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(η^6-Benzene)chlorido[(*S*)-2-(4-isopropyl-4,5-dihydrooxazol-2-yl)phenolato]ruthenium(II)

Monsuru T. Kelani,* Alfred Muller and Koop Lammertsma

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

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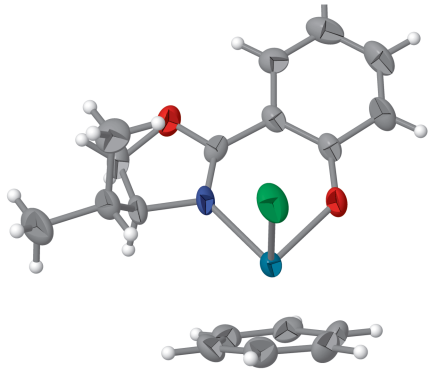
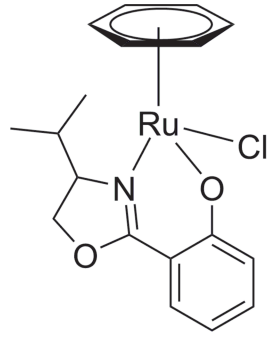
The title compound, $[Ru(C_{12}H_{14}NO_2)Cl(\eta^6\text{-}C_6H_6)]$, exhibits a half-sandwich tripod stand structure and crystallizes in the orthorhombic space group $P2_12_12_1$. The arene group is η^6 π-coordinated to the Ru atom with a centroid-to-metal distance of 1.6590 (5) Å, with the (*S*)-2-(4-isopropyl-4,5-dihydrooxazol-2-yl)-phenolate chelate ligand forming a bite angle of 86.88 (19)° through its N and phenolate O atoms. The pseudo-octahedral geometry assumed by the complex is completed by a chloride ligand. The coordination of the optically pure bidentate ligand induces metal centered chirality onto the complex with a Flack parameter of −0.056.

3D view



Chemical scheme



Structure description

Ruthenium complexes have profound applications in various studies relating to chemotherapeutics (Chan *et al.*, 2017), catalysis (Chavarot *et al.*, 2003; Hamelin *et al.*, 2007), electrochemistry (Ryabov *et al.*, 2005), and photochemistry (Huisman *et al.*, 2016). The optically pure salicyloxazoline coordinating ligand of the complex is often employed as an auxiliary ligand towards the enantioselective synthesis of chiral-at-metal complexes. The approach relies on the leaving propensity of the benzene and the halo ligands for replacement in the octahedral geometry with another achiral ligand system as a strategy in most cases. The choice of the salicyloxazoline ligand is due to its reversible coordination upon acid protonation of its phenolate leaving the stereochemistry of the metal complex preserved (Gong *et al.*, 2013). Thus, the use of the compound is extremely helpful in the synthesis of enantiomerically pure transition-metal complexes with metal-centred chirality (Gong *et al.*, 2009, 2010). The title compound (Fig. 1) features an optically pure bidentate salicyloxazoline and a chloride ligand within a pseudo-octahedral confinement of the three-legged stool while an arene ring occupying the seat of the stool completes the coordination sphere of the ruthenium(II) complex. The bite angle, 86.88 (19)°, of the bidentate ligand is comparable to those of its cymene analogues, 86.68°

Table 1
Selected torsion angles (°).

O2—C1—C2—N1	−16.4 (7)	C8—C7—C12—O1	179.3 (6)
O2—C1—C2—C3	103.6 (6)	O2—C6—N1—Ru1	174.7 (4)
C6—C7—C8—C9	179.4 (6)	C3—C2—N1—Ru1	71.5 (7)
C10—C11—C12—O1	−179.3 (7)	C7—C6—O2—C1	174.8 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.93	2.38	2.725 (9)	102
C17—H17···Cl1^{i}	0.93	2.80	3.440 (8)	127
C18—H18···O1^{i}	0.93	2.54	3.405 (8)	156

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

(Brunner *et al.*, 1998), 88.29° (Davenport *et al.*, 2004) and mesitylene analogue, 86.91° (Davenport *et al.*, 2004) reported in the literature. The Ru forms bond lengths of 2.4176 (19), 2.063 (5) and 2.083 (6) Å to Cl1, O1 and N1, respectively. The crystal packing features weak C—H···*X* hydrogen bonding (*X* = O or Cl) in a manner in which each molecular unit is skewed like a satellite dish. Selected torsion angles are given in Table 1 and details of the hydrogen-bonding geometry in Table 2.

