1—N2—C6—C1	6.7 (2)	O4—S3—C27—F3	56.79 (18)
N1—C1—C6—N2	1.3 (3)	O6—S3—C27—F2	56.59 (19)
C2—C1—C6—N2	−179.2 (2)	O5—S3—C27—F2	177.32 (17)
N1—C1—C6—C7	−177.8 (2)	O4—S3—C27—F2	−62.81 (19)
C2—C1—C6—C7	1.7 (4)	O9A—S4A—C28A—F6A	−67.7 (12)
N2—C6—C7—C8	−1.2 (4)	O7A—S4A—C28A—F6A	54.1 (11)
C1—C6—C7—C8	177.8 (2)	O8A—S4A—C28A—F6A	176.8 (13)
C6—C7—C8—C9	−1.0 (4)	O9A—S4A—C28A—F4A	177.6 (10)
C7—C8—C9—C10	2.1 (4)	O7A—S4A—C28A—F4A	−60.6 (10)
C6—N2—C10—C9	−1.1 (4)	O8A—S4A—C28A—F4A	62.1 (12)
Ru1—N2—C10—C9	174.88 (18)	O9A—S4A—C28A—F5A	52.1 (14)
C8—C9—C10—N2	−1.1 (4)	O7A—S4A—C28A—F5A	173.9 (13)
C15—N3—C11—C12	2.9 (5)	O8A—S4A—C28A—F5A	−63.5 (15)
Ru1—N3—C11—C12	178.7 (3)	O8B—S4B—C28B—F4B	71.2 (17)
C15—N3—C11—C16	177.0 (3)	O9B—S4B—C28B—F4B	−44 (2)
Ru1—N3—C11—C16	−7.2 (3)	O7B—S4B—C28B—F4B	−178.8 (17)
N3—C11—C12—C13	−1.3 (7)	O8B—S4B—C28B—F5B	175.8 (18)
C16—C11—C12—C13	−174.7 (4)	O9B—S4B—C28B—F5B	61 (2)
C11—C12—C13—C14	0.3 (9)	O7B—S4B—C28B—F5B	−74.2 (18)
C12—C13—C14—C15	−1.0 (9)	O8B—S4B—C28B—F6B	−47.7 (17)
C11—N3—C15—C14	−3.7 (6)	O9B—S4B—C28B—F6B	−162.9 (19)
Ru1—N3—C15—C14	−178.7 (3)	O7B—S4B—C28B—F6B	62.3 (16)
C13—C14—C15—N3	2.7 (8)	O9C—S4C—C28C—F6C	54.8 (13)
Ru1—O1—C16—C17	−170.77 (17)	O8C—S4C—C28C—F6C	175.4 (12)
Ru1—O1—C16—C11	10.7 (3)	O7C—S4C—C28C—F6C	−77.4 (10)
N3—C11—C16—O1	−2.2 (4)	O9C—S4C—C28C—F4C	−168.2 (13)
C12—C11—C16—O1	171.7 (3)	O8C—S4C—C28C—F4C	−47.6 (12)
N3—C11—C16—C17	179.4 (2)	O7C—S4C—C28C—F4C	59.5 (10)
C12—C11—C16—C17	−6.7 (5)	O9C—S4C—C28C—F5C	−59.5 (12)
O1—C16—C17—C18	−42.3 (3)	O8C—S4C—C28C—F5C	61.0 (11)
C11—C16—C17—C18	136.2 (3)	O7C—S4C—C28C—F5C	168.2 (9)
O1—C16—C17—C22	134.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O5	0.95	2.56	3.436 (3)	152
C26—H26*A*···O5	0.98	2.57	3.543 (3)	171
C4—H4···O4	0.95	2.55	3.184 (3)	125
C5—H5···O4	0.95	2.63	3.236 (3)	122
C9—H9···O4^{i}	0.95	2.54	3.314 (3)	139
C25—H25*A*···F2^{i}	0.98	2.65	3.067 (2)	106
C25—H25*C*···O6^{ii}	0.98	2.49	3.404 (3)	156
C26—H26*B*···O6^{ii}	0.98	2.67	3.530 (3)	146

