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Two isomers of [1-benzyl-4-(pyridin-2-yl-κN)-1*H*-1,2,3-triazole-κN^3]dichloridobis(dimethyl sulfoxide-κS)ruthenium(II)

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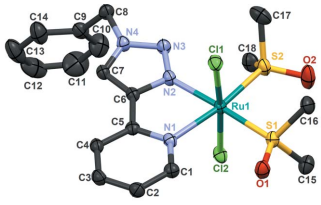
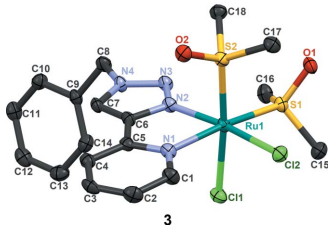
The structures of two isomers of the title compound, $[RuCl_2(C_{14}H_{12}N_4)(C_2H_6OS)_2]$, **2** and **3**, are reported. Isomers **2** and **3** are produced by reaction of the pyridyltriazole ligand 1-benzyl-4-(pyridin-2-yl)-1*H*-1,2,3-triazole (bpt) (**1**) with *fac*-$[RuCl_2(DMSO\text{-}S)_3(DMSO\text{-}O)]$. Reaction in acetone produces *ca* 95% **2**, which is the *OC*-6-14 isomer, with *cis* DMSO and *trans* chlorido ligands, and 5% **3** (the *OC*-6-32 isomer, with *cis* DMSO and *cis* chlorido ligands, and the pyridyl moiety of bpt *trans* to DMSO). Reaction in refluxing toluene initially forms **2**, which slowly isomerizes to **3**.

1. Chemical context

Many 1,2,3-triazole-based ligands have been prepared by copper(I) catalysis of reaction of alkynes with azides; see, for example, Crowley *et al.* (2010). Continuing our research concerning multifunctional chelating ligands in the construction of supramolecular metal–organic frameworks, we used bis(pyridyltriazole) ligands to make macrocyclic Cu^{II} dimers that have found application in hosting small molecules such as DABCO and oxalate (Pokharel *et al.*, 2013, 2014). As an extension of this work, we were also interested in Ru^{II} pyridyltriazole complexes. Ru^{II}–polypyridine coordination compounds have been employed in dye-sensitized solar cells, optical sensors, and photoredox catalysts (Grätzel, 2009; Orellana & García-Fresnadillo, 2004; Prier *et al.*, 2013). In contrast, only a small number of Ru^{II}–pyridyltriazole complexes have been examined to ascertain whether incorporation of triazole could result in improvements compared to the polypyridine complexes. Triazole is a stronger π acceptor analog of pyridine, because of its three electronegative nitrogen atoms, leading to Ru complexes with different photophysical and electrochemical properties (Schulze *et al.*, 2009; Felici *et al.*, 2009; Elliott *et al.*, 2016). Kumar *et al.* (2016) used benzylpyridytriazole (bpt, **1**) to synthesize the homoleptic Ru^{II} complex $Ru(bpt)_3^{2+}$.



2



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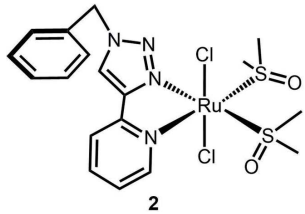
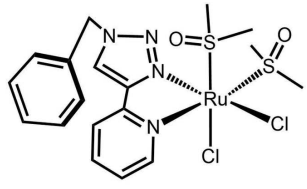


2



3

Our intention was to make an Ru^{II} complex with one or two pyridyltriazoles per metal atom along with weakly ligated coordination sites to facilitate other types of chemistry. In this

Table 1
Selected bond distances for complexes **2** and **3**, the distance between Ru and the mean plane of the pyridyltriazole (Å), the N1—Ru—N2 angle, and the angle between the pyridyltriazole and benzyl mean planes (°).

	complex **2**	complex **3**
Ru1—N1 (pyridine)	2.1714 (18)	2.126 (3)
Ru1—N2 (triazole)	2.0890 (19)	2.044 (3)
Ru1—Cl1	2.3835 (6)	2.4175 (9)
Ru1—Cl2	2.4157 (6)	2.4167 (9)
Ru1—S1	2.2814 (6)	2.2530 (9)
Ru1—S2	2.2440 (6)	2.2434 (9)
Ru1···mean plane of pyridyltriazole	0.0728 (2)	0.048 (3)
N1—Ru—N2	77.10 (7)	78.32 (12)
pyridyltriazole plane···benzyl plane	77.75 (7)	69.52 (10)

paper, we report the synthesis of two isomers of $Ru(bpt)(DMSO)_2Cl_2$, **2** and **3** (see Fig. 1). Compound **2** is the kinetic product of the reaction, and it slowly isomerizes to the thermodynamically more stable **3**.

2. Structural commentary

Complexation of $RuCl_2(DMSO)_4$ and bpt in refluxing acetone gave compound **2** in good yield. Although enough bpt was present in the mixture to replace all DMSO molecules, the product contains only one molecule of bpt per Ru atom. The Ru^{II} cation in **2** adopts a distorted octahedral geometry and beside one bpt, two S-bonded DMSO molecules occupy equatorial positions, and chlorides are coordinated in axial positions. This is the *OC*-6-14 isomer, according to Chemical Abstracts stereochemical notation (Brown *et al.*, 1975; Connelly & Damhus, 2005). The lengths of important bonds, the distances of the Ru atoms from the mean planes of the bpt ligands, and the angles between the pyridyltriazole and benzyl mean planes, are reported in Table 1. We performed 2D NMR analysis to fully assign the peaks in the ^{1}H and ^{1}C NMR spectra. The HMBC spectrum shows cross coupling of H3, but not H2, with C5. This assignment, along with information from HSQC, NOESY, and COSY spectra (see supporting information), led to consistent assignments for the remaining atoms in **2**. In this structure, the DMSO molecules are bonded through S, with S1—Ru1—S2 = 91.27 (2)°, and they are in slightly different environments, in agreement with the NMR data.

Compound **3**, the thermodynamically stable product of complexation of $RuCl_2(DMSO)_4$ and bpt, forms under reflux in toluene. During the reaction we detected **2** by ^{1}H NMR as an intermediate, and it gradually isomerizes to **3**. The atoms *trans* to the two DMSO and chlorido ligands are similar or identical in **2**, but different in **3** (which is the *OC*-6-32 isomer). However, bond lengths and angles in **2** and **3** are only slightly different (see Table 1). The ^{1}H NMR resonances for the two DMSO ligands differ by more in **3** (four singlet peaks) than they do in **2**, as expected. Unlike in **2**, the benzylic methylene hydrogens in **3** are inequivalent, and they appear as a multiplet at 5.67 ppm.

