

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

[1-*tert*-Butyl-3-(pyridin-2-ylmethyl- κ N)-imidazol-2-ylidene- κ C¹]carbonyl-dichlorido(dimethyl sulfoxide- κ S)-ruthenium(II)

Yong Cheng,* Wen-Qian Hua and Ying-Hua Zhou

College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, People's Republic of China

Correspondence e-mail: chyong2008happy@163.com

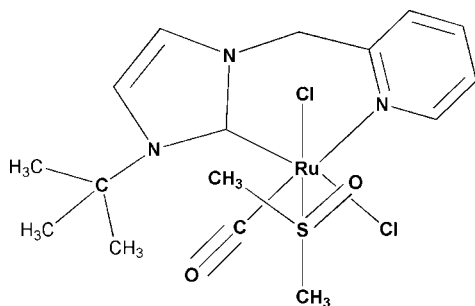
Received 3 July 2011; accepted 14 October 2011

 Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 16.5.

In the title complex, $[\text{RuCl}_2(\text{C}_{13}\text{H}_{17}\text{N}_3)(\text{C}_2\text{H}_6\text{OS})(\text{CO})]$, the coordination environment around the Ru atom is slightly distorted octahedral. The Cl atoms are mutually *trans* to the dimethyl sulfoxide ligand and the imidazole carbene C atom, respectively. The carbonyl ligand is located *trans* to the pyridine N atom.

Related literature

For general background to N-heterocyclic carbene (NHC) complexes, see: Hahn *et al.* (2006); Lee *et al.* (2007); Mas-Marza *et al.* (2005); Kaufhold *et al.* (2008); Araki *et al.* (2008); Son *et al.* (2004); Poyatos *et al.* (2006). For our previous work on Ru-NHC complexes, see: Cheng, Sun *et al.* (2009); Cheng, Xu *et al.* (2009).



Experimental

Crystal data

$[\text{RuCl}_2(\text{C}_{13}\text{H}_{17}\text{N}_3)(\text{C}_2\text{H}_6\text{OS})(\text{CO})]$	$V = 3877.1 (7) \text{ \AA}^3$
$M_r = 493.40$	$Z = 8$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 14.3297 (14) \text{ \AA}$	$\mu = 1.21 \text{ mm}^{-1}$
$b = 15.7428 (16) \text{ \AA}$	$T = 291 \text{ K}$
$c = 17.1867 (16) \text{ \AA}$	$0.26 \times 0.22 \times 0.20 \text{ mm}$

Data collection

Bruker SMART APEX CCD diffractometer	20132 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3815 independent reflections
$T_{\min} = 0.74, T_{\max} = 0.79$	3401 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$	231 parameters
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\max} = 0.33 \text{ e \AA}^{-3}$
3815 reflections	$\Delta\rho_{\min} = -1.30 \text{ e \AA}^{-3}$

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

This work was supported by the National Basic Research Program of China (No. 2006CB806104 and 2007CB925102). We are also grateful to the Doctoral Startup Foundation of Anhui Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZB2017).

References

- Araki, K., Kuwata, S. & Ikariya, T. (2008). *Organometallics*, **27**, 2176–2178.
- Bruker (1997). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cheng, Y., Sun, J.-F., Yang, H.-L., Xu, H.-J., Li, Y.-Z., Chen, X.-T. & Xue, Z.-L. (2009). *Organometallics*, **28**, 819–823.
- Cheng, Y., Xu, H.-J., Sun, J.-F., Li, Y.-Z., Chen, X.-T. & Xue, Z.-L. (2009). *Dalton Trans.* pp. 7132–7140.
- Hahn, F. E. (2006). *Angew. Chem. Int. Ed.* **45**, 1348–1352.
- Kaufhold, O., Hahn, F. E., Pape, T. & Hepp, A. (2008). *J. Organomet. Chem.* **693**, 3435–3440.
- Lee, H. M., Lee, C.-C. & Cheng, P.-Y. (2007). *Curr. Org. Chem.* **11**, 1491–1524.
- Mas-Marza, E., Sanau, M. & Peris, E. (2005). *Inorg. Chem.* **44**, 9961–9967.
- Poyatos, M., Maise-Francis, A., Bellemin-Laponnaz, S., Peris, E. & Gade, L. H. (2006). *J. Organomet. Chem.* **691**, 2713–2720.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Son, K. H., Park, S. U., Lee, Y.-S., Kim, B. Y., Choi, C. H., Lah, M. S., Jang, Y. H., Jang, D.-J. & Chung, Y. K. (2004). *Inorg. Chem.* **43**, 6896–6898.