C25—H25*C*···O6^{ii}	0.98	2.49	3.404 (3)	1556
C26—H26*B*···O6^{ii}	0.98	2.67	3.530 (3)	146

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

(Squeezed_model)

Crystal data

$C_{28}H_{29}F_6N_3O_9RuS_4$
M_r = 894.85
Monoclinic, $P2_1/c$
a = 17.3772 (4) Å
b = 12.2931 (2) Å
c = 16.3443 (4) Å
β = 98.895 (2)°
V = 3449.47 (13) Å^3
Z = 4
F(000) = 1808.00
D_x = 1.723 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 31997 reflections
θ = 2.2–30.5°
μ = 0.79 mm^{-1}
T = 173 K
Block, orange
0.10 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury70 diffractometer
Detector resolution: 14.629 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.921, T_{max} = 0.962
42165 measured reflections
9317 independent reflections
8290 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.019
θ_{max} = 30.4°, θ_{min} = 2.0°
h = −23→23
k = −16→16
l = −23→22

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.071
S = 1.05
9317 reflections
392 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 3.2481P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.21892 (2)	0.05017 (2)	0.20103 (2)	0.02636 (4)
S1	0.27378 (4)	−0.04295 (4)	0.10370 (3)	0.04980 (16)

S2	0.10234 (3)	0.03559 (3)	0.11611 (3)	0.02876 (9)
S3	0.07627 (3)	0.46067 (4)	0.18348 (3)	0.03408 (10)
F1	0.03507 (9)	0.58331 (11)	0.05157 (7)	0.0488 (3)
F2	0.04294 (9)	0.66787 (9)	0.16804 (8)	0.0479 (3)
F3	0.14705 (8)	0.62215 (11)	0.12006 (8)	0.0489 (3)
O1	0.24409 (8)	0.19932 (10)	0.14977 (8)	0.0332 (3)
O2	0.23263 (14)	−0.14250 (13)	0.07011 (10)	0.0683 (6)
O3	0.10620 (9)	0.06063 (12)	0.02799 (8)	0.0404 (3)
O4	0.12550 (11)	0.48452 (12)	0.26071 (9)	0.0484 (4)
O5	0.10880 (11)	0.38527 (12)	0.13066 (10)	0.0479 (4)
O6	−0.00432 (10)	0.44374 (13)	0.19013 (10)	0.0483 (4)
N2	0.20000 (9)	−0.08312 (11)	0.27273 (9)	0.0272 (3)
N1	0.17312 (9)	0.12391 (11)	0.29822 (8)	0.0248 (3)
N3	0.32653 (10)	0.09260 (15)	0.27153 (12)	0.0407 (4)
C1	0.16540 (11)	0.05712 (14)	0.36240 (10)	0.0280 (3)
C2	0.14500 (13)	0.09717 (16)	0.43552 (11)	0.0369 (4)
H2	0.1394	0.0492	0.4798	0.044*
C3	0.13283 (14)	0.20795 (16)	0.44327 (12)	0.0399 (5)
H3	0.1196	0.2368	0.4932	0.048*
C4	0.14025 (12)	0.27582 (15)	0.37749 (12)	0.0350 (4)
H4	0.1317	0.3518	0.3813	0.042*
C5	0.16035 (11)	0.23127 (14)	0.30601 (11)	0.0293 (4)
H5	0.1653	0.2780	0.2608	0.035*
C6	0.17960 (11)	−0.05895 (14)	0.34786 (10)	0.0283 (3)
C7	0.17188 (14)	−0.13966 (15)	0.40550 (11)	0.0384 (4)
H7	0.1587	−0.1210	0.4580	0.046*
C8	0.18354 (14)	−0.24735 (16)	0.38619 (12)	0.0415 (5)
H8	0.1792	−0.3032	0.4254	0.050*
C9	0.20157 (13)	−0.27230 (15)	0.30937 (12)	0.0381 (4)
H9	0.2082	−0.3458	0.2940	0.046*
C10	0.20995 (13)	−0.18874 (14)	0.25485 (11)	0.0347 (4)
H10	0.2233	−0.2066	0.2023	0.042*
C11	0.35012 (13)	0.1962 (2)	0.25811 (17)	0.0520 (6)
C12	0.41880 (17)	0.2384 (3)	0.3007 (2)	0.0890 (12)
H12	0.4349	0.3101	0.2901	0.107*
C13	0.4635 (2)	0.1735 (4)	0.3593 (3)	0.1220 (19)
H13	0.5106	0.2009	0.3894	0.146*
C14	0.43982 (19)	0.0708 (3)	0.3736 (3)	0.0986 (14)
H14	0.4704	0.0253	0.4128	0.118*
C15	0.37040 (15)	0.0341 (2)	0.32992 (19)	0.0651 (8)
H15	0.3529	−0.0364	0.3420	0.078*
C16	0.29956 (12)	0.25231 (17)	0.18902 (14)	0.0402 (5)
C17	0.31303 (13)	0.36515 (17)	0.16368 (15)	0.0438 (5)
C18	0.30677 (16)	0.3878 (2)	0.07994 (17)	0.0542 (6)
H18	0.2957	0.3310	0.0404	0.065*
C19	0.31671 (18)	0.4937 (2)	0.0538 (2)	0.0654 (8)
H19	0.3138	0.5086	−0.0036	0.079*
C20	0.33052 (17)	0.5763 (2)	0.1096 (2)	0.0704 (9)