Two other isomers of the title compound, with DMSO ligands *trans* and Cl ligands *cis* (the *OC*-6-43 isomer) or with *cis* DMSO and Cl ligands and pyridyl *trans* to Cl (*OC*-6-42), are possible. We did not observe any other materials in the NMR spectra or in the isolated products that were attributable to these isomers.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Cl2^{i}	0.95	2.49	3.438 (2)	172

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

Table 3
Hydrogen-bond geometry (Å, °) for **3**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.95	2.11	3.031 (4)	164

Symmetry code: (i) $x+1, y, z$.

3. Supramolecular features

The packing structure of **2** shows a non-classical hydrogen bond between Cl2 and H7 (see Table 2). The methine hydrogen (H7) is relatively acidic, showing a downfield ^{1}H

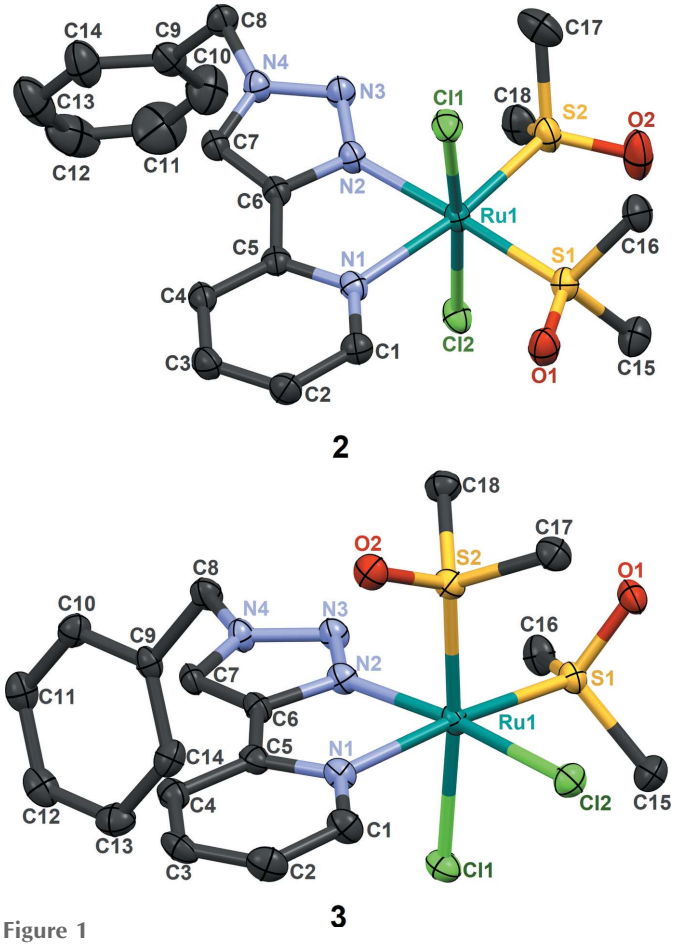


Figure 1
X-ray structures of **2** and **3.** Displacement ellipsoids are drawn at the 50% probability level, and hydrogen atoms are omitted for clarity.

Table 4
Experimental details.

	2	3
Crystal data		
Chemical formula	$[RuCl_2(C_{14}H_{12}N_4)(C_2H_6OS)_2]$	$[RuCl_2(C_{14}H_{12}N_4)(C_2H_6OS)_2]$
M_r	564.50	564.50
Crystal system, space group	Orthorhombic, *Pbca*	Triclinic, $P\overline{1}$
Temperature (K)	90	90
a, *b*, *c* (Å)	21.3094 (11), 9.4213 (5), 22.5267 (12)	9.3535 (14), 9.4900 (15), 13.904 (2)
α, β, γ (°)	90, 90, 90	98.893 (5), 106.772 (5), 106.276 (5)
V (Å^3)	4522.5 (4)	1096.4 (3)
Z	8	2
Radiation type	Cu *Kα*	Cu *Kα*
μ (mm^{-1})	9.70	10.01
Crystal size (mm)	0.71 × 0.16 × 0.04	0.67 × 0.63 × 0.45
Data collection		
Diffractometer	Bruker Kappa APEXII CCD DUO	Bruker Kappa APEXII CCD DUO
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.349, 0.715	0.062, 0.094
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34572, 3970, 3628	9693, 3704, 3657
R_{int}	0.043	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596	0.596
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.025, 0.067, 1.04	0.037, 0.103, 1.16
No. of reflections	3970	3704
No. of parameters	266	266
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −0.46	2.21, −0.63

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2012), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

NMR peak at 7.93 ppm. Li & Flood (2008) took advantage of this C—H(triazole)···Cl interaction in preparing a neutral, macrocyclic receptor for chloride ions. Hydrogen bonds to triazole H atoms were also used by White & Beer (2012) in creating a host system that can strongly bind halides. The packing structure of **3** also shows a close interaction of H7, this time with O1 (see Table 3).

4. Database survey

A survey of the Cambridge Structural Database (version 5.40; Groom *et al.*, 2016) yielded 31 Ru complexes with pyridyltriazole-based ligands. [Hits with bis(triazolyl)pyridine ligands were not included in the analysis.] All of the Ru centers in these structures have the +2 oxidation state and an approximately octahedral geometry. In these structures, the average N(pyridine)—Ru—N(triazole) angle, Ru—N(pyridine), and Ru—N(triazole) bond lengths are 78.4 (5)°, 2.088 (10) Å, and 2.040 (17) Å, respectively; the maximum deviation of Ru from the mean plane of the pyridyltriazole ligand is 0.319 Å. The corresponding values for **2** and **3** are listed in Table 1, showing that their structural characteristics are similar to those of the reported structures in the literature.

5. Synthesis and crystallization

General. $RuCl_3{\cdot}3H_2O$ was purchased from Pressure Chemical; other reagents and solvents were purchased from Aldrich, Alfa Aesar, Acros Organics, or Combi-Blocks, and used without further purification. Bpt (**1**) was synthesized according to the procedure of Crowley *et al.* (2010) and purified by trituration with ether. The Ru starting material was *fac*-$[RuCl_2(DMSO\text{-}S)_3(DMSO\text{-}O)]$, prepared following the literature procedure (Evans *et al.*, 1973) and characterized by comparison with the ^{1}H NMR spectra of Bratsos & Alessio (2010). Elsewhere in this manuscript, it is referred to as $RuCl_2(DMSO)_4$ for simplicity. NMR spectra were recorded on a Bruker AV-400 MHz spectrometer and are reported in ppm, with coupling constants in Hz. Electrospray ionization mass spectra (ESI-MS) were measured on an Agilent 6210 instrument.