supporting information

Acta Cryst. (2011). E67, m1573 [doi:10.1107/S1600536811042590]

[1-*tert*-Butyl-3-(pyridin-2-ylmethyl- κ N)imidazol-2-ylidene- κ C¹]carbonyl-dichlorido(dimethyl sulfoxide- κ S)ruthenium(II)

Yong Cheng, Wen-Qian Hua and Ying-Hua Zhou

S1. Comment

N-Heterocyclic carbenes (NHCs) complexes have attracted increasing attention as they have been proven to act as efficient homogeneous catalyst (Hahn *et al.* 2006). Pyridine-functionalized bidentate carbene ligands have been frequently used as versatile ancillary ligands in organometallic complexes in recent years (Lee *et al.* 2007). A lot of bidentate pyridinefunctionalized NHC complexes have been prepared, some of which showed catalytic activities in reactions such as hydrosilylation of acetylenes, cyclization of acetylenic carboxylic acids, hydrogen transfer to ketones (Mas-Marza *et al.* 2005). However, few reports have been published on Ru complexes containing bidentate pyridine-functionalized NHC ligands (Kaufhold *et al.* 2008, Araki *et al.* 2008, Son *et al.* 2004, Poyatos *et al.* 2006). We have reported the synthesis and characterization of pyridine functionalized Ru(II)-NHC nitrosyl or carbonyl complexes and their catalytic activity in hydrogen transfer of ketones (Cheng, Sun *et al.*, 2009; Cheng, Xu *et al.*, 2009). Herein, we report a new pyridine functionalized Ru-NHC carbonyl complex with dimethyl sulfoxide.

The structure of the title complex shows that the coordination geometry around the ruthenium atom can be rationalized as a slightly distorted octahedron. Two chloride atoms occupy mutually *trans* to the dimethylsulfoxide and imidazole carbene carbon respectively. The CO group is located *trans* to the pyridine nitrogen (Fig.1).

S2. Experimental

A mixture of 3-*tert*-butyl-1-picolylimidazolium Bromide (1.0 mmol), silver oxide (1.0 mmol) and CH₂Cl₂ (30 ml) was stirred at room temperature for 12 h, and was then filtered through Celite to remove unreacted silver oxide and insoluble residues. [Ru(CO)₂Cl₂]_n (1.0 mmol) was added to the pale yellow solution, stirred for 12 h at room temperature and then filtered through Celite to remove the silver halide. The products were chromatographed using silica gel. Elution with CH₂Cl₂: MeOH (40:1) afforded a pale yellow band that contained the *trans*-[(3-*tert*-butyl-1-picolylimidazol-2-ylidene)biscolorodicarbonylruthenium], Removal of the volatiles under vacuum gave the products as pale yellow powders.

Exposured the saturated dimethyl sulfoxide solution of the *trans*-[(3-*tert*-butyl-1-picolylimidazol-2-ylidene)biscolorodicarbonylruthenium] in air, yellow-rectangle crystals were obtained one month later, which were title complex confirmed by X-ray structure determination. It shows that dimethyl sulfoxide displaced one molecule of CO in previous compound, and the structure converted from *trans* to *cis*.

S3. Refinement

The structures were solved by direct methods and refined on F² against all reflections by full-matrix least-squares methods with *SHELXTL* program. The hydrogen atoms in the compound were positioned geometrically (C—H = 0.93 Å and O—H = 0.83 Å) and refined in the riding-model approximation, with *U*_{iso}(H) set to 1.2*U*_{eq}(O). All non-hydrogen atoms were refined with anisotropic thermal parameters. The highest peak and deepest hole residual peak in the final

difference Fourier map are located at 0.33 Å and 1.30 Å, respectively, from atom Ru.