H20	0.3363	0.6486	0.0909	0.084*
C21	0.33610 (17)	0.5550 (2)	0.1931 (2)	0.0714 (9)
H21	0.3455	0.6127	0.2319	0.086*
C22	0.32804 (16)	0.4488 (2)	0.2206 (2)	0.0585 (6)
H22	0.3328	0.4339	0.2782	0.070*
C23	0.3718 (2)	−0.0814 (3)	0.1402 (2)	0.0882 (13)
H23A	0.3733	−0.1289	0.1886	0.106*
H23B	0.4031	−0.0162	0.1558	0.106*
H23C	0.3931	−0.1203	0.0963	0.106*
C24	0.28800 (18)	0.0412 (2)	0.01821 (15)	0.0621 (8)
H24A	0.2379	0.0715	−0.0075	0.075*
H24B	0.3102	−0.0023	−0.0226	0.075*
H24C	0.3237	0.1007	0.0378	0.075*
C25	0.05595 (14)	−0.09282 (15)	0.11908 (12)	0.0382 (4)
H25A	0.0906	−0.1501	0.1045	0.046*
H25B	0.0075	−0.0932	0.0794	0.046*
H25C	0.0441	−0.1060	0.1749	0.046*
C26	0.02972 (12)	0.12184 (16)	0.14662 (13)	0.0371 (4)
H26A	0.0462	0.1979	0.1442	0.045*
H26B	0.0224	0.1040	0.2033	0.045*
H26C	−0.0194	0.1113	0.1091	0.045*
C27	0.07526 (13)	0.58962 (15)	0.12773 (12)	0.0356 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.03765 (8)	0.02051 (7)	0.02267 (7)	0.00532 (5)	0.01014 (5)	0.00555 (5)
S1	0.0815 (4)	0.0381 (3)	0.0382 (3)	0.0271 (3)	0.0355 (3)	0.0154 (2)
S2	0.0468 (3)	0.02038 (18)	0.01935 (18)	−0.00077 (17)	0.00577 (17)	0.00437 (14)
S3	0.0546 (3)	0.01982 (19)	0.0294 (2)	0.00343 (18)	0.0115 (2)	0.00172 (16)
F1	0.0737 (9)	0.0423 (7)	0.0292 (6)	0.0041 (6)	0.0038 (6)	0.0052 (5)
F2	0.0807 (9)	0.0225 (5)	0.0433 (7)	0.0104 (6)	0.0188 (6)	0.0011 (5)
F3	0.0626 (8)	0.0413 (7)	0.0456 (7)	−0.0065 (6)	0.0172 (6)	0.0078 (6)
O1	0.0417 (7)	0.0264 (6)	0.0340 (7)	0.0029 (5)	0.0139 (6)	0.0078 (5)
O2	0.1423 (19)	0.0322 (8)	0.0403 (9)	0.0156 (10)	0.0448 (11)	−0.0021 (7)
O3	0.0637 (9)	0.0365 (7)	0.0208 (6)	−0.0040 (7)	0.0062 (6)	0.0096 (5)
O4	0.0786 (12)	0.0312 (7)	0.0331 (7)	−0.0002 (7)	0.0007 (7)	0.0051 (6)
O5	0.0772 (11)	0.0265 (7)	0.0434 (8)	0.0106 (7)	0.0200 (8)	−0.0022 (6)
O6	0.0577 (10)	0.0394 (8)	0.0512 (9)	−0.0023 (7)	0.0191 (8)	0.0080 (7)
N2	0.0412 (8)	0.0200 (6)	0.0213 (7)	0.0040 (6)	0.0073 (6)	0.0036 (5)
N1	0.0344 (7)	0.0190 (6)	0.0211 (6)	0.0014 (5)	0.0049 (5)	0.0010 (5)
N3	0.0319 (8)	0.0408 (9)	0.0492 (10)	0.0052 (7)	0.0058 (7)	0.0147 (8)
C1	0.0417 (9)	0.0216 (7)	0.0209 (7)	0.0005 (7)	0.0052 (7)	0.0003 (6)
C2	0.0607 (13)	0.0280 (9)	0.0237 (8)	0.0012 (8)	0.0119 (8)	0.0002 (7)
C3	0.0631 (13)	0.0302 (9)	0.0283 (9)	0.0046 (9)	0.0133 (9)	−0.0057 (7)
C4	0.0494 (11)	0.0232 (8)	0.0326 (9)	0.0029 (8)	0.0067 (8)	−0.0044 (7)
C5	0.0382 (9)	0.0203 (7)	0.0294 (8)	0.0013 (7)	0.0049 (7)	0.0010 (6)
C6	0.0432 (10)	0.0212 (7)	0.0206 (7)	0.0018 (7)	0.0057 (7)	0.0015 (6)