Synthesis of (*OC*-6-14)-Ru(bpt)(DMSO)$_2$Cl$_2$, 2. $RuCl_2(DMSO)_4$ (101.5 mg, 0.2095 mmol) and bpt (98.3 mg, 0.416 mmol) were mixed with 20 mL acetone and the mixture refluxed for 12 h under nitrogen. The bright-yellow solution was allowed to cool to room temperature and the acetone evaporated *in vacuo*. Excess bpt was removed from the product as follows: The solid was sonicated with 5 mL of ether, the suspension centrifuged, and the solvent decanted. This process was repeated twice more. The resulting yellow solid was dried in air; yield 110 mg (93%). This material contains *ca* 95% **2** and 5% **3** by NMR. Yellow single crystals of **2** were obtained by vapor diffusion of ether into a solution of the complex in ethanol–chloroform (1:1 *v*/*v*). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.59 (*d*, *J* = 5.04, H1), 7.93 (*s*, H7), 7.81 (*td*, J_1 = 7.68 Hz, J_2 = 1.32 Hz, H3), 7.64 (*d*, *J* = 7.56, H4), 7.46–7.51 (*m*, H2, H11, H12, H13), 7.35–7.39 (*m*, H10, H14), 5.65 (*s*, H8), 3.60 (*s*, DMSO), 3.58 (*s*, DMSO). ^{13}C NMR (100 MHz, $CDCl_3$)

δ 155.64 (C1), 148.92, 148.82 (C5, C6), 137.37(C3), 131. 94 (C9), 129.90, 129.70 (C11/C13, C12), 128.84 (C10/C14), 124.73 (C2), 122.39 (C7), 120.77 (C4), 56.20 (C8), 46.42 (DMSO), 44.53 (DMSO). ESI–MS: *m*/*z* $[Ru(bpt)(DMSO)_2Cl_2+Na]^+$ 580.9665 (calculated: 580.9686).

Synthesis of (*OC*-6-32)-Ru(bpt)(DMSO)$_2$Cl$_2$, 3. $RuCl_2(DMSO)_4$ (513.5 mg, 1.059 mmol) and bpt (361.5 mg, 1.530 mmol) were mixed with 15 mL toluene and the mixture refluxed for 16 days under nitrogen, then cooled to room temperature. The resulting yellow suspension was filtered and the solid washed with fresh toluene and ether, then dried in air. Yield 590 mg (98%) of yellow solid **3**. For crystallization, a sample was mixed with acetonitrile, heated to boiling, allowed to cool, centrifuged, and the yellow decantate used for ether vapor diffusion. After a day, yellow cube-shaped crystals were obtained. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.86 (*d*, *J* = 5.68, H1), 7.96 (*s*, H7), 7.87 (*td*, J_1 = 7.68 Hz, J_2 = 1.48 Hz, H3), 7.66 (*d*, *J* = 7.76 Hz, H4), 7.43–7.53 (*m*, H2, H12, H11, H13), 7.32–7.37 (*m*, H10, H14), 5.67 (*m*, H8), 3.69 (*s*, DMSO), 3.55 (*s*, DMSO), 3.12 (*s*, DMSO), 3.07 (*s*, DMSO). ^{13}C NMR (100 MHz, DMSO-d^6) δ 152.02, 149.91, 149.52, 138.72, 135.27, 129.45, 129.20, 128.77, 125.69, 124.53, 121.39, 55.45, 46.55, 45.20, 44.70, 43.91. ESI–MS: *m*/*z* $[Ru(bpt)(DMSO)_2Cl_2+Na]^+$ 580.9670 (calculated: 580.9686).

6. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 4. In both structures, H atoms were placed in idealized positions and treated with a riding model, with C—H distances of 0.95 Å for Csp^2, 0.99 Å for CH_2, and 0.98 Å for methyl groups. U_{iso}(H) values were set to either 1.2 or 1.5 (CH_3) times U_{eq} of the attached atom. The largest peaks in the final difference maps of **2** and **3** are located 0.914 and 0.887 Å, respectively, from Ru1.

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supporting information

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Two isomers of [1-benzyl-4-(pyridin-2-yl-κN)-1*H*-1,2,3-triazole-κN^3]dichloridobis(dimethyl sulfoxide-κS)ruthenium(II)

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(*OC*-6-14)-[1-Benzyl-4-(pyridin-2-yl-κN)-1*H*-1,2,3-triazole-κN^3]dichloridobis(dimethyl sulfoxide-κS)ruthenium(II) (2)

Crystal data

$[RuCl_2(C_{14}H_{12}N_4)(C_2H_6OS)_2]$
$M_r = 564.50$
Orthorhombic, *Pbca*
$a = 21.3094$ (11) Å
$b = 9.4213$ (5) Å
$c = 22.5267$ (12) Å
$V = 4522.5$ (4) Å^3
$Z = 8$
$F(000) = 2288$
$D_x = 1.658$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 9998 reflections
$\theta = 3.9$–66.5°
$\mu = 9.70$ mm^{-1}
$T = 90$ K
Needle, yellow
0.71 × 0.16 × 0.04 mm