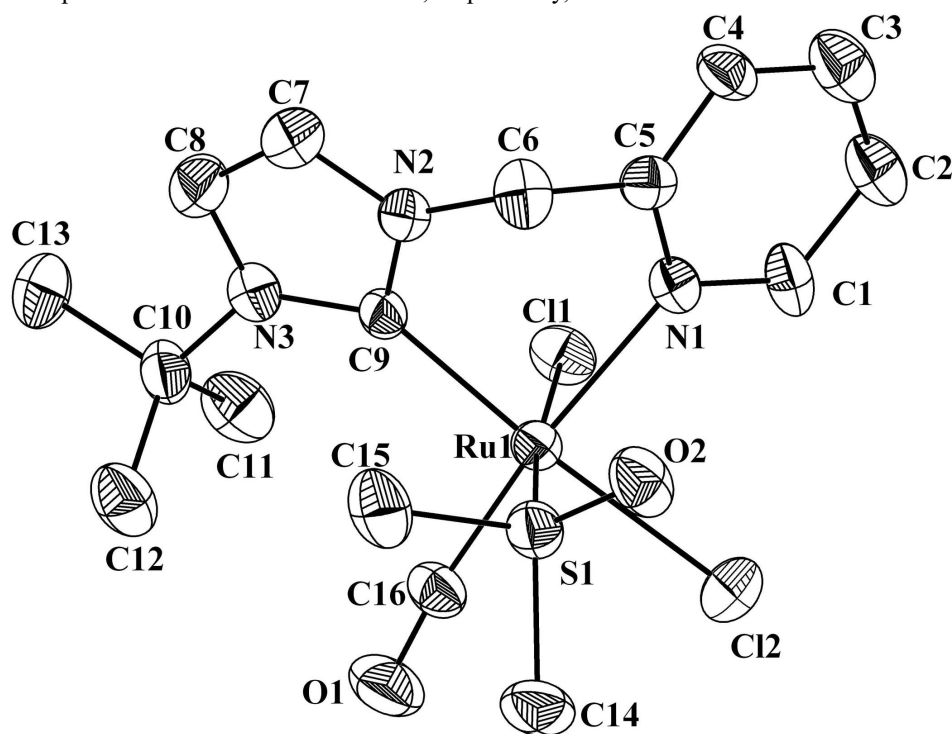


Figure 1

View of the title complex showing 30% probability ellipsoids. Hydrogen atoms are omitted for clarity. [symmetry codes: (i) $-x + 1/2, -y, z + 1/2$; (ii) $-x, y + 1/2, -z + 1/2$]

[1-*tert*-Butyl-3-(pyridin-2-ylmethyl- κ N)imidazol-2-ylidene- κ C¹]carbonyldichlorido(dimethyl sulfoxide- κ S)ruthenium(II)

Crystal data

[RuCl₂(C₁₃H₁₇N₃)(C₂H₆OS)(CO)]

$M_r = 493.40$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 14.3297$ (14) Å

$b = 15.7428$ (16) Å

$c = 17.1867$ (16) Å

$V = 3877.1$ (7) Å³

$Z = 8$

$F(000) = 2000$

$D_x = 1.691$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2216 reflections

$\theta = 2.3$ – 23.2°

$\mu = 1.21$ mm⁻¹

$T = 291$ K

Cuboid, yellow

$0.26 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: sealed tube

Graphite monochromator

ϕ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.74, T_{\max} = 0.79$

20132 measured reflections

3815 independent reflections

3401 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.0^\circ, \theta_{\min} = 2.3^\circ$

