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{2-[(2-Aminophenyl)iminomethyl]-4-bromophenolato-κ^3N,N',O}chlorido-bis(dimethyl sulfoxide-κS)ruthenium(II)

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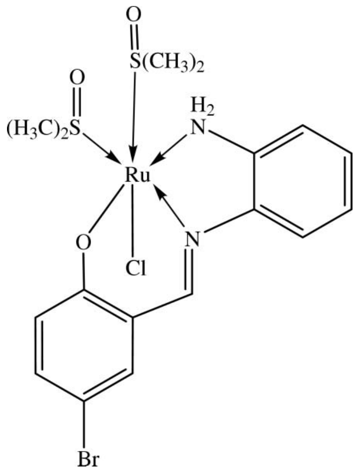
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.105; data-to-parameter ratio = 23.3.

The title compound, $[Ru(C_{13}H_{10}BrN_2O)Cl(C_2H_6OS)_2]$, shows a distorted octahedral Ru^{II} coordination with the N_2O tridentate Schiff base ligand and one dimethyl sulfoxide (DMSO) molecule bonded in the equatorial plane, and the Cl and another DMSO ligand occupying the axial positions. In the crystal structure, molecules are linked by N—H⋯Cl and N—H⋯O hydrogen bonds into one-dimensional chains along the [100] direction. The crystal structure is further stabilized by weak C—H⋯O and C—H⋯Cl interactions. C—H⋯π interactions are also observed in the crystal structure.

Related literature

For related structures, see, for example: Calligaris (2004); Otero *et al.* (2003); Rusanova *et al.* (2006). For related literature on Schiff base coordination complexes and applications of Ru^{II} complexes, see: Eltayeb *et al.* (2007*a*,*b*); Kovacs *et al.* (2007); Liu *et al.* (2007); Lyons *et al.* (1998); Otero *et al.* (2003). For bond length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Ru(C_{13}H_{10}BrN_2O)Cl(C_2H_6OS)_2]$
M_r = 582.92
Triclinic, $P\overline{1}$
a = 8.1302 (3) Å
b = 12.0908 (4) Å
c = 12.2445 (6) Å
α = 115.774 (3)°
β = 101.712 (3)°
γ = 98.135 (2)°
V = 1024.67 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.07 mm^{-1}
T = 100.0 (1) K
0.13 × 0.11 × 0.10 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.686, T_{max} = 0.755
19338 measured reflections
5964 independent reflections
4532 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.105
S = 1.07
5964 reflections
256 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 benzene rings, respectively.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1*N*1⋯Cl1^{i}	0.95 (5)	2.34 (5)	3.235 (4)	157 (4)
N1—H2*N*1⋯O2^{ii}	0.91 (5)	2.22 (5)	2.975 (5)	141 (4)
C2—H2*A*⋯O2^{ii}	0.93	2.58	3.267 (5)	131
C5—H5*A*⋯O3^{iii}	0.93	2.40	3.323 (6)	174
C7—H7*A*⋯O3^{iii}	0.93	2.35	3.263 (5)	168
C16—H16*B*⋯Cl1	0.96	2.83	3.222 (4)	106
C14—H14*A*⋯*Cg*2^{iv}	0.96	2.73	3.634 (5)	157
C16—H16*B*⋯*Cg*1^{i}	0.96	3.09	3.561 (5)	112

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2450).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.

Calligaris, M. (2004). *Coord. Chem. Rev.* **248**, 351–375.

Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Ibrahim, K. (2007*a*). *Acta Cryst.* E**63**, m1633–m1634.

Eltayeb, N. E., Teoh, S. G., Chantrapromma, S., Fun, H.-K. & Ibrahim, K. (2007*b*). *Acta Cryst.* E**63**, m1672–m1673.

Kovacs, M., Fodor, L., Brown, W. R. & Horvath, A. (2007). *Radiat. Phys. Chem.* **76**, 1236–1243.

Liu, P., Tam, W. & Goddard, J. D. (2007). *Tetrahedron*, **63**, 7659–7666.