Data collection

Bruker Kappa APEXII CCD DUO diffractometer
Radiation source: IμS microfocus
QUAZAR multilayer optics monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
$T_{min} = 0.349$, $T_{max} = 0.715$
34572 measured reflections
3970 independent reflections
3628 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 66.7°$, $\theta_{min} = 3.9°$
$h = -24\rightarrow23$
$k = -11\rightarrow9$
$l = -26\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.067$
$S = 1.04$
3970 reflections
266 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 3.2772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.09298 (2)	0.17864 (2)	0.37532 (2)	0.02143 (8)
Cl1	0.08456 (3)	0.01442 (6)	0.45541 (2)	0.02897 (14)
Cl2	0.11140 (3)	0.34903 (6)	0.29710 (2)	0.02744 (13)
S1	0.04525 (3)	0.34440 (6)	0.43372 (2)	0.02548 (13)
S2	0.00095 (3)	0.11879 (7)	0.33388 (3)	0.02991 (14)
O2	−0.05488 (9)	0.2095 (2)	0.34285 (9)	0.0476 (5)
O1	0.08383 (8)	0.4194 (2)	0.47853 (8)	0.0336 (4)
N1	0.18911 (8)	0.2124 (2)	0.40402 (8)	0.0224 (4)
N2	0.14267 (8)	0.0257 (2)	0.32734 (8)	0.0240 (4)
N3	0.12683 (9)	−0.0753 (2)	0.28984 (8)	0.0264 (4)
N4	0.18058 (9)	−0.1375 (2)	0.27335 (8)	0.0240 (4)
C1	0.21032 (11)	0.3039 (2)	0.44464 (10)	0.0261 (5)
H1	0.180986	0.362842	0.464654	0.031*
C2	0.27331 (12)	0.3162 (3)	0.45875 (11)	0.0301 (5)
H2	0.286609	0.383822	0.487405	0.036*
C3	0.31690 (11)	0.2297 (3)	0.43097 (11)	0.0297 (5)
H3	0.360309	0.237149	0.440043	0.036*
C4	0.29572 (11)	0.1328 (3)	0.38988 (10)	0.0256 (5)
H4	0.324292	0.070938	0.370413	0.031*
C5	0.23209 (11)	0.1268 (3)	0.37732 (9)	0.0230 (5)
C6	0.20593 (10)	0.0266 (2)	0.33525 (9)	0.0223 (5)
C7	0.23052 (10)	−0.0784 (2)	0.30006 (9)	0.0235 (4)
H7	0.273411	−0.103661	0.295568	0.028*
C8	0.18019 (11)	−0.2548 (3)	0.23009 (10)	0.0281 (5)
H8A	0.136727	−0.271837	0.216302	0.034*
H8AB	0.195534	−0.342585	0.249364	0.034*
C18	0.00697 (12)	0.1011 (3)	0.25524 (11)	0.0365 (6)
H18A	−0.033416	0.069712	0.239103	0.055*
H18B	0.039385	0.031020	0.245612	0.055*
H18C	0.018252	0.192946	0.237803	0.055*
C17	−0.02254 (14)	−0.0564 (3)	0.35314 (13)	0.0459 (7)
H17A	−0.058689	−0.084239	0.328895	0.069*
H17B	−0.034137	−0.059392	0.395224	0.069*
H17C	0.012264	−0.122196	0.345925	0.069*
C9	0.22158 (12)	−0.2194 (3)	0.17743 (10)	0.0317 (5)
C10	0.19814 (17)	−0.1376 (4)	0.13231 (13)	0.0518 (8)
H10	0.155735	−0.106577	0.133446	0.062*
C11	0.2363 (2)	−0.1000 (4)	0.08503 (15)	0.0686 (11)
H11	0.219937	−0.043315	0.053763	0.082*

C12	0.29860 (18)	−0.1453 (4)	0.08322 (15)	0.0614 (10)
H12	0.325403	−0.115599	0.051885	0.074*
C13	0.32091 (16)	−0.2331 (5)	0.12711 (14)	0.0592 (10)
H13	0.362443	−0.269291	0.124741	0.071*
C14	0.28276 (13)	−0.2694 (4)	0.17521 (13)	0.0476 (7)
H14	0.298593	−0.327775	0.206148	0.057*
C15	0.00646 (13)	0.4811 (3)	0.39304 (11)	0.0349 (6)
H15A	0.037764	0.541872	0.373815	0.052*
H15B	−0.019102	0.538224	0.420192	0.052*
H15C	−0.020607	0.438318	0.362755	0.052*
C16	−0.02029 (12)	0.2740 (3)	0.47367 (11)	0.0336 (5)
H16A	−0.050315	0.232593	0.445651	0.050*
H16B	−0.040715	0.350377	0.496027	0.050*
H16C	−0.005731	0.200585	0.501229	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01644 (12)	0.02583 (12)	0.02202 (11)	0.00089 (6)	0.00003 (6)	−0.00100 (6)
Cl1	0.0250 (3)	0.0305 (3)	0.0313 (3)	0.0012 (2)	0.0041 (2)	0.0048 (2)
Cl2	0.0217 (3)	0.0355 (3)	0.0251 (3)	0.0012 (2)	−0.0010 (2)	0.0042 (2)
S1	0.0226 (3)	0.0286 (3)	0.0251 (3)	0.0031 (2)	0.0023 (2)	−0.0011 (2)
S2	0.0197 (3)	0.0379 (3)	0.0321 (3)	0.0011 (2)	−0.0021 (2)	−0.0057 (2)
O2	0.0265 (9)	0.0660 (13)	0.0503 (12)	0.0126 (9)	−0.0099 (8)	−0.0207 (10)
O1	0.0288 (9)	0.0383 (10)	0.0337 (9)	0.0039 (7)	0.0007 (7)	−0.0093 (8)
N1	0.0207 (9)	0.0259 (10)	0.0207 (9)	−0.0012 (7)	0.0015 (7)	0.0031 (7)
N2	0.0191 (9)	0.0286 (10)	0.0245 (9)	0.0002 (7)	−0.0009 (7)	−0.0011 (8)
N3	0.0218 (10)	0.0306 (11)	0.0268 (9)	0.0013 (8)	−0.0001 (7)	−0.0046 (8)
N4	0.0216 (9)	0.0277 (10)	0.0226 (9)	0.0011 (8)	0.0015 (7)	−0.0017 (8)
C1	0.0265 (12)	0.0273 (12)	0.0247 (11)	−0.0001 (9)	−0.0007 (9)	−0.0005 (9)
C2	0.0267 (13)	0.0300 (13)	0.0336 (13)	−0.0012 (9)	−0.0051 (10)	−0.0039 (10)
C3	0.0212 (11)	0.0316 (13)	0.0364 (12)	−0.0021 (10)	−0.0051 (9)	0.0017 (10)
C4	0.0198 (11)	0.0278 (12)	0.0293 (11)	0.0014 (9)	0.0001 (9)	0.0037 (10)
C5	0.0237 (12)	0.0230 (11)	0.0223 (11)	0.0006 (9)	0.0009 (8)	0.0043 (8)
C6	0.0191 (11)	0.0262 (12)	0.0217 (10)	−0.0002 (9)	−0.0001 (8)	0.0035 (9)
C7	0.0191 (11)	0.0270 (12)	0.0244 (10)	0.0002 (9)	0.0006 (8)	0.0019 (9)
C8	0.0272 (12)	0.0303 (13)	0.0269 (11)	0.0000 (10)	0.0001 (9)	−0.0064 (10)
C18	0.0297 (13)	0.0474 (15)	0.0325 (13)	−0.0005 (11)	−0.0077 (10)	−0.0054 (11)
C17	0.0371 (15)	0.0541 (18)	0.0465 (16)	−0.0165 (13)	−0.0054 (13)	0.0020 (14)
C9	0.0311 (13)	0.0375 (13)	0.0265 (12)	−0.0047 (11)	0.0033 (10)	−0.0103 (10)
C10	0.055 (2)	0.063 (2)	0.0378 (15)	0.0074 (16)	0.0089 (13)	0.0044 (14)
C11	0.090 (3)	0.072 (3)	0.0439 (18)	0.000 (2)	0.0190 (18)	0.0109 (17)
C12	0.071 (2)	0.069 (2)	0.0434 (18)	−0.0280 (19)	0.0284 (17)	−0.0162 (16)
C13	0.0360 (17)	0.086 (3)	0.055 (2)	−0.0121 (17)	0.0139 (13)	−0.0219 (19)
C14	0.0331 (15)	0.065 (2)	0.0445 (15)	0.0003 (14)	0.0061 (12)	−0.0093 (15)
C15	0.0346 (14)	0.0381 (15)	0.0319 (12)	0.0091 (11)	0.0035 (11)	0.0016 (11)
C16	0.0276 (12)	0.0384 (14)	0.0348 (12)	0.0010 (11)	0.0108 (10)	−0.0016 (11)