C7	0.0675 (14)	0.0266 (9)	0.0225 (8)	0.0022 (9)	0.0119 (9)	0.0048 (7)
C8	0.0709 (15)	0.0246 (9)	0.0295 (9)	0.0001 (9)	0.0097 (9)	0.0090 (7)
C9	0.0634 (13)	0.0197 (8)	0.0306 (9)	0.0043 (8)	0.0056 (9)	0.0030 (7)
C10	0.0587 (12)	0.0224 (8)	0.0241 (8)	0.0067 (8)	0.0095 (8)	0.0012 (7)
C11	0.0338 (11)	0.0485 (13)	0.0732 (16)	−0.0016 (9)	0.0066 (11)	0.0239 (12)
C12	0.0449 (15)	0.078 (2)	0.134 (3)	−0.0196 (14)	−0.0173 (17)	0.050 (2)
C13	0.0526 (18)	0.114 (3)	0.179 (4)	−0.027 (2)	−0.046 (2)	0.076 (3)
C14	0.0547 (17)	0.092 (3)	0.134 (3)	−0.0068 (17)	−0.0337 (19)	0.058 (2)
C15	0.0406 (12)	0.0655 (17)	0.084 (2)	0.0029 (12)	−0.0055 (12)	0.0411 (15)
C16	0.0380 (10)	0.0345 (10)	0.0508 (12)	0.0034 (8)	0.0154 (9)	0.0109 (9)
C17	0.0386 (11)	0.0330 (10)	0.0607 (14)	0.0006 (8)	0.0106 (10)	0.0094 (10)
C18	0.0653 (16)	0.0358 (11)	0.0614 (15)	−0.0004 (11)	0.0094 (12)	0.0124 (11)
C19	0.0731 (18)	0.0432 (14)	0.0769 (19)	−0.0032 (13)	0.0022 (15)	0.0248 (13)
C20	0.0600 (16)	0.0336 (12)	0.110 (3)	−0.0071 (11)	−0.0093 (16)	0.0202 (14)
C21	0.0610 (17)	0.0405 (13)	0.108 (3)	−0.0067 (12)	−0.0001 (17)	−0.0079 (15)
C22	0.0548 (15)	0.0461 (13)	0.0732 (18)	−0.0079 (11)	0.0051 (13)	0.0001 (12)
C23	0.095 (2)	0.098 (2)	0.086 (2)	0.068 (2)	0.0578 (19)	0.0509 (19)
C24	0.093 (2)	0.0563 (15)	0.0486 (13)	0.0328 (14)	0.0476 (14)	0.0269 (11)
C25	0.0627 (13)	0.0238 (8)	0.0273 (9)	−0.0092 (8)	0.0044 (9)	0.0035 (7)
C26	0.0411 (10)	0.0304 (9)	0.0390 (10)	0.0041 (8)	0.0037 (8)	0.0028 (8)
C27	0.0545 (12)	0.0252 (8)	0.0290 (9)	0.0025 (8)	0.0117 (8)	0.0020 (7)