Lyons, C. H., Abbas, E. D., Lee, J.-K. & Rubner, M. F. (1998). *J. Am. Chem. Soc.* **120**, 12100–12107.

Otero, L., Noblia, P., Gambino, D., Cerecetto, H., Gonzalez, M., Ellena, J. A. & Piro, O. E. (2003). *Inorg. Chim. Acta*, **344**, 85–94.

Rusanova, J., Rusanov, E., Gorelsky, S. I., Christendat, D., Popescu, R., Farah, A. A., Beaulac, R., Reber, C. & Lever, A. B. P. (2006). *Inorg. Chem.* **45**, 6246–6262.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, m2269-m2270 [**doi:10.1107/S160053680703718X**]

{2-[(2-Aminophenyl)iminomethyl]-4-bromophenolato-κ^3*N*,*N'*,*O*}chloridobis(dimethyl sulfoxide-κ*S*)ruthenium(II)

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

Ruthenium chemistry is an interesting branch of chemistry due to the diverse properties of ruthenium and its photophysics and redox chemistry. Ruthenium complexes can be used as catalysts (Liu *et al.*, 2007), luminescence materials (Kovacs *et al.*, 2007), light emitting diodes (Lyons *et al.*, 1998) and against Chagas' disease (Otero *et al.*, 2003). Our current interest in the chemistry of ruthenium complexes is because of its properties as light emitting diodes. As a continuation of our research on Schiff base complexes (Eltayeb *et al.*, 2007*a*; 2007*b*), we extend our studies to the ruthenium complexes with Schiff base ligands and herein the crystal structure of the title compound was reported.

The title complex molecule is characterized by a distort octahedral Ru^{II} coordination, with the N_2O tridentate Schiff-base ligand and one S-DMSO in the basal plane and another S-DMSO and Cl occupied in the axial positions (Fig. 1). The Ru(II) is in the same plane with the N1/N2/O1/S1 basal plane. The cyclic skeleton of the tridentate Schiff-base ligand is not planar as indicated by the dihedral angle between the two benzene rings of 14.5 (2)°. Bond lengths and angles observed in the structure are in normal ranges (Allen *et al.*, 1987). The bond lengths and angles of the Schiff base ligand are comparable with the related structures (Eltayeb *et al.*, 2007*a*; 2007*b*). The Ru—S bond distances [Ru1—S1 = 2.2511 (9)Å and Ru1—S2 = 2.2206 (9) Å] are typical for the complexes of ruthenium with S-coordinated DMSO in the coordination sphere (Calligaris, 2004; Otero *et al.*, 2003). The Cl atom is pushed toward the Schiff-base ligand side of the complex with a S2—Ru1—Cl1 bond angle of 172.75 (3)° for steric reason. The endocyclic N1—Ru1—N2 and N2—Ru1—O1 bond angles are 81.38 (12)° and 93.33 (11)° because of the chelate nature of the ligand.

In the crystal structure of the title compound (Fig. 2), the molecules are connected by N—H···Cl and N—H···O hydrogen bonds into 1-D chains along the [1 0 0] direction. The crystal is stabilized by intermolecular N—H···Cl and N—H···O hydrogen bonds together with weak C—H···O and C—H···Cl interactions (Table 1). C—H···π interactions are also observed (Table 1); Cg_1 and Cg_2 are the centroids of C1–C6 and C8–C13 benzene rings, respectively.

Experimental

The title compound was synthesized by adding 5-bromo-2-hydroxybenzaldehyde (0.402 g, 2 mmol) into a solution of *o*-phenylenediamine (0.108 g, 1 mmol) in ethanol 95% (20 ml). The mixture was refluxed with stirring for half an hour. Dichlorotetrakis(dimethylsulfoxide)ruthenium(II) (0.484 g, 1 mmol) in ethanol (20 ml) was then added. The mixture was refluxed with heating and stirring for two hours. A dark brown-red solution was obtained, wherein brown single crystals suitable for *x*-ray structure determination were formed after one week of slow evaporation of the solvent.