Geometric parameters (Å, º)

Ru1—N2	2.0890 (19)	C6—C7	1.371 (3)
Ru1—N1	2.1714 (18)	C7—H7	0.9500
Ru1—S2	2.2440 (6)	C8—C9	1.515 (3)
Ru1—S1	2.2814 (6)	C8—H8A	0.9900
Ru1—Cl1	2.3835 (6)	C8—H8AB	0.9900
Ru1—Cl2	2.4157 (6)	C18—H18A	0.9800
S1—O1	1.4814 (18)	C18—H18B	0.9800
S1—C15	1.784 (3)	C18—H18C	0.9800
S1—C16	1.789 (2)	C17—H17A	0.9800
S2—O2	1.4786 (19)	C17—H17B	0.9800
S2—C17	1.779 (3)	C17—H17C	0.9800
S2—C18	1.784 (3)	C9—C10	1.370 (4)
N1—C1	1.336 (3)	C9—C14	1.387 (4)
N1—C5	1.360 (3)	C10—C11	1.386 (5)
N2—N3	1.317 (3)	C10—H10	0.9500
N2—C6	1.360 (3)	C11—C12	1.396 (6)
N3—N4	1.339 (3)	C11—H11	0.9500
N4—C7	1.344 (3)	C12—C13	1.374 (6)
N4—C8	1.473 (3)	C12—H12	0.9500
C1—C2	1.384 (4)	C13—C14	1.397 (4)
C1—H1	0.9500	C13—H13	0.9500
C2—C3	1.385 (4)	C14—H14	0.9500
C2—H2	0.9500	C15—H15A	0.9800
C3—C4	1.376 (4)	C15—H15B	0.9800
C3—H3	0.9500	C15—H15C	0.9800
C4—C5	1.386 (3)	C16—H16A	0.9800
C4—H4	0.9500	C16—H16B	0.9800
C5—C6	1.449 (3)	C16—H16C	0.9800
N2—Ru1—N1	77.10 (7)	N2—C6—C5	118.1 (2)
N2—Ru1—S2	93.13 (5)	C7—C6—C5	134.5 (2)
N1—Ru1—S2	170.10 (5)	N4—C7—C6	104.79 (19)
N2—Ru1—S1	175.11 (5)	N4—C7—H7	127.6
N1—Ru1—S1	98.55 (5)	C6—C7—H7	127.6
S2—Ru1—S1	91.27 (2)	N4—C8—C9	110.5 (2)
N2—Ru1—Cl1	88.98 (5)	N4—C8—H8A	109.6
N1—Ru1—Cl1	86.60 (5)	C9—C8—H8A	109.6
S2—Ru1—Cl1	94.93 (2)	N4—C8—H8AB	109.6
S1—Ru1—Cl1	88.52 (2)	C9—C8—H8AB	109.6
N2—Ru1—Cl2	89.92 (5)	H8A—C8—H8AB	108.1
N1—Ru1—Cl2	88.09 (5)	S2—C18—H18A	109.5
S2—Ru1—Cl2	90.32 (2)	S2—C18—H18B	109.5
S1—Ru1—Cl2	92.19 (2)	H18A—C18—H18B	109.5
Cl1—Ru1—Cl2	174.69 (2)	S2—C18—H18C	109.5
O1—S1—C15	105.23 (12)	H18A—C18—H18C	109.5
O1—S1—C16	105.50 (11)	H18B—C18—H18C	109.5

C15—S1—C16	99.46 (13)	S2—C17—H17A	109.5
O1—S1—Ru1	118.17 (7)	S2—C17—H17B	109.5
C15—S1—Ru1	113.87 (9)	H17A—C17—H17B	109.5
C16—S1—Ru1	112.62 (9)	S2—C17—H17C	109.5
O2—S2—C17	106.05 (14)	H17A—C17—H17C	109.5
O2—S2—C18	104.33 (12)	H17B—C17—H17C	109.5
C17—S2—C18	100.13 (14)	C10—C9—C14	120.5 (3)
O2—S2—Ru1	120.08 (8)	C10—C9—C8	119.5 (2)
C17—S2—Ru1	112.19 (10)	C14—C9—C8	120.1 (3)
C18—S2—Ru1	111.94 (9)	C9—C10—C11	120.0 (3)
C1—N1—C5	117.23 (19)	C9—C10—H10	120.0
C1—N1—Ru1	128.13 (16)	C11—C10—H10	120.0
C5—N1—Ru1	114.63 (15)	C10—C11—C12	120.2 (4)
N3—N2—C6	110.02 (18)	C10—C11—H11	119.9
N3—N2—Ru1	134.47 (14)	C12—C11—H11	119.9
C6—N2—Ru1	115.51 (15)	C13—C12—C11	119.5 (3)
N2—N3—N4	105.96 (17)	C13—C12—H12	120.3
N3—N4—C7	111.83 (18)	C11—C12—H12	120.3
N3—N4—C8	120.44 (18)	C12—C13—C14	120.3 (3)
C7—N4—C8	127.72 (19)	C12—C13—H13	119.9
N1—C1—C2	122.6 (2)	C14—C13—H13	119.9
N1—C1—H1	118.7	C9—C14—C13	119.5 (3)
C2—C1—H1	118.7	C9—C14—H14	120.3
C1—C2—C3	119.8 (2)	C13—C14—H14	120.3
C1—C2—H2	120.1	S1—C15—H15A	109.5
C3—C2—H2	120.1	S1—C15—H15B	109.5
C4—C3—C2	118.3 (2)	H15A—C15—H15B	109.5
C4—C3—H3	120.8	S1—C15—H15C	109.5
C2—C3—H3	120.8	H15A—C15—H15C	109.5
C3—C4—C5	119.0 (2)	H15B—C15—H15C	109.5
C3—C4—H4	120.5	S1—C16—H16A	109.5
C5—C4—H4	120.5	S1—C16—H16B	109.5
N1—C5—C4	123.0 (2)	H16A—C16—H16B	109.5
N1—C5—C6	114.6 (2)	S1—C16—H16C	109.5
C4—C5—C6	122.4 (2)	H16A—C16—H16C	109.5
N2—C6—C7	107.39 (19)	H16B—C16—H16C	109.5