Synthesis and crystallization

$[\eta^6$-$C_6H_6)_2RuCl_2]_2$ (200 mg, 0.40 mmol, 1 eq), (*S*)-isopropyl-2-(2-hydroxyphenyl)oxazoline (174 mg, 0.84 mmol, 2 eq) and K_2CO_3 (122 mg, 0.88 mmol, 2 eq) were dissolved in acetonitrile and refluxed for 3 h with continuous stirring. The reaction mixture was cooled to room temperature and then concentrated *in vacuo* under reduced pressure to obtain a single enantiomer of the expected compound. The crude product was purified using column chromatography with silica gel to obtain an orange crystalline compound. Yield, 165 mg (46%, 0.4 mmol). ^{1}H NMR (DMSO-d_6) δ 7.24 (*d*, *J* = 7.5 Hz, 1H), 7.05 (*t*, *J* = 7.0 and 7.5 Hz, 1H), 6.62 (*d*, *J* = 8.5 Hz, 1H), 6.28 (*t*, *J* = 7.5 Hz, 1H), 5.71 (*s*, 6H), 4.84 (*d*, *J* = 9.0 Hz, 1H), 4.59 (*dd*, *J* = 3.0 and 8.0 Hz, 1H), 4.41 (*t*, *J* = 9.0 Hz, 1H), 2.56 (*m*, *J* = 6.0 and 7.5 Hz, 1H), 1.0 (*d*, *J* = 7.0 Hz, 3H), 0.68 (*d*, *J* = 6.5 Hz, 3H); ^{13}C NMR (DMSO-d_6) δ 164.50, 133.10, 128.57, 128.26, 122.00, 112.40, 108.80, 83.33, 74.71, 67.07, 29.23, 19.12, 14.82; FTIR (neat, cm^{-1}) 3067, 1540, 1522, 1489, 1446, 1349, 1255, 1183, 1140, 1069, 826, 763; Elemental analysis calculated for $C_{18}H_{20}ClNO_2Ru$: C, 51.61; H, 4.81; N, 3.34. Found: C, 50.73; H, 4.95; N, 3.64.

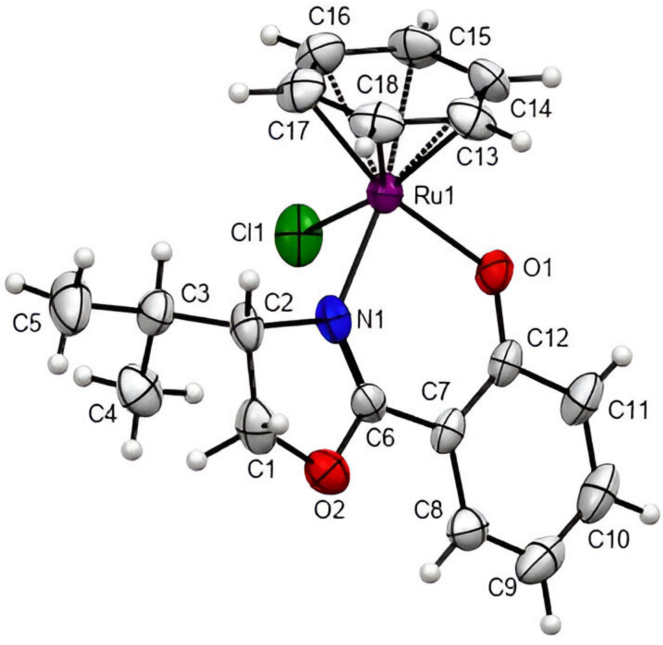


Figure 1
ORTEP drawing of the title compound with 50% probability displacement ellipsoids.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ru(C_{12}H_{14}NO_2)Cl(C_6H_6)]$
M_r	418.87
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, *b*, *c* (Å)	6.5669 (18), 9.414 (3), 27.570 (9)
V (Å^3)	1704.5 (9)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	1.09
Crystal size (mm)	0.47 × 0.18 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.662, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9005, 4074, 2937
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.089, 0.98
No. of reflections	4074
No. of parameters	210
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.41
Absolute structure	Flack *x* determined using 934 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.05 (6)