Refinement

H atoms of the NH_2 group were located from the difference map and isotropically refined. The remainning H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual peak is located 0.82 Å from S1 and the deepest hole is located 0.77 Å from Ru1.

Figures

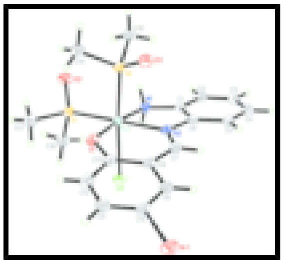

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

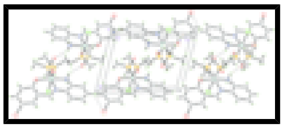

Fig. 2. The crystal packing of (I), viewed along the *c* axis. Hydrogen bond were drawn as dash lines.

{2-[(2-Aminophenyl)iminomethyl]-4-bromophenolato- κ^3*N*,*N*',*O*}chloridobis(dimethyl sulfoxide-κ*S*)ruthenium(II)

Crystal data

$[Ru(C_{13}H_{10}BrN_2O)Cl(C_2H_6OS)_2]$	$Z = 2$
$M_r = 582.92$	$F_{000} = 580$
Triclinic, $P\bar{1}$	$D_x = 1.889$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
a = 8.1302 (3) Å	Cell parameters from 5964 reflections
b = 12.0908 (4) Å	θ = 2.7–30.0°
c = 12.2445 (6) Å	μ = 3.07 mm^{-1}
α = 115.774 (3)°	*T* = 100.0 (1) K
β = 101.712 (3)°	Block, black
γ = 98.135 (2)°	0.13 × 0.11 × 0.10 mm
V = 1024.67 (8) Å^3	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	5964 independent reflections
Radiation source: fine-focus sealed tube	4532 reflections with $I > 2\sigma(I)$

Monochromator: graphite

Detector resolution: 8.33 pixels mm^{-1}

T = 100.0(1) K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

T_{min} = 0.686, T_{max} = 0.755

19338 measured reflections

R_{int} = 0.039

θ_{max} = 30.0°

θ_{min} = 2.7°

$h = -11 \rightarrow 11$

$k = -16 \rightarrow 16$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.041

$wR(F^2)$ = 0.105

S = 1.07

5964 reflections

256 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.8835P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.25 e Å^{-3}

$\Delta\rho_{min}$ = −0.96 e Å^{-3}

Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Ru1	0.79226 (3)	0.36415 (3)	0.12373 (3)	0.01612 (9)
Br1	1.39210 (5)	0.12129 (4)	0.45490 (4)	0.03040 (12)
Cl1	1.03365 (11)	0.35010 (9)	0.03345 (9)	0.02261 (19)
S1	0.59540 (11)	0.26471 (9)	−0.06999 (9)	0.0213 (2)
S2	0.59443 (11)	0.37706 (9)	0.22689 (9)	0.02027 (19)
O1	0.8085 (3)	0.1943 (2)	0.1222 (2)	0.0208 (5)
O2	0.4362 (3)	0.3112 (3)	−0.0816 (3)	0.0273 (6)
O3	0.6586 (3)	0.4040 (3)	0.3597 (3)	0.0292 (6)