C6—N2—N3—N4	−0.8 (2)	C4—C5—C6—N2	177.9 (2)
Ru1—N2—N3—N4	179.26 (15)	N1—C5—C6—C7	−178.5 (2)
N2—N3—N4—C7	0.4 (2)	C4—C5—C6—C7	0.5 (4)
N2—N3—N4—C8	−178.75 (19)	N3—N4—C7—C6	0.1 (2)
C5—N1—C1—C2	1.7 (3)	C8—N4—C7—C6	179.2 (2)
Ru1—N1—C1—C2	−179.42 (18)	N2—C6—C7—N4	−0.6 (2)
N1—C1—C2—C3	−1.1 (4)	C5—C6—C7—N4	177.1 (2)
C1—C2—C3—C4	−0.2 (4)	N3—N4—C8—C9	123.2 (2)
C2—C3—C4—C5	0.9 (4)	C7—N4—C8—C9	−55.9 (3)
C1—N1—C5—C4	−1.0 (3)	N4—C8—C9—C10	−82.9 (3)
Ru1—N1—C5—C4	179.97 (17)	N4—C8—C9—C14	96.9 (3)

C1—N1—C5—C6	177.95 (19)	C14—C9—C10—C11	−2.3 (5)
Ru1—N1—C5—C6	−1.1 (2)	C8—C9—C10—C11	177.5 (3)
C3—C4—C5—N1	−0.3 (3)	C9—C10—C11—C12	0.0 (6)
C3—C4—C5—C6	−179.2 (2)	C10—C11—C12—C13	3.2 (6)
N3—N2—C6—C7	0.9 (2)	C11—C12—C13—C14	−4.1 (5)
Ru1—N2—C6—C7	−179.16 (14)	C10—C9—C14—C13	1.4 (5)
N3—N2—C6—C5	−177.21 (18)	C8—C9—C14—C13	−178.4 (3)
Ru1—N2—C6—C5	2.7 (2)	C12—C13—C14—C9	1.9 (5)
N1—C5—C6—N2	−1.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Cl2^{i}	0.95	2.49	3.438 (2)	172

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

(*OC*-6-32)-[1-Benzyl-4-(pyridin-2-yl-*κN*)-1*H*-1,2,3-triazole-*κN*^{3}]dichloridobis(dimethyl sulfoxide-*κS*)ruthenium(II) (3)

Crystal data

$[RuCl_2(C_{14}H_{12}N_4)(C_2H_6OS)_2]$
M_r = 564.50
Triclinic, $P\overline{1}$
a = 9.3535 (14) Å
b = 9.4900 (15) Å
c = 13.904 (2) Å
α = 98.893 (5)°
β = 106.772 (5)°
γ = 106.276 (5)°
V = 1096.4 (3) Å^3
Z = 2
F(000) = 572
D_x = 1.710 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 7943 reflections
θ = 3.4–66.9°
μ = 10.01 mm^{-1}
T = 90 K
Cubic, yellow
0.67 × 0.63 × 0.45 mm

Data collection

Bruker Kappa APEXII CCD DUO diffractometer
Radiation source: I*μ*S microfocus
QUAZAR multilayer optics monochromator
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
T_{min} = 0.062, T_{max} = 0.094
9693 measured reflections
3704 independent reflections
3657 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 66.9°, θ_{min} = 3.4°
h = −10→11
k = −10→11
l = −16→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.16
3704 reflections
266 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 2.1529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.34993 (3)	0.83627 (3)	0.70658 (2)	0.01710 (13)
Cl1	0.47441 (11)	0.82110 (10)	0.88125 (7)	0.0249 (2)
C1	0.4322 (5)	0.5485 (4)	0.6392 (3)	0.0251 (8)
H1	0.326454	0.492417	0.631964	0.030*
C3	0.6834 (5)	0.5504 (4)	0.6309 (3)	0.0249 (8)
H3	0.751793	0.498296	0.617920	0.030*
N3	0.6204 (4)	1.1465 (4)	0.7637 (3)	0.0211 (6)
C5	0.6319 (4)	0.7785 (4)	0.6771 (3)	0.0201 (7)
S1	0.22838 (10)	0.98237 (10)	0.76998 (7)	0.0195 (2)
S2	0.25606 (10)	0.85272 (10)	0.54247 (7)	0.0201 (2)
Cl2	0.11642 (10)	0.61922 (10)	0.67424 (7)	0.0240 (2)
C2	0.5301 (5)	0.4707 (4)	0.6218 (3)	0.0281 (8)
H2	0.492296	0.362796	0.603645	0.034*
N2	0.5625 (4)	0.9976 (3)	0.7295 (2)	0.0197 (6)
O1	0.0918 (3)	1.0056 (3)	0.6943 (2)	0.0237 (6)
O2	0.3217 (3)	0.7874 (3)	0.4691 (2)	0.0248 (6)
N1	0.4805 (4)	0.7007 (3)	0.6660 (2)	0.0197 (6)
N4	0.7735 (4)	1.1863 (3)	0.7691 (2)	0.0198 (6)
C4	0.7360 (5)	0.7070 (4)	0.6590 (3)	0.0227 (8)
H4	0.841005	0.764702	0.665853	0.027*
C6	0.6756 (4)	0.9424 (4)	0.7130 (3)	0.0186 (7)
C7	0.8119 (4)	1.0644 (4)	0.7384 (3)	0.0193 (7)
H7	0.911618	1.063422	0.735085	0.023*
C8	0.8771 (4)	1.3460 (4)	0.8080 (3)	0.0227 (8)
H8A	0.818548	1.408213	0.831416	0.027*
H8B	0.907011	1.381665	0.750905	0.027*
C9	1.0257 (4)	1.3673 (4)	0.8971 (3)	0.0197 (7)
C10	1.1666 (5)	1.4801 (4)	0.9085 (3)	0.0231 (8)
H10	1.168318	1.539792	0.859658	0.028*
C13	1.1646 (5)	1.3045 (5)	1.0502 (3)	0.0282 (9)
H13	1.163861	1.242858	1.097911	0.034*
C11	1.3043 (5)	1.5055 (4)	0.9911 (3)	0.0254 (8)
H11	1.399325	1.583829	0.999096	0.030*
C12	1.3051 (5)	1.4179 (5)	1.0621 (3)	0.0272 (8)
H12	1.400003	1.435062	1.118164	0.033*
C15	0.1582 (5)	0.9144 (5)	0.8671 (3)	0.0285 (8)
H15A	0.104786	0.979669	0.892022	0.043*
H15B	0.248383	0.916245	0.925322	0.043*
H15C	0.083077	0.810137	0.837040	0.043*