Geometric parameters (Å, º)

Ru1—N2	2.0702 (14)	C8—C9	1.375 (3)
Ru1—O1	2.0900 (12)	C8—H8	0.9500
Ru1—N1	2.0904 (14)	C9—C10	1.382 (3)
Ru1—N3	2.1047 (18)	C9—H9	0.9500
Ru1—S2	2.2789 (5)	C10—H10	0.9500
Ru1—S1	2.2844 (5)	C11—C12	1.386 (4)
S1—O2	1.480 (2)	C11—C16	1.489 (3)
S1—C23	1.780 (3)	C12—C13	1.387 (4)
S1—C24	1.786 (2)	C12—H12	0.9500
S2—O3	1.4843 (13)	C13—C14	1.359 (5)
S2—C25	1.7765 (19)	C13—H13	0.9500
S2—C26	1.778 (2)	C14—C15	1.379 (4)
S3—O6	1.4364 (17)	C14—H14	0.9500
S3—O5	1.4405 (15)	C15—H15	0.9500
S3—O4	1.4414 (16)	C16—C17	1.477 (3)
S3—C27	1.8270 (19)	C17—C22	1.384 (4)
F1—C27	1.332 (2)	C17—C18	1.384 (3)
F2—C27	1.338 (2)	C18—C19	1.390 (3)
F3—C27	1.334 (2)	C18—H18	0.9500
O1—C16	1.254 (3)	C19—C20	1.360 (4)
N2—C10	1.348 (2)	C19—H19	0.9500
N2—C6	1.363 (2)	C20—C21	1.378 (5)
N1—C5	1.348 (2)	C20—H20	0.9500
N1—C1	1.355 (2)	C21—C22	1.395 (4)

N3—C15	1.336 (3)	C21—H21	0.9500
N3—C11	1.366 (3)	C22—H22	0.9500
C1—C2	1.388 (2)	C23—H23A	0.9800
C1—C6	1.474 (2)	C23—H23B	0.9800
C2—C3	1.387 (3)	C23—H23C	0.9800
C2—H2	0.9500	C24—H24A	0.9800
C3—C4	1.383 (3)	C24—H24B	0.9800
C3—H3	0.9500	C24—H24C	0.9800
C4—C5	1.383 (3)	C25—H25A	0.9800
C4—H4	0.9500	C25—H25B	0.9800
C5—H5	0.9500	C25—H25C	0.9800
C6—C7	1.389 (2)	C26—H26A	0.9800
C7—C8	1.383 (3)	C26—H26B	0.9800
C7—H7	0.9500	C26—H26C	0.9800