N1	0.8072 (4)	0.5441 (3)	0.1349 (3)	0.0183 (6)
N2	0.9799 (4)	0.4710 (3)	0.2943 (3)	0.0175 (6)
C1	0.9182 (4)	0.6432 (4)	0.2601 (4)	0.0203 (7)
C2	0.9370 (5)	0.7702 (4)	0.2943 (4)	0.0230 (8)
H2A	0.8733	0.7940	0.2398	0.028*
C3	1.0502 (5)	0.8609 (4)	0.4092 (4)	0.0278 (9)
H3A	1.0655	0.9466	0.4320	0.033*
C4	1.1415 (5)	0.8257 (4)	0.4911 (4)	0.0277 (9)
H4A	1.2166	0.8882	0.5694	0.033*
C5	1.1232 (5)	0.6986 (4)	0.4588 (4)	0.0223 (8)
H5A	1.1857	0.6758	0.5147	0.027*
C6	1.0095 (4)	0.6048 (3)	0.3406 (3)	0.0199 (7)
C7	1.0733 (5)	0.4251 (4)	0.3538 (4)	0.0211 (8)
H7A	1.1549	0.4828	0.4313	0.025*
C8	1.0621 (5)	0.2923 (4)	0.3104 (3)	0.0216 (8)
C9	1.1924 (5)	0.2684 (4)	0.3865 (4)	0.0213 (8)
H9A	1.2708	0.3362	0.4599	0.026*
C10	1.2053 (5)	0.1465 (4)	0.3538 (4)	0.0251 (8)
C11	1.0886 (5)	0.0434 (4)	0.2437 (4)	0.0264 (8)
H11A	1.0990	−0.0388	0.2208	0.032*
C12	0.9588 (5)	0.0641 (4)	0.1699 (4)	0.0241 (8)
H12A	0.8812	−0.0055	0.0976	0.029*
C13	0.9381 (4)	0.1883 (4)	0.1995 (3)	0.0210 (8)
C14	0.4181 (5)	0.2370 (4)	0.1500 (4)	0.0286 (9)
H14A	0.3430	0.2444	0.2027	0.043*
H14B	0.4630	0.1642	0.1362	0.043*
H14C	0.3536	0.2270	0.0700	0.043*
C15	0.4777 (5)	0.4921 (4)	0.2296 (4)	0.0278 (9)
H15A	0.3881	0.4874	0.2690	0.042*
H15B	0.4260	0.4751	0.1442	0.042*
H15C	0.5562	0.5756	0.2769	0.042*
C16	0.6823 (5)	0.2727 (4)	−0.1903 (4)	0.0294 (9)
H16A	0.5905	0.2366	−0.2687	0.044*
H16B	0.7691	0.2260	−0.2017	0.044*
H16C	0.7339	0.3600	−0.1649	0.044*
C17	0.5297 (5)	0.0960 (4)	−0.1386 (4)	0.0340 (10)
H17A	0.4620	0.0601	−0.2258	0.051*
H17B	0.4608	0.0732	−0.0929	0.051*
H17C	0.6308	0.0638	−0.1342	0.051*
H1N1	0.861 (5)	0.552 (4)	0.076 (4)	0.023 (11)*
H2N1	0.701 (6)	0.560 (4)	0.125 (4)	0.039 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01129 (13)	0.02104 (16)	0.01781 (15)	0.00654 (11)	0.00418 (10)	0.01019 (12)
Br1	0.0246 (2)	0.0381 (2)	0.0317 (2)	0.01639 (18)	0.00366 (17)	0.0190 (2)
Cl1	0.0189 (4)	0.0307 (5)	0.0251 (5)	0.0111 (4)	0.0107 (3)	0.0160 (4)