C14	1.0261 (5)	1.2809 (4)	0.9692 (3)	0.0244 (8)
H14	0.930278	1.204961	0.962791	0.029*
C16	0.3581 (5)	1.1661 (4)	0.8480 (3)	0.0254 (8)
H16A	0.403859	1.224247	0.805103	0.038*
H16B	0.443670	1.156519	0.904175	0.038*
H16C	0.298350	1.218801	0.877788	0.038*
C17	0.0452 (5)	0.7802 (4)	0.4819 (3)	0.0255 (8)
H17A	0.015495	0.804549	0.414508	0.038*
H17B	−0.002664	0.826346	0.526319	0.038*
H17C	0.006768	0.669736	0.471409	0.038*
C18	0.2932 (5)	1.0468 (4)	0.5377 (3)	0.0250 (8)
H18A	0.238266	1.050697	0.467030	0.037*
H18B	0.407723	1.098936	0.557126	0.037*
H18C	0.253771	1.096943	0.586229	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01527 (18)	0.01563 (18)	0.01954 (18)	0.00614 (12)	0.00501 (12)	0.00265 (12)
Cl1	0.0253 (5)	0.0278 (5)	0.0212 (4)	0.0119 (4)	0.0045 (4)	0.0065 (4)
C1	0.026 (2)	0.0198 (19)	0.0272 (19)	0.0087 (16)	0.0064 (16)	0.0024 (15)
C3	0.030 (2)	0.0251 (19)	0.0220 (18)	0.0183 (17)	0.0048 (16)	0.0033 (15)
N3	0.0177 (15)	0.0198 (16)	0.0245 (15)	0.0066 (12)	0.0062 (12)	0.0042 (12)
C5	0.0216 (18)	0.0227 (19)	0.0171 (17)	0.0106 (15)	0.0055 (14)	0.0055 (14)
S1	0.0180 (4)	0.0210 (4)	0.0202 (4)	0.0082 (3)	0.0070 (3)	0.0037 (3)
S2	0.0211 (4)	0.0185 (4)	0.0203 (4)	0.0076 (3)	0.0063 (3)	0.0036 (3)
Cl2	0.0215 (4)	0.0200 (4)	0.0269 (4)	0.0035 (3)	0.0074 (4)	0.0050 (3)
C2	0.033 (2)	0.0187 (18)	0.029 (2)	0.0088 (16)	0.0065 (17)	0.0027 (15)
N2	0.0198 (15)	0.0174 (15)	0.0207 (15)	0.0066 (12)	0.0061 (12)	0.0028 (12)
O1	0.0199 (13)	0.0305 (14)	0.0233 (13)	0.0134 (11)	0.0072 (11)	0.0055 (11)
O2	0.0282 (14)	0.0210 (13)	0.0255 (13)	0.0094 (11)	0.0106 (11)	0.0030 (11)
N1	0.0196 (15)	0.0180 (15)	0.0192 (15)	0.0071 (12)	0.0041 (12)	0.0025 (12)
N4	0.0139 (14)	0.0192 (15)	0.0237 (15)	0.0044 (12)	0.0052 (12)	0.0034 (12)
C4	0.0232 (19)	0.027 (2)	0.0197 (17)	0.0120 (16)	0.0070 (15)	0.0048 (15)
C6	0.0184 (17)	0.0201 (18)	0.0183 (16)	0.0099 (14)	0.0057 (14)	0.0029 (14)
C7	0.0150 (17)	0.0234 (18)	0.0221 (17)	0.0101 (14)	0.0070 (14)	0.0055 (14)
C8	0.0204 (18)	0.0178 (18)	0.0292 (19)	0.0069 (15)	0.0072 (16)	0.0062 (15)
C9	0.0175 (17)	0.0180 (17)	0.0232 (18)	0.0084 (14)	0.0064 (15)	0.0014 (14)
C10	0.0242 (19)	0.0185 (18)	0.0268 (19)	0.0060 (15)	0.0106 (16)	0.0052 (15)
C13	0.035 (2)	0.028 (2)	0.0224 (19)	0.0129 (18)	0.0102 (17)	0.0073 (16)
C11	0.0207 (19)	0.0211 (19)	0.029 (2)	0.0053 (15)	0.0064 (16)	−0.0007 (15)
C12	0.024 (2)	0.028 (2)	0.0235 (19)	0.0101 (16)	0.0021 (16)	−0.0026 (16)
C15	0.029 (2)	0.033 (2)	0.029 (2)	0.0115 (18)	0.0154 (17)	0.0117 (17)
C14	0.0238 (19)	0.0244 (19)	0.0242 (19)	0.0054 (16)	0.0114 (16)	0.0037 (15)
C16	0.025 (2)	0.0235 (19)	0.0262 (19)	0.0094 (16)	0.0094 (16)	−0.0014 (15)
C17	0.0237 (19)	0.025 (2)	0.0231 (18)	0.0073 (16)	0.0039 (15)	0.0036 (15)
C18	0.029 (2)	0.0223 (19)	0.0256 (19)	0.0100 (16)	0.0104 (16)	0.0071 (15)

Geometric parameters (Å, º)