$h = -16 \rightarrow 17$

$k = -12 \rightarrow 19$

$l = -17 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.110$
 $S = 1.06$
 3815 reflections
 231 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
 $w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.99P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.30 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The single crystals was mounted on a glass fibre with silicon grease. Diffraction data were collected on a Bruker *SMART* Apex CCD diffractometer using graphite-monochromated MoK α ($\lambda = 0.71073 \text{ \AA}$) radiation and corrected for absorption using *SADABS* program.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7924 (2)	0.1922 (3)	0.4198 (2)	0.0412 (8)
H1	0.7884	0.1378	0.4404	0.049*
C2	0.8640 (3)	0.2469 (3)	0.4455 (3)	0.0460 (10)
H2	0.9069	0.2292	0.4827	0.055*
C3	0.8685 (3)	0.3279 (3)	0.4137 (3)	0.0504 (10)
H3	0.9157	0.3649	0.4291	0.060*
C4	0.8029 (2)	0.3541 (2)	0.3591 (2)	0.0374 (8)
H4	0.8046	0.4085	0.3380	0.045*
C5	0.7357 (2)	0.2968 (2)	0.33735 (19)	0.0307 (7)
C6	0.6614 (3)	0.3243 (2)	0.2791 (2)	0.0389 (8)
H6A	0.6010	0.3249	0.3047	0.047*
H6B	0.6748	0.3817	0.2617	0.047*
C7	0.6571 (3)	0.3016 (3)	0.1371 (2)	0.0487 (10)
H7	0.6625	0.3586	0.1233	0.058*
C8	0.6478 (3)	0.2344 (3)	0.0883 (2)	0.0485 (10)
H8	0.6465	0.2366	0.0343	0.058*
C9	0.6444 (2)	0.1815 (2)	0.21162 (19)	0.0276 (6)
C10	0.6203 (3)	0.0776 (3)	0.0934 (2)	0.0403 (8)
C11	0.6801 (3)	0.0038 (3)	0.1278 (3)	0.0501 (10)
H11A	0.7451	0.0162	0.1208	0.075*
H11B	0.6650	-0.0483	0.1016	0.075*
H11C	0.6670	-0.0020	0.1824	0.075*

C12	0.5139 (3)	0.0597 (3)	0.1032 (3)	0.0512 (10)
H12A	0.4976	0.0628	0.1573	0.077*
H12B	0.4998	0.0040	0.0837	0.077*
H12C	0.4789	0.1013	0.0746	0.077*
C13	0.6446 (3)	0.0843 (3)	0.0066 (2)	0.0577 (12)
H13A	0.6002	0.1206	-0.0188	0.087*
H13B	0.6425	0.0288	-0.0166	0.087*
H13C	0.7061	0.1076	0.0008	0.087*
C14	0.4160 (3)	0.1148 (3)	0.3901 (3)	0.0518 (11)
H14A	0.4441	0.0782	0.4280	0.078*
H14B	0.3913	0.0812	0.3482	0.078*
H14C	0.3664	0.1466	0.4139	0.078*
C15	0.4341 (3)	0.2282 (3)	0.2722 (3)	0.0524 (10)
H15A	0.3793	0.2559	0.2920	0.079*
H15B	0.4158	0.1823	0.2387	0.079*
H15C	0.4709	0.2682	0.2433	0.079*
C16	0.5656 (2)	0.0265 (2)	0.2880 (2)	0.0351 (7)
Cl1	0.78532 (6)	0.05000 (6)	0.29450 (6)	0.0388 (2)
Cl2	0.63074 (7)	0.05755 (7)	0.44994 (6)	0.0496 (3)
N1	0.72873 (19)	0.21741 (17)	0.36515 (15)	0.0303 (6)
N2	0.65692 (19)	0.26818 (19)	0.21148 (17)	0.0325 (6)
N3	0.6403 (2)	0.1616 (2)	0.13376 (18)	0.0364 (7)
O1	0.5227 (2)	-0.03364 (19)	0.27652 (19)	0.0556 (8)
O2	0.51299 (19)	0.25707 (19)	0.40880 (16)	0.0488 (7)
Ru1	0.636122 (18)	0.119715 (16)	0.318107 (15)	0.02810 (12)
S1	0.50232 (6)	0.18683 (6)	0.35263 (5)	0.0356 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0356 (18)	0.053 (2)	0.0345 (18)	0.0042 (16)	-0.0116 (14)	-0.0115 (16)
C2	0.041 (2)	0.047 (2)	0.050 (2)	-0.0011 (16)	-0.0079 (16)	-0.0176 (19)
C3	0.043 (2)	0.054 (2)	0.054 (3)	-0.0021 (18)	-0.0030 (17)	-0.020 (2)
C4	0.0343 (17)	0.0377 (19)	0.0402 (19)	-0.0088 (15)	0.0031 (14)	-0.0128 (16)
C5	0.0319 (16)	0.0288 (16)	0.0316 (16)	0.0009 (13)	0.0054 (13)	-0.0038 (13)
C6	0.0436 (19)	0.0327 (18)	0.040 (2)	0.0098 (15)	-0.0052 (16)	-0.0053 (15)
C7	0.056 (2)	0.049 (2)	0.041 (2)	-0.0112 (19)	-0.0021 (18)	0.0076 (18)
C8	0.066 (3)	0.044 (2)	0.036 (2)	-0.0120 (19)	-0.0048 (18)	0.0055 (17)
C9	0.0219 (15)	0.0351 (17)	0.0259 (16)	-0.0020 (12)	-0.0013 (11)	-0.0008 (13)
C10	0.0396 (19)	0.051 (2)	0.0300 (18)	-0.0049 (17)	-0.0043 (14)	-0.0075 (16)
C11	0.035 (2)	0.051 (2)	0.064 (3)	0.0041 (17)	-0.0020 (18)	-0.010 (2)
C12	0.034 (2)	0.063 (3)	0.057 (2)	0.0003 (18)	-0.0081 (17)	-0.010 (2)
C13	0.068 (3)	0.075 (3)	0.030 (2)	-0.009 (2)	0.0055 (18)	-0.010 (2)
C14	0.037 (2)	0.063 (3)	0.055 (3)	-0.0163 (18)	0.0153 (18)	-0.011 (2)
C15	0.035 (2)	0.066 (3)	0.057 (2)	0.0095 (18)	-0.0167 (18)	-0.002 (2)
C16	0.0285 (16)	0.0331 (18)	0.0437 (19)	-0.0018 (14)	-0.0075 (14)	0.0018 (15)
Cl1	0.0302 (4)	0.0355 (4)	0.0508 (5)	0.0019 (3)	-0.0024 (3)	-0.0006 (4)
Cl2	0.0601 (6)	0.0520 (6)	0.0366 (5)	-0.0054 (4)	-0.0026 (4)	0.0137 (4)