S1	0.0160 (4)	0.0264 (5)	0.0195 (5)	0.0088 (4)	0.0024 (3)	0.0095 (4)
S2	0.0150 (4)	0.0280 (5)	0.0217 (5)	0.0085 (4)	0.0067 (3)	0.0138 (4)
O1	0.0145 (11)	0.0244 (14)	0.0230 (14)	0.0068 (10)	0.0028 (10)	0.0115 (11)
O2	0.0223 (13)	0.0395 (16)	0.0247 (15)	0.0195 (12)	0.0052 (11)	0.0167 (13)
O3	0.0235 (13)	0.0435 (17)	0.0223 (14)	0.0120 (13)	0.0074 (11)	0.0160 (13)
N1	0.0155 (14)	0.0196 (16)	0.0239 (17)	0.0072 (12)	0.0053 (12)	0.0134 (14)
N2	0.0149 (13)	0.0234 (16)	0.0170 (15)	0.0071 (12)	0.0069 (11)	0.0104 (13)
C1	0.0129 (15)	0.0246 (19)	0.0223 (19)	0.0083 (14)	0.0071 (13)	0.0086 (16)
C2	0.0205 (17)	0.025 (2)	0.032 (2)	0.0090 (15)	0.0131 (16)	0.0182 (17)
C3	0.0250 (19)	0.031 (2)	0.026 (2)	0.0098 (17)	0.0118 (16)	0.0094 (18)
C4	0.0216 (18)	0.029 (2)	0.023 (2)	0.0048 (16)	0.0078 (15)	0.0044 (17)
C5	0.0187 (17)	0.026 (2)	0.0219 (19)	0.0072 (15)	0.0067 (14)	0.0108 (16)
C6	0.0155 (16)	0.0236 (19)	0.0204 (19)	0.0093 (14)	0.0080 (14)	0.0080 (16)
C7	0.0177 (16)	0.026 (2)	0.0218 (19)	0.0079 (15)	0.0065 (14)	0.0128 (16)
C8	0.0190 (17)	0.033 (2)	0.0187 (18)	0.0114 (15)	0.0083 (14)	0.0143 (17)
C9	0.0190 (17)	0.027 (2)	0.0199 (19)	0.0098 (15)	0.0054 (14)	0.0119 (16)
C10	0.0187 (17)	0.037 (2)	0.026 (2)	0.0132 (17)	0.0067 (15)	0.0187 (19)
C11	0.0230 (18)	0.027 (2)	0.032 (2)	0.0107 (16)	0.0084 (16)	0.0154 (18)
C12	0.0201 (17)	0.026 (2)	0.028 (2)	0.0056 (15)	0.0051 (15)	0.0149 (17)
C13	0.0148 (16)	0.031 (2)	0.0200 (19)	0.0082 (15)	0.0063 (14)	0.0135 (17)
C14	0.0239 (19)	0.030 (2)	0.031 (2)	0.0014 (16)	0.0107 (17)	0.0144 (18)
C15	0.0231 (19)	0.035 (2)	0.030 (2)	0.0150 (17)	0.0124 (16)	0.0156 (19)
C16	0.029 (2)	0.042 (2)	0.024 (2)	0.0126 (18)	0.0112 (17)	0.0184 (19)
C17	0.029 (2)	0.034 (2)	0.028 (2)	0.0077 (18)	0.0037 (18)	0.0073 (19)

Geometric parameters (Å, °)

Ru1—N2	2.040 (3)	C4—H4A	0.9300
Ru1—O1	2.069 (2)	C5—C6	1.402 (5)
Ru1—N1	2.104 (3)	C5—H5A	0.9300
Ru1—S2	2.2206 (9)	C7—C8	1.437 (5)
Ru1—S1	2.2511 (9)	C7—H7A	0.9300
Ru1—Cl1	2.4319 (9)	C8—C9	1.412 (5)
Br1—C10	1.905 (3)	C8—C13	1.429 (5)
S1—O2	1.488 (3)	C9—C10	1.375 (5)
S1—C17	1.781 (4)	C9—H9A	0.9300
S1—C16	1.790 (4)	C10—C11	1.398 (5)
S2—O3	1.474 (3)	C11—C12	1.370 (5)
S2—C15	1.784 (4)	C11—H11A	0.9300
S2—C14	1.786 (4)	C12—C13	1.428 (5)
O1—C13	1.298 (4)	C12—H12A	0.9300
N1—C1	1.461 (5)	C14—H14A	0.9600
N1—H1N1	0.95 (4)	C14—H14B	0.9600
N1—H2N1	0.90 (5)	C14—H14C	0.9600
N2—C7	1.289 (4)	C15—H15A	0.9600
N2—C6	1.426 (5)	C15—H15B	0.9600
C1—C2	1.381 (5)	C15—H15C	0.9600
C1—C6	1.392 (5)	C16—H16A	0.9600
C2—C3	1.370 (5)	C16—H16B	0.9600

C2—H2A	0.9300	C16—H16C	0.9600
C3—C4	1.377 (6)	C17—H17A	0.9600
C3—H3A	0.9300	C17—H17B	0.9600
C4—C5	1.387 (5)	C17—H17C	0.9600