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

Refinement

Details of the crystal data collection, solution and refinement are provided in Table 3.

Acknowledgements

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References

Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Brunner, H., Nuber, B. & Prommesberger, M. (1998). *Tetrahedron Asymmetry*, **9**, 3223–3229.
Chan, H., Ghrayche, J. B., Wei, J. & Renfrew, A. K. (2017). *Eur. J. Inorg. Chem.* pp. 1679–1686.
Chavarot, M., Ménage, S., Hamelin, O., Charnay, F., Pécaut, J. & Fontecave, M. (2003). *Inorg. Chem.* **42**, 4810–4816.
Davenport, A. J., Davies, D. L., Fawcett, J. & Russell, D. R. (2004). *Dalton Trans.* pp. 1481–1492.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gong, L., Mulcahy, S. P., Devarajan, D., Harms, K., Frenking, G. & Meggers, E. (2010). *Inorg. Chem.* **49**, 7692–7699.
Gong, L., Mulcahy, S. P., Harms, K. & Meggers, E. (2009). *J. Am. Chem. Soc.* **131**, 9602–9603.
Gong, L., Wenzel, M. & Meggers, E. (2013). *Acc. Chem. Res.* **46**, 2635–2644.
Hamelin, O., Rimboud, M., Pécaut, J. & Fontecave, M. (2007). *Inorg. Chem.* **46**, 5354–5360.
Huisman, M., White, J. K., Lewalski, V. G., Podgorski, I., Turro, C. & Kodanko, J. J. (2016). *Chem. Commun.* **52**, 12590–12593.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Ryabov, A. D., Le Lagadec, R., Estevez, H., Toscano, R. A., Hernandez, S., Alexandrova, L., Kurova, V. S., Fischer, A., Sirlin, C. & Pfeffer, M. (2005). *Inorg. Chem.* **44**, 1626–1634.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2024). **9**, x240720 [https://doi.org/10.1107/S241431462400720X]

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Crystal data

$[Ru(C_{12}H_{14}NO_2)Cl(C_6H_6)]$
M_r = 418.87
Orthorhombic, $P2_12_12_1$
a = 6.5669 (18) Å
b = 9.414 (3) Å
c = 27.570 (9) Å
V = 1704.5 (9) Å^3
Z = 4
$F(000)$ = 848
D_x = 1.632 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1424 reflections
θ = 2.6–22.4°
μ = 1.09 mm^{-1}
T = 293 K
Plate, orange
0.47 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Detector resolution: φ and ω scans pixels mm^{-1}
Bruker APEXII CCD scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.662, T_{max} = 0.746
9005 measured reflections
4074 independent reflections
2937 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 28.3°, θ_{min} = 2.3°
h = −8→6
k = −12→12
l = −36→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.089
S = 0.98
4074 reflections
210 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack x determined using 934 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.05 (6)