N2—Ru1—O1	169.32 (6)	N2—C10—C9	123.11 (17)
N2—Ru1—N1	78.50 (5)	N2—C10—H10	118.4
O1—Ru1—N1	92.98 (5)	C9—C10—H10	118.4
N2—Ru1—N3	95.26 (6)	N3—C11—C12	121.6 (2)
O1—Ru1—N3	77.22 (6)	N3—C11—C16	113.4 (2)
N1—Ru1—N3	83.51 (7)	C12—C11—C16	124.7 (2)
N2—Ru1—S2	94.50 (4)	C11—C12—C13	118.6 (3)
O1—Ru1—S2	92.65 (4)	C11—C12—H12	120.7
N1—Ru1—S2	95.15 (4)	C13—C12—H12	120.7
N3—Ru1—S2	169.67 (5)	C14—C13—C12	120.1 (3)
N2—Ru1—S1	96.74 (4)	C14—C13—H13	120.0
O1—Ru1—S1	91.42 (4)	C12—C13—H13	120.0
N1—Ru1—S1	174.50 (4)	C13—C14—C15	118.6 (3)
N3—Ru1—S1	94.26 (6)	C13—C14—H14	120.7
S2—Ru1—S1	87.93 (2)	C15—C14—H14	120.7
O2—S1—C23	106.70 (16)	N3—C15—C14	123.4 (3)
O2—S1—C24	107.83 (13)	N3—C15—H15	118.3
C23—S1—C24	100.07 (14)	C14—C15—H15	118.3
O2—S1—Ru1	116.31 (8)	O1—C16—C17	119.14 (19)
C23—S1—Ru1	112.37 (12)	O1—C16—C11	117.65 (18)
C24—S1—Ru1	112.18 (8)	C17—C16—C11	123.2 (2)
O3—S2—C25	107.43 (9)	C22—C17—C18	119.5 (2)
O3—S2—C26	106.80 (9)	C22—C17—C16	122.1 (2)
C25—S2—C26	100.23 (10)	C18—C17—C16	118.3 (2)
O3—S2—Ru1	113.91 (7)	C17—C18—C19	119.8 (3)
C25—S2—Ru1	114.69 (7)	C17—C18—H18	120.1
C26—S2—Ru1	112.64 (7)	C19—C18—H18	120.1
O6—S3—O5	115.44 (10)	C20—C19—C18	120.7 (3)
O6—S3—O4	114.63 (10)	C20—C19—H19	119.6
O5—S3—O4	114.90 (10)	C18—C19—H19	119.6
O6—S3—C27	103.25 (10)	C19—C20—C21	120.0 (3)
O5—S3—C27	103.52 (9)	C19—C20—H20	120.0
O4—S3—C27	102.64 (9)	C21—C20—H20	120.0

C16—O1—Ru1	116.26 (12)	C20—C21—C22	120.1 (3)
C10—N2—C6	117.74 (15)	C20—C21—H21	119.9
C10—N2—Ru1	127.07 (12)	C22—C21—H21	119.9
C6—N2—Ru1	115.07 (11)	C17—C22—C21	119.8 (3)
C5—N1—C1	118.87 (15)	C17—C22—H22	120.1
C5—N1—Ru1	125.74 (12)	C21—C22—H22	120.1
C1—N1—Ru1	114.86 (11)	S1—C23—H23A	109.5
C15—N3—C11	117.7 (2)	S1—C23—H23B	109.5
C15—N3—Ru1	128.20 (17)	H23A—C23—H23B	109.5
C11—N3—Ru1	113.98 (14)	S1—C23—H23C	109.5
N1—C1—C2	121.36 (16)	H23A—C23—H23C	109.5
N1—C1—C6	115.02 (14)	H23B—C23—H23C	109.5
C2—C1—C6	123.62 (16)	S1—C24—H24A	109.5
C3—C2—C1	119.32 (17)	S1—C24—H24B	109.5
C3—C2—H2	120.3	H24A—C24—H24B	109.5
C1—C2—H2	120.3	S1—C24—H24C	109.5
C4—C3—C2	119.19 (17)	H24A—C24—H24C	109.5
C4—C3—H3	120.4	H24B—C24—H24C	109.5
C2—C3—H3	120.4	S2—C25—H25A	109.5
C3—C4—C5	118.95 (17)	S2—C25—H25B	109.5
C3—C4—H4	120.5	H25A—C25—H25B	109.5
C5—C4—H4	120.5	S2—C25—H25C	109.5
N1—C5—C4	122.31 (16)	H25A—C25—H25C	109.5
N1—C5—H5	118.8	H25B—C25—H25C	109.5
C4—C5—H5	118.8	S2—C26—H26A	109.5
N2—C6—C7	121.42 (16)	S2—C26—H26B	109.5
N2—C6—C1	115.46 (14)	H26A—C26—H26B	109.5
C7—C6—C1	123.11 (16)	S2—C26—H26C	109.5
C8—C7—C6	119.74 (17)	H26A—C26—H26C	109.5
C8—C7—H7	120.1	H26B—C26—H26C	109.5
C6—C7—H7	120.1	F1—C27—F3	106.99 (16)
C9—C8—C7	118.95 (17)	F1—C27—F2	107.62 (17)
C9—C8—H8	120.5	F3—C27—F2	107.49 (16)
C7—C8—H8	120.5	F1—C27—S3	112.25 (14)
C8—C9—C10	118.98 (17)	F3—C27—S3	111.71 (14)
C8—C9—H9	120.5	F2—C27—S3	110.53 (13)
C10—C9—H9	120.5		