Ru1—N2	2.044 (3)	C6—C7	1.370 (5)
Ru1—N1	2.126 (3)	C7—H7	0.9500
Ru1—S2	2.2434 (9)	C8—C9	1.509 (5)
Ru1—S1	2.2530 (9)	C8—H8A	0.9900
Ru1—Cl2	2.4167 (9)	C8—H8B	0.9900
Ru1—Cl1	2.4175 (9)	C9—C14	1.390 (5)
C1—N1	1.341 (5)	C9—C10	1.394 (5)
C1—C2	1.377 (6)	C10—C11	1.387 (6)
C1—H1	0.9500	C10—H10	0.9500
C3—C4	1.379 (6)	C13—C14	1.384 (6)
C3—C2	1.380 (6)	C13—C12	1.393 (6)
C3—H3	0.9500	C13—H13	0.9500
N3—N2	1.315 (4)	C11—C12	1.385 (6)
N3—N4	1.351 (4)	C11—H11	0.9500
C5—N1	1.351 (5)	C12—H12	0.9500
C5—C4	1.390 (5)	C15—H15A	0.9800
C5—C6	1.456 (5)	C15—H15B	0.9800
S1—O1	1.497 (3)	C15—H15C	0.9800
S1—C16	1.777 (4)	C14—H14	0.9500
S1—C15	1.793 (4)	C16—H16A	0.9800
S2—O2	1.477 (3)	C16—H16B	0.9800
S2—C17	1.782 (4)	C16—H16C	0.9800
S2—C18	1.792 (4)	C17—H17A	0.9800
C2—H2	0.9500	C17—H17B	0.9800
N2—C6	1.364 (5)	C17—H17C	0.9800
N4—C7	1.348 (5)	C18—H18A	0.9800
N4—C8	1.466 (5)	C18—H18B	0.9800
C4—H4	0.9500	C18—H18C	0.9800
N2—Ru1—N1	78.32 (12)	N2—C6—C5	117.9 (3)
N2—Ru1—S2	90.28 (9)	C7—C6—C5	135.0 (3)
N1—Ru1—S2	91.60 (8)	N4—C7—C6	105.0 (3)
N2—Ru1—S1	100.24 (9)	N4—C7—H7	127.5
N1—Ru1—S1	173.01 (8)	C6—C7—H7	127.5
S2—Ru1—S1	95.26 (3)	N4—C8—C9	111.4 (3)
N2—Ru1—Cl2	171.78 (9)	N4—C8—H8A	109.3
N1—Ru1—Cl2	93.49 (9)	C9—C8—H8A	109.3
S2—Ru1—Cl2	90.60 (3)	N4—C8—H8B	109.3
S1—Ru1—Cl2	87.81 (3)	C9—C8—H8B	109.3
N2—Ru1—Cl1	85.57 (9)	H8A—C8—H8B	108.0
N1—Ru1—Cl1	84.32 (8)	C14—C9—C10	119.0 (3)
S2—Ru1—Cl1	174.69 (3)	C14—C9—C8	122.3 (3)
S1—Ru1—Cl1	88.75 (3)	C10—C9—C8	118.7 (3)
Cl2—Ru1—Cl1	93.04 (3)	C11—C10—C9	120.1 (4)
N1—C1—C2	122.5 (4)	C11—C10—H10	119.9
N1—C1—H1	118.8	C9—C10—H10	119.9

C2—C1—H1	118.8	C14—C13—C12	120.4 (4)
C4—C3—C2	119.0 (4)	C14—C13—H13	119.8
C4—C3—H3	120.5	C12—C13—H13	119.8
C2—C3—H3	120.5	C12—C11—C10	120.8 (4)
N2—N3—N4	105.3 (3)	C12—C11—H11	119.6
N1—C5—C4	122.5 (3)	C10—C11—H11	119.6
N1—C5—C6	113.6 (3)	C11—C12—C13	119.0 (4)
C4—C5—C6	123.8 (3)	C11—C12—H12	120.5
O1—S1—C16	106.23 (18)	C13—C12—H12	120.5
O1—S1—C15	106.64 (18)	S1—C15—H15A	109.5
C16—S1—C15	97.9 (2)	S1—C15—H15B	109.5
O1—S1—Ru1	117.75 (11)	H15A—C15—H15B	109.5
C16—S1—Ru1	114.42 (13)	S1—C15—H15C	109.5
C15—S1—Ru1	111.80 (14)	H15A—C15—H15C	109.5
O2—S2—C17	107.02 (17)	H15B—C15—H15C	109.5
O2—S2—C18	105.76 (17)	C13—C14—C9	120.6 (4)
C17—S2—C18	99.59 (19)	C13—C14—H14	119.7
O2—S2—Ru1	116.22 (12)	C9—C14—H14	119.7
C17—S2—Ru1	115.64 (13)	S1—C16—H16A	109.5
C18—S2—Ru1	110.93 (13)	S1—C16—H16B	109.5
C1—C2—C3	119.5 (4)	H16A—C16—H16B	109.5
C1—C2—H2	120.2	S1—C16—H16C	109.5
C3—C2—H2	120.2	H16A—C16—H16C	109.5
N3—N2—C6	110.8 (3)	H16B—C16—H16C	109.5
N3—N2—Ru1	134.0 (2)	S2—C17—H17A	109.5
C6—N2—Ru1	115.0 (2)	S2—C17—H17B	109.5
C1—N1—C5	117.9 (3)	H17A—C17—H17B	109.5
C1—N1—Ru1	126.7 (3)	S2—C17—H17C	109.5
C5—N1—Ru1	115.1 (2)	H17A—C17—H17C	109.5
C7—N4—N3	111.9 (3)	H17B—C17—H17C	109.5
C7—N4—C8	127.9 (3)	S2—C18—H18A	109.5
N3—N4—C8	120.2 (3)	S2—C18—H18B	109.5
C3—C4—C5	118.5 (4)	H18A—C18—H18B	109.5
C3—C4—H4	120.7	S2—C18—H18C	109.5
C5—C4—H4	120.7	H18A—C18—H18C	109.5
N2—C6—C7	107.1 (3)	H18B—C18—H18C	109.5

N1—C1—C2—C3	−0.7 (6)	C4—C5—C6—N2	−178.9 (3)
C4—C3—C2—C1	1.1 (6)	N1—C5—C6—C7	177.5 (4)
N4—N3—N2—C6	−0.2 (4)	C4—C5—C6—C7	−0.5 (6)
N4—N3—N2—Ru1	174.8 (2)	N3—N4—C7—C6	−0.3 (4)
C2—C1—N1—C5	−0.8 (6)	C8—N4—C7—C6	177.8 (3)
C2—C1—N1—Ru1	−174.9 (3)	N2—C6—C7—N4	0.2 (4)
C4—C5—N1—C1	1.9 (5)	C5—C6—C7—N4	−178.2 (4)
C6—C5—N1—C1	−176.1 (3)	C7—N4—C8—C9	−53.0 (5)
C4—C5—N1—Ru1	176.7 (3)	N3—N4—C8—C9	125.0 (3)
C6—C5—N1—Ru1	−1.3 (4)	N4—C8—C9—C14	−34.4 (5)
N2—N3—N4—C7	0.3 (4)	N4—C8—C9—C10	147.0 (3)

N2—N3—N4—C8	−178.0 (3)	C14—C9—C10—C11	−0.3 (5)
C2—C3—C4—C5	0.0 (5)	C8—C9—C10—C11	178.3 (3)
N1—C5—C4—C3	−1.5 (5)	C9—C10—C11—C12	1.2 (6)
C6—C5—C4—C3	176.3 (3)	C10—C11—C12—C13	−0.7 (6)
N3—N2—C6—C7	0.0 (4)	C14—C13—C12—C11	−0.7 (6)
Ru1—N2—C6—C7	−176.1 (2)	C12—C13—C14—C9	1.6 (6)
N3—N2—C6—C5	178.7 (3)	C10—C9—C14—C13	−1.1 (5)
Ru1—N2—C6—C5	2.7 (4)	C8—C9—C14—C13	−179.6 (4)
N1—C5—C6—N2	−0.9 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.95	2.11	3.031 (4)	164

Symmetry code: (i) *x*+1, *y*, *z*.