N1	0.0292 (14)	0.0306 (14)	0.0309 (14)	0.0006 (11)	-0.0028 (10)	-0.0047 (11)
N2	0.0327 (14)	0.0343 (15)	0.0306 (14)	-0.0040 (12)	-0.0035 (11)	0.0037 (12)
N3	0.0383 (16)	0.0379 (16)	0.0331 (16)	-0.0044 (12)	-0.0029 (11)	-0.0039 (13)
O1	0.0553 (17)	0.0423 (16)	0.069 (2)	-0.0183 (14)	-0.0067 (15)	-0.0039 (14)
O2	0.0422 (14)	0.0581 (17)	0.0462 (15)	-0.0040 (13)	0.0044 (12)	-0.0214 (13)
Ru1	0.02643 (17)	0.02881 (18)	0.02905 (18)	-0.00223 (10)	-0.00179 (9)	0.00097 (10)
S1	0.0285 (4)	0.0435 (5)	0.0348 (4)	-0.0005 (3)	0.0018 (3)	-0.0040 (4)

Geometric parameters (Å, °)

C1—N1	1.368 (4)	C10—C12	1.560 (5)
C1—C2	1.409 (5)	C11—H11A	0.9600
C1—H1	0.9300	C11—H11B	0.9600
C2—C3	1.389 (6)	C11—H11C	0.9600
C2—H2	0.9300	C12—H12A	0.9600
C3—C4	1.391 (6)	C12—H12B	0.9600
C3—H3	0.9300	C12—H12C	0.9600
C4—C5	1.372 (5)	C13—H13A	0.9600
C4—H4	0.9300	C13—H13B	0.9600
C5—N1	1.341 (4)	C13—H13C	0.9600
C5—C6	1.526 (5)	C14—S1	1.797 (4)
C6—N2	1.461 (4)	C14—H14A	0.9600
C6—H6A	0.9700	C14—H14B	0.9600
C6—H6B	0.9700	C14—H14C	0.9600
C7—C8	1.357 (6)	C15—S1	1.815 (4)
C7—N2	1.383 (5)	C15—H15A	0.9600
C7—H7	0.9300	C15—H15B	0.9600
C8—N3	1.391 (5)	C15—H15C	0.9600
C8—H8	0.9300	C16—O1	1.146 (4)
C9—N2	1.376 (4)	C16—Ru1	1.855 (3)
C9—N3	1.376 (5)	Cl1—Ru1	2.4372 (9)
C9—Ru1	2.076 (3)	Cl2—Ru1	2.4692 (10)
C10—N3	1.521 (5)	N1—Ru1	2.186 (3)
C10—C13	1.536 (5)	O2—S1	1.476 (3)
C10—C11	1.560 (6)	Ru1—S1	2.2682 (9)
N1—C1—C2	121.6 (4)	C10—C13—H13B	109.5
N1—C1—H1	119.2	H13A—C13—H13B	109.5
C2—C1—H1	119.2	C10—C13—H13C	109.5
C3—C2—C1	118.1 (4)	H13A—C13—H13C	109.5
C3—C2—H2	120.9	H13B—C13—H13C	109.5
C1—C2—H2	120.9	S1—C14—H14A	109.5
C2—C3—C4	120.4 (4)	S1—C14—H14B	109.5
C2—C3—H3	119.8	H14A—C14—H14B	109.5
C4—C3—H3	119.8	S1—C14—H14C	109.5
C5—C4—C3	117.5 (4)	H14A—C14—H14C	109.5
C5—C4—H4	121.2	H14B—C14—H14C	109.5
C3—C4—H4	121.2	S1—C15—H15A	109.5

N1—C5—C4	124.7 (3)	S1—C15—H15B	109.5