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. The structure solution and refinement were implemented using WinGX software program (Farrugia, 2012). The highest peak and deepest hole are 0.66 and -0.41 e Å^{-3}, respectively, which are 1.13 and 0.83 Å away from the ruthenium center. The refinement of the hydrogen atoms was performed isotropically in their idealized geometry while sitting and riding on their anisotropically refined parent atoms with $U_{iso} = 1.2U_{eq}$ for the aromatic and methine protons, and $U_{iso} = 1.5U_{eq}$ for the methyl protons.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2589 (12)	1.2854 (9)	0.8188 (3)	0.047 (2)
H1A	0.379457	1.320678	0.835165	0.057*
H1B	0.267789	1.309492	0.784613	0.057*
C2	0.2375 (11)	1.1261 (8)	0.8256 (2)	0.0362 (17)
H2	0.364617	1.086811	0.838471	0.043*
C3	0.1761 (10)	1.0454 (9)	0.7791 (2)	0.0409 (19)
H3	0.137753	0.948622	0.788452	0.049*
C4	−0.0048 (18)	1.1122 (8)	0.7531 (2)	0.0508 (17)
H4A	0.030043	1.206761	0.743036	0.076*
H4B	−0.119213	1.115928	0.774774	0.076*
H4C	−0.039225	1.056171	0.725238	0.076*
C5	0.3629 (12)	1.0355 (12)	0.7454 (3)	0.070 (3)
H5A	0.333602	0.971968	0.719131	0.105*
H5B	0.477509	1.000471	0.763443	0.105*
H5C	0.393965	1.128034	0.732786	0.105*
C6	−0.0089 (13)	1.2403 (6)	0.86639 (19)	0.0312 (13)
C7	−0.1874 (9)	1.2786 (7)	0.8950 (2)	0.0316 (16)
C8	−0.2721 (11)	1.4153 (8)	0.8885 (2)	0.0394 (17)
H8	−0.212165	1.477639	0.866531	0.047*
C9	−0.4400 (11)	1.4573 (9)	0.9137 (3)	0.053 (2)
H9	−0.498466	1.545825	0.908180	0.064*
C10	−0.5219 (15)	1.3655 (9)	0.9478 (3)	0.056 (2)
H10	−0.632514	1.395362	0.966250	0.067*
C11	−0.4456 (10)	1.2333 (9)	0.9552 (3)	0.047 (2)
H11	−0.506447	1.174317	0.978042	0.057*
C12	−0.2755 (10)	1.1833 (8)	0.9288 (2)	0.0319 (16)
C13	0.2044 (11)	0.9128 (8)	0.9641 (2)	0.0424 (19)
H13	0.238607	0.979015	0.987744	0.051*
C14	0.0350 (12)	0.8234 (7)	0.9705 (2)	0.042 (2)
H14	−0.041486	0.830265	0.998837	0.050*
C15	−0.0200 (14)	0.7245 (7)	0.9352 (2)	0.0456 (18)
H15	−0.130235	0.664262	0.940233	0.055*
C16	0.0933 (11)	0.7167 (8)	0.8916 (3)	0.047 (2)
H16	0.052812	0.654450	0.867215	0.057*