C5—N1—C1—C2	−0.2 (3)	C11—C12—C13—C14	0.3 (8)
Ru1—N1—C1—C2	171.93 (15)	C12—C13—C14—C15	−1.1 (8)
C5—N1—C1—C6	179.31 (16)	C11—N3—C15—C14	−3.7 (5)
Ru1—N1—C1—C6	−8.5 (2)	Ru1—N3—C15—C14	−178.8 (3)
N1—C1—C2—C3	−0.5 (3)	C13—C14—C15—N3	2.9 (7)
C6—C1—C2—C3	−180.0 (2)	Ru1—O1—C16—C17	−170.77 (15)
C1—C2—C3—C4	0.9 (3)	Ru1—O1—C16—C11	10.8 (2)
C2—C3—C4—C5	−0.6 (3)	N3—C11—C16—O1	−2.3 (3)
C1—N1—C5—C4	0.5 (3)	C12—C11—C16—O1	171.8 (3)
Ru1—N1—C5—C4	−170.68 (14)	N3—C11—C16—C17	179.3 (2)

C3—C4—C5—N1	−0.1 (3)	C12—C11—C16—C17	−6.5 (4)
C10—N2—C6—C7	2.2 (3)	O1—C16—C17—C22	134.7 (2)
Ru1—N2—C6—C7	−174.17 (16)	C11—C16—C17—C22	−46.9 (3)
C10—N2—C6—C1	−176.87 (17)	O1—C16—C17—C18	−42.3 (3)
Ru1—N2—C6—C1	6.7 (2)	C11—C16—C17—C18	136.0 (3)
N1—C1—C6—N2	1.2 (2)	C22—C17—C18—C19	0.9 (4)
C2—C1—C6—N2	−179.24 (18)	C16—C17—C18—C19	178.0 (2)
N1—C1—C6—C7	−177.82 (19)	C17—C18—C19—C20	−1.8 (4)
C2—C1—C6—C7	1.7 (3)	C18—C19—C20—C21	1.1 (5)
N2—C6—C7—C8	−1.3 (3)	C19—C20—C21—C22	0.4 (5)
C1—C6—C7—C8	177.7 (2)	C18—C17—C22—C21	0.5 (4)
C6—C7—C8—C9	−0.9 (4)	C16—C17—C22—C21	−176.5 (2)
C7—C8—C9—C10	2.1 (3)	C20—C21—C22—C17	−1.2 (4)
C6—N2—C10—C9	−1.0 (3)	O6—S3—C27—F1	−63.58 (16)
Ru1—N2—C10—C9	174.89 (16)	O5—S3—C27—F1	57.13 (17)
C8—C9—C10—N2	−1.1 (3)	O4—S3—C27—F1	176.98 (15)
C15—N3—C11—C12	2.7 (4)	O6—S3—C27—F3	176.23 (14)
Ru1—N3—C11—C12	178.5 (3)	O5—S3—C27—F3	−63.06 (16)
C15—N3—C11—C16	177.1 (2)	O4—S3—C27—F3	56.79 (16)
Ru1—N3—C11—C16	−7.1 (3)	O6—S3—C27—F2	56.58 (17)
N3—C11—C12—C13	−1.1 (6)	O5—S3—C27—F2	177.29 (15)
C16—C11—C12—C13	−174.8 (4)	O4—S3—C27—F2	−62.86 (17)