N2—Ru1—O1	93.33 (11)	C4—C5—H5A	120.4
N2—Ru1—N1	81.38 (12)	C6—C5—H5A	120.4
O1—Ru1—N1	173.35 (10)	C1—C6—C5	118.5 (3)
N2—Ru1—S2	88.91 (8)	C1—C6—N2	116.3 (3)
O1—Ru1—S2	89.22 (7)	C5—C6—N2	125.2 (3)
N1—Ru1—S2	94.67 (9)	N2—C7—C8	125.5 (3)
N2—Ru1—S1	173.20 (9)	N2—C7—H7A	117.2
O1—Ru1—S1	92.61 (7)	C8—C7—H7A	117.2
N1—Ru1—S1	92.46 (9)	C9—C8—C13	119.7 (3)
S2—Ru1—S1	94.48 (3)	C9—C8—C7	114.0 (3)
N2—Ru1—Cl1	85.04 (8)	C13—C8—C7	126.3 (3)
O1—Ru1—Cl1	87.14 (7)	C10—C9—C8	121.1 (4)
N1—Ru1—Cl1	88.38 (9)	C10—C9—H9A	119.5
S2—Ru1—Cl1	172.75 (3)	C8—C9—H9A	119.5
S1—Ru1—Cl1	91.95 (3)	C9—C10—C11	120.2 (3)
O2—S1—C17	108.13 (18)	C9—C10—Br1	119.0 (3)
O2—S1—C16	105.03 (18)	C11—C10—Br1	120.6 (3)
C17—S1—C16	97.9 (2)	C12—C11—C10	119.7 (4)
O2—S1—Ru1	116.15 (12)	C12—C11—H11A	120.1
C17—S1—Ru1	114.69 (15)	C10—C11—H11A	120.1
C16—S1—Ru1	113.08 (14)	C11—C12—C13	122.6 (4)
O3—S2—C15	106.04 (18)	C11—C12—H12A	118.7
O3—S2—C14	106.19 (18)	C13—C12—H12A	118.7
C15—S2—C14	99.9 (2)	O1—C13—C12	116.3 (3)
O3—S2—Ru1	116.07 (11)	O1—C13—C8	127.1 (3)
C15—S2—Ru1	113.99 (14)	C12—C13—C8	116.6 (3)
C14—S2—Ru1	113.06 (14)	S2—C14—H14A	109.5
C13—O1—Ru1	121.4 (2)	S2—C14—H14B	109.5
C1—N1—Ru1	109.8 (2)	H14A—C14—H14B	109.5
C1—N1—H1N1	106 (2)	S2—C14—H14C	109.5
Ru1—N1—H1N1	111 (2)	H14A—C14—H14C	109.5
C1—N1—H2N1	107 (3)	H14B—C14—H14C	109.5
Ru1—N1—H2N1	111 (3)	S2—C15—H15A	109.5
H1N1—N1—H2N1	112 (4)	S2—C15—H15B	109.5
C7—N2—C6	121.3 (3)	H15A—C15—H15B	109.5
C7—N2—Ru1	124.5 (3)	S2—C15—H15C	109.5
C6—N2—Ru1	114.0 (2)	H15A—C15—H15C	109.5
C2—C1—C6	121.6 (3)	H15B—C15—H15C	109.5
C2—C1—N1	120.7 (3)	S1—C16—H16A	109.5
C6—C1—N1	117.7 (3)	S1—C16—H16B	109.5
C3—C2—C1	119.4 (4)	H16A—C16—H16B	109.5
C3—C2—H2A	120.3	S1—C16—H16C	109.5
C1—C2—H2A	120.3	H16A—C16—H16C	109.5
C2—C3—C4	120.2 (4)	H16B—C16—H16C	109.5
C2—C3—H3A	119.9	S1—C17—H17A	109.5

C4—C3—H3A	119.9	S1—C17—H17B	109.5
C3—C4—C5	121.1 (4)	H17A—C17—H17B	109.5
C3—C4—H4A	119.4	S1—C17—H17C	109.5
C5—C4—H4A	119.4	H17A—C17—H17C	109.5
C4—C5—C6	119.2 (4)	H17B—C17—H17C	109.5