C17	0.2667 (11)	0.8025 (8)	0.8847 (3)	0.0443 (19)
H17	0.343741	0.794385	0.856557	0.053*
C18	0.3229 (10)	0.9013 (8)	0.9212 (3)	0.043 (2)
H18	0.437009	0.958522	0.916953	0.052*
N1	0.0747 (7)	1.1175 (6)	0.86312 (18)	0.0311 (14)
O1	−0.2134 (7)	1.0558 (5)	0.93758 (15)	0.0381 (11)
O2	0.0756 (7)	1.3444 (5)	0.84022 (17)	0.0456 (14)
Cl1	−0.2594 (3)	0.8953 (2)	0.84198 (6)	0.0507 (5)
Ru1	0.00224 (9)	0.93480 (5)	0.90217 (2)	0.02858 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.044 (5)	0.057 (5)	0.040 (4)	−0.015 (4)	0.012 (4)	0.001 (4)
C2	0.027 (4)	0.054 (5)	0.027 (3)	0.001 (4)	0.008 (3)	0.000 (3)
C3	0.040 (4)	0.047 (5)	0.036 (4)	0.006 (4)	0.010 (3)	−0.003 (4)
C4	0.052 (4)	0.061 (5)	0.039 (3)	−0.005 (8)	−0.013 (4)	−0.001 (3)
C5	0.061 (6)	0.106 (9)	0.044 (5)	0.030 (6)	0.012 (4)	−0.004 (5)
C6	0.041 (4)	0.028 (3)	0.025 (3)	−0.010 (5)	−0.001 (4)	−0.001 (2)
C7	0.027 (4)	0.037 (4)	0.030 (4)	0.000 (3)	0.000 (3)	−0.012 (3)
C8	0.045 (4)	0.038 (4)	0.036 (4)	0.003 (4)	−0.008 (3)	−0.004 (3)
C9	0.054 (6)	0.048 (5)	0.058 (5)	0.017 (4)	−0.015 (4)	−0.021 (4)
C10	0.045 (5)	0.066 (5)	0.055 (4)	0.011 (6)	0.008 (5)	−0.026 (4)
C11	0.043 (6)	0.049 (5)	0.051 (4)	0.002 (4)	0.014 (3)	−0.017 (4)
C12	0.029 (4)	0.038 (4)	0.029 (3)	−0.001 (3)	0.003 (3)	−0.013 (3)
C13	0.040 (4)	0.047 (5)	0.040 (4)	−0.002 (4)	−0.014 (3)	0.008 (4)
C14	0.050 (6)	0.041 (4)	0.035 (3)	−0.003 (4)	0.007 (4)	0.012 (3)
C15	0.046 (5)	0.035 (4)	0.056 (4)	−0.010 (5)	0.008 (5)	0.013 (3)
C16	0.052 (5)	0.035 (4)	0.056 (5)	0.001 (4)	0.001 (4)	−0.003 (4)
C17	0.029 (4)	0.045 (5)	0.059 (5)	0.008 (4)	0.009 (4)	0.001 (4)
C18	0.027 (4)	0.044 (5)	0.059 (5)	0.001 (3)	−0.004 (3)	0.010 (4)
N1	0.019 (3)	0.047 (4)	0.028 (3)	−0.008 (3)	0.005 (2)	0.001 (3)
O1	0.039 (3)	0.037 (3)	0.039 (2)	0.001 (3)	0.017 (2)	−0.002 (2)
O2	0.049 (3)	0.043 (3)	0.046 (3)	−0.007 (2)	0.012 (2)	0.008 (2)
Cl1	0.0276 (10)	0.0772 (16)	0.0475 (10)	−0.0096 (10)	−0.0033 (8)	−0.0106 (10)
Ru1	0.0237 (2)	0.0325 (2)	0.0295 (2)	−0.0020 (4)	0.0034 (3)	−0.0008 (2)

Geometric parameters (Å, º)

C1—O2	1.452 (8)	C9—C10	1.386 (11)
C1—C2	1.519 (10)	C9—H9	0.9300
C1—H1A	0.9700	C10—C11	1.357 (11)
C1—H1B	0.9700	C10—H10	0.9300
C2—N1	1.490 (7)	C11—C12	1.414 (9)
C2—C3	1.542 (9)	C11—H11	0.9300
C2—H2	0.9800	C12—O1	1.291 (8)
C3—C4	1.523 (12)	C13—C14	1.406 (9)
C3—C5	1.541 (9)	C13—C18	1.420 (9)

C3—H3	0.9800	C13—H13	0.9300
C4—H4A	0.9600	C14—C15	1.396 (9)
C4—H4B	0.9600	C14—H14	0.9300
C4—H4C	0.9600	C15—C16	1.416 (10)
C5—H5A	0.9600	C15—H15	0.9300
C5—H5B	0.9600	C16—C17	1.409 (10)
C5—H5C	0.9600	C16—H16	0.9300
C6—N1	1.282 (8)	C17—C18	1.418 (10)
C6—O2	1.338 (7)	C17—H17	0.9300
C6—C7	1.458 (10)	C18—H18	0.9300
C7—C8	1.413 (9)	N1—Ru1	2.084 (6)
C7—C12	1.418 (9)	O1—Ru1	2.063 (5)
C8—C9	1.363 (9)	Cl1—Ru1	2.4176 (19)
C8—H8	0.9300		