N1—C5—C6	116.5 (3)	H15A—C15—H15B	109.5
C4—C5—C6	118.8 (3)	S1—C15—H15C	109.5
N2—C6—C5	112.4 (3)	H15A—C15—H15C	109.5
N2—C6—H6A	109.1	H15B—C15—H15C	109.5
C5—C6—H6A	109.1	O1—C16—Ru1	173.5 (3)
N2—C6—H6B	109.1	C5—N1—C1	117.7 (3)
C5—C6—H6B	109.1	C5—N1—Ru1	124.7 (2)
H6A—C6—H6B	107.9	C1—N1—Ru1	117.1 (2)
C8—C7—N2	105.9 (4)	C9—N2—C7	112.3 (3)
C8—C7—H7	127.1	C9—N2—C6	127.2 (3)
N2—C7—H7	127.1	C7—N2—C6	120.3 (3)
C7—C8—N3	107.7 (4)	C9—N3—C8	110.8 (3)
C7—C8—H8	126.2	C9—N3—C10	130.5 (3)
N3—C8—H8	126.2	C8—N3—C10	118.4 (3)
N2—C9—N3	103.3 (3)	C16—Ru1—C9	98.96 (14)
N2—C9—Ru1	118.3 (2)	C16—Ru1—N1	171.94 (13)
N3—C9—Ru1	138.4 (3)	C9—Ru1—N1	87.79 (11)
N3—C10—C13	109.9 (3)	C16—Ru1—S1	88.94 (11)
N3—C10—C11	111.8 (3)	C9—Ru1—S1	93.48 (9)
C13—C10—C11	107.2 (3)	N1—Ru1—S1	95.09 (7)
N3—C10—C12	107.0 (3)	C16—Ru1—Cl1	94.29 (11)
C13—C10—C12	109.8 (3)	C9—Ru1—Cl1	90.81 (9)
C11—C10—C12	111.2 (3)	N1—Ru1—Cl1	81.13 (7)
C10—C11—H11A	109.5	S1—Ru1—Cl1	174.18 (3)
C10—C11—H11B	109.5	C16—Ru1—Cl2	85.74 (12)
H11A—C11—H11B	109.5	C9—Ru1—Cl2	175.13 (10)
C10—C11—H11C	109.5	N1—Ru1—Cl2	87.62 (8)
H11A—C11—H11C	109.5	S1—Ru1—Cl2	85.31 (4)
H11B—C11—H11C	109.5	Cl1—Ru1—Cl2	90.09 (3)
C10—C12—H12A	109.5	O2—S1—C14	108.05 (19)
C10—C12—H12B	109.5	O2—S1—C15	106.6 (2)
H12A—C12—H12B	109.5	C14—S1—C15	97.4 (2)
C10—C12—H12C	109.5	O2—S1—Ru1	115.63 (11)
H12A—C12—H12C	109.5	C14—S1—Ru1	112.44 (15)
H12B—C12—H12C	109.5	C15—S1—Ru1	115.05 (15)
C10—C13—H13A	109.5		
N1—C1—C2—C3	0.0 (6)	C13—C10—N3—C8	19.2 (5)
C1—C2—C3—C4	1.0 (6)	C11—C10—N3—C8	138.1 (4)
C2—C3—C4—C5	-1.1 (6)	C12—C10—N3—C8	-99.9 (4)
C3—C4—C5—N1	0.1 (5)	N2—C9—Ru1—C16	153.9 (2)
C3—C4—C5—C6	178.5 (3)	N3—C9—Ru1—C16	-25.5 (4)
N1—C5—C6—N2	-56.8 (4)	N2—C9—Ru1—N1	-30.6 (2)
C4—C5—C6—N2	124.7 (3)	N3—C9—Ru1—N1	150.1 (3)
N2—C7—C8—N3	1.1 (5)	N2—C9—Ru1—S1	64.4 (2)
C4—C5—N1—C1	0.9 (5)	N3—C9—Ru1—S1	-115.0 (3)
C6—C5—N1—C1	-177.5 (3)	N2—C9—Ru1—Cl1	-111.7 (2)