O1—Ru1—S1—O2	129.94 (15)	S2—Ru1—N2—C6	−87.7 (2)
N1—Ru1—S1—O2	−54.37 (16)	Cl1—Ru1—N2—C6	96.3 (2)
S2—Ru1—S1—O2	40.52 (14)	Ru1—N1—C1—C2	−174.7 (3)
Cl1—Ru1—S1—O2	−142.83 (14)	Ru1—N1—C1—C6	8.1 (4)
O1—Ru1—S1—C17	2.55 (18)	C6—C1—C2—C3	1.1 (6)
N1—Ru1—S1—C17	178.24 (19)	N1—C1—C2—C3	−176.0 (3)
S2—Ru1—S1—C17	−86.87 (17)	C1—C2—C3—C4	−1.5 (6)
Cl1—Ru1—S1—C17	89.78 (17)	C2—C3—C4—C5	1.0 (6)
O1—Ru1—S1—C16	−108.52 (17)	C3—C4—C5—C6	−0.1 (6)
N1—Ru1—S1—C16	67.17 (18)	C2—C1—C6—C5	−0.3 (5)
S2—Ru1—S1—C16	162.06 (16)	N1—C1—C6—C5	176.9 (3)
Cl1—Ru1—S1—C16	−21.29 (16)	C2—C1—C6—N2	−179.6 (3)
N2—Ru1—S2—O3	−22.80 (16)	N1—C1—C6—N2	−2.4 (5)
O1—Ru1—S2—O3	70.55 (15)	C4—C5—C6—C1	−0.2 (5)
N1—Ru1—S2—O3	−104.06 (16)	C4—C5—C6—N2	179.0 (3)
S1—Ru1—S2—O3	163.10 (14)	C7—N2—C6—C1	171.1 (3)
N2—Ru1—S2—C15	100.87 (17)	Ru1—N2—C6—C1	−4.9 (4)
O1—Ru1—S2—C15	−165.78 (17)	C7—N2—C6—C5	−8.2 (5)
N1—Ru1—S2—C15	19.61 (17)	Ru1—N2—C6—C5	175.8 (3)
S1—Ru1—S2—C15	−73.23 (15)	C6—N2—C7—C8	−175.3 (3)
N2—Ru1—S2—C14	−145.87 (17)	Ru1—N2—C7—C8	0.3 (5)
O1—Ru1—S2—C14	−52.52 (17)	N2—C7—C8—C9	173.2 (3)
N1—Ru1—S2—C14	132.87 (17)	N2—C7—C8—C13	−4.9 (6)
S1—Ru1—S2—C14	40.03 (16)	C13—C8—C9—C10	1.8 (6)
N2—Ru1—O1—C13	−14.2 (3)	C7—C8—C9—C10	−176.4 (3)
S2—Ru1—O1—C13	−103.1 (3)	C8—C9—C10—C11	0.0 (6)
S1—Ru1—O1—C13	162.5 (3)	C8—C9—C10—Br1	176.4 (3)
Cl1—Ru1—O1—C13	70.6 (3)	C9—C10—C11—C12	−1.4 (6)
N2—Ru1—N1—C1	−8.0 (2)	Br1—C10—C11—C12	−177.7 (3)
S2—Ru1—N1—C1	80.1 (2)	C10—C11—C12—C13	0.9 (6)
S1—Ru1—N1—C1	174.9 (2)	Ru1—O1—C13—C12	−165.0 (2)
Cl1—Ru1—N1—C1	−93.3 (2)	Ru1—O1—C13—C8	14.8 (5)
O1—Ru1—N2—C7	7.3 (3)	C11—C12—C13—O1	−179.3 (4)
N1—Ru1—N2—C7	−168.7 (3)	C11—C12—C13—C8	0.9 (6)
S2—Ru1—N2—C7	96.4 (3)	C9—C8—C13—O1	178.0 (3)
Cl1—Ru1—N2—C7	−79.6 (3)	C7—C8—C13—O1	−4.0 (6)
O1—Ru1—N2—C6	−176.8 (2)	C9—C8—C13—C12	−2.2 (5)
N1—Ru1—N2—C6	7.2 (2)	C7—C8—C13—C12	175.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N1···Cl1^{i}	0.95 (5)	2.34 (5)	3.235 (4)	157 (4)