C4—C5—N1—Ru1	-170.0 (3)	N3—C9—Ru1—C11	69.0 (3)
C6—C5—N1—Ru1	11.6 (4)	C5—N1—Ru1—C9	26.9 (3)
C2—C1—N1—C5	-0.9 (5)	C1—N1—Ru1—C9	-144.0 (3)
C2—C1—N1—Ru1	170.7 (3)	C5—N1—Ru1—S1	-66.4 (3)
N3—C9—N2—C7	2.2 (4)	C1—N1—Ru1—S1	122.7 (2)
Ru1—C9—N2—C7	-177.3 (3)	C5—N1—Ru1—C11	118.1 (3)
N3—C9—N2—C6	176.7 (3)	C1—N1—Ru1—C11	-52.9 (2)
Ru1—C9—N2—C6	-2.8 (4)	C5—N1—Ru1—C12	-151.5 (3)
C8—C7—N2—C9	-2.1 (4)	C1—N1—Ru1—C12	37.6 (2)
C8—C7—N2—C6	-177.0 (3)	C16—Ru1—S1—O2	158.69 (19)
C5—C6—N2—C9	55.1 (5)	C9—Ru1—S1—O2	-102.40 (17)
C5—C6—N2—C7	-130.8 (4)	N1—Ru1—S1—O2	-14.31 (16)
N2—C9—N3—C8	-1.5 (4)	C12—Ru1—S1—O2	72.87 (15)
Ru1—C9—N3—C8	177.9 (3)	C16—Ru1—S1—C14	33.9 (2)
N2—C9—N3—C10	-174.9 (3)	C9—Ru1—S1—C14	132.85 (19)
Ru1—C9—N3—C10	4.5 (6)	N1—Ru1—S1—C14	-139.06 (19)
C7—C8—N3—C9	0.3 (5)	C12—Ru1—S1—C14	-51.88 (17)
C7—C8—N3—C10	174.6 (3)	C16—Ru1—S1—C15	-76.3 (2)
C13—C10—N3—C9	-167.8 (3)	C9—Ru1—S1—C15	22.6 (2)
C11—C10—N3—C9	-48.9 (5)	N1—Ru1—S1—C15	110.71 (19)
C12—C10—N3—C9	73.0 (5)	C12—Ru1—S1—C15	-162.11 (18)