N1—H2N1···O2$^{\mathrm{ii}}$	0.91 (5)	2.22 (5)	2.975 (5)	141 (4)
C2—H2A···O2$^{\mathrm{ii}}$	0.93	2.58	3.267 (5)	131
C5—H5A···O3$^{\mathrm{iii}}$	0.93	2.40	3.323 (6)	174
C7—H7A···O3$^{\mathrm{iii}}$	0.93	2.35	3.263 (5)	168
C16—H16B···Cl1	0.96	2.83	3.222 (4)	106
C14—H14A···Cg2$^{\mathrm{iv}}$	0.96	2.73	3.634 (5)	157
C16—H16B···Cg1$^{\mathrm{i}}$	0.96	3.09	3.561 (5)	112

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

Fig. 1

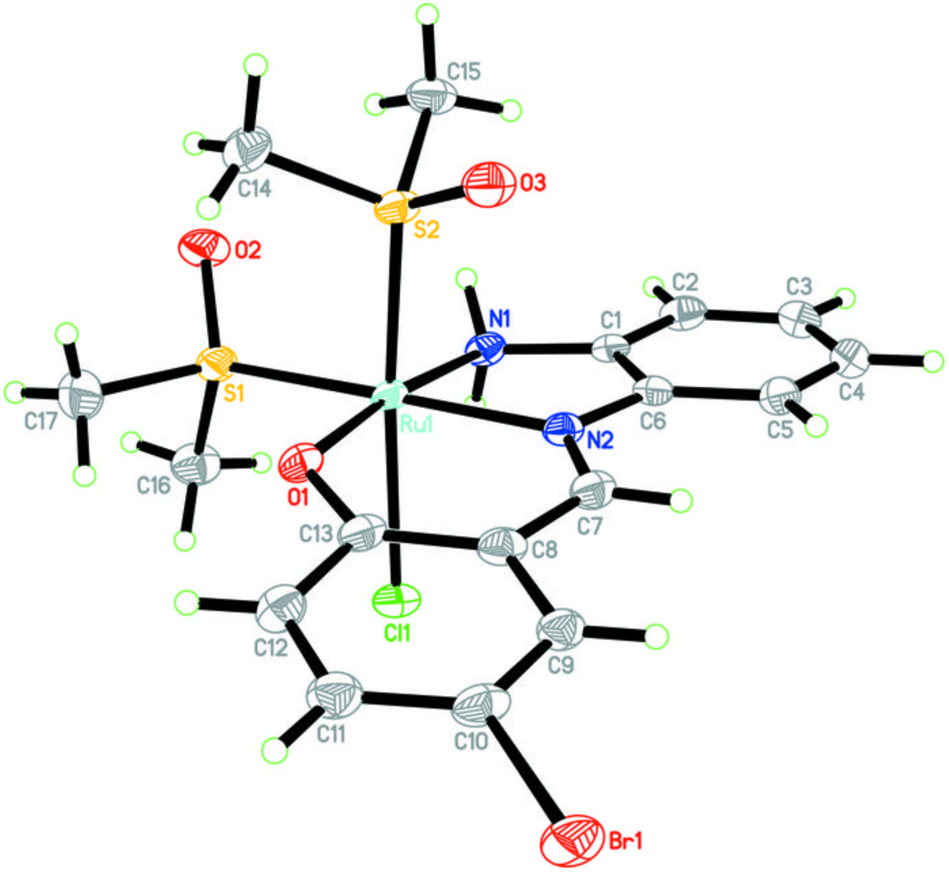
C15
C14
O3
S2
O2
N1
C2
C3
C1
C4
C17
S1
Ru1
C6
C5
N2
C16
O1
C7
C13
C8
Cl1
C9
C12
C11
C10
Br1

Fig. 2