O2—C1—C2	104.5 (6)	C8—C9—C10	118.6 (8)
O2—C1—H1A	110.9	C8—C9—H9	120.7
C2—C1—H1A	110.9	C10—C9—H9	120.7
O2—C1—H1B	110.9	C11—C10—C9	122.0 (8)
C2—C1—H1B	110.9	C11—C10—H10	119.0
H1A—C1—H1B	108.9	C9—C10—H10	119.0
N1—C2—C1	101.9 (6)	C10—C11—C12	121.4 (8)
N1—C2—C3	111.3 (5)	C10—C11—H11	119.3
C1—C2—C3	114.1 (6)	C12—C11—H11	119.3
N1—C2—H2	109.8	O1—C12—C11	117.5 (7)
C1—C2—H2	109.8	O1—C12—C7	125.7 (6)
C3—C2—H2	109.8	C11—C12—C7	116.7 (7)
C4—C3—C5	111.3 (6)	C14—C13—C18	119.6 (7)
C4—C3—C2	113.0 (6)	C14—C13—H13	120.2
C5—C3—C2	108.8 (6)	C18—C13—H13	120.2
C4—C3—H3	107.9	C15—C14—C13	121.0 (7)
C5—C3—H3	107.9	C15—C14—H14	119.5
C2—C3—H3	107.9	C13—C14—H14	119.5
C3—C4—H4A	109.5	C14—C15—C16	119.5 (7)
C3—C4—H4B	109.5	C14—C15—H15	120.3
H4A—C4—H4B	109.5	C16—C15—H15	120.3
C3—C4—H4C	109.5	C17—C16—C15	120.6 (7)
H4A—C4—H4C	109.5	C17—C16—H16	119.7
H4B—C4—H4C	109.5	C15—C16—H16	119.7
C3—C5—H5A	109.5	C16—C17—C18	119.5 (7)
C3—C5—H5B	109.5	C16—C17—H17	120.3
H5A—C5—H5B	109.5	C18—C17—H17	120.3
C3—C5—H5C	109.5	C17—C18—C13	119.8 (7)
H5A—C5—H5C	109.5	C17—C18—H18	120.1
H5B—C5—H5C	109.5	C13—C18—H18	120.1
N1—C6—O2	116.4 (7)	C6—N1—C2	107.9 (6)
N1—C6—C7	127.3 (6)	C6—N1—Ru1	127.6 (4)
O2—C6—C7	116.3 (6)	C2—N1—Ru1	124.5 (5)

C8—C7—C12	120.0 (6)	C12—O1—Ru1	129.9 (4)
C8—C7—C6	118.3 (6)	C6—O2—C1	106.5 (6)
C12—C7—C6	121.8 (6)	O1—Ru1—N1	86.9 (2)
C9—C8—C7	121.2 (7)	O1—Ru1—Cl1	85.52 (14)
C9—C8—H8	119.4	N1—Ru1—Cl1	86.26 (15)
C7—C8—H8	119.4		

O2—C1—C2—N1	−16.4 (7)	C6—C7—C12—C11	178.7 (6)
O2—C1—C2—C3	103.6 (6)	C18—C13—C14—C15	−0.7 (11)
N1—C2—C3—C4	65.7 (8)	C13—C14—C15—C16	−1.7 (11)
C1—C2—C3—C4	−48.8 (9)	C14—C15—C16—C17	3.3 (11)
N1—C2—C3—C5	−170.2 (6)	C15—C16—C17—C18	−2.5 (11)
C1—C2—C3—C5	75.2 (8)	C16—C17—C18—C13	0.1 (11)
N1—C6—C7—C8	−171.5 (7)	C14—C13—C18—C17	1.5 (11)
O2—C6—C7—C8	7.7 (9)	O2—C6—N1—C2	−5.5 (8)
N1—C6—C7—C12	8.9 (11)	C7—C6—N1—C2	173.7 (6)
O2—C6—C7—C12	−172.0 (6)	O2—C6—N1—Ru1	174.7 (4)
C12—C7—C8—C9	−0.9 (10)	C7—C6—N1—Ru1	−6.2 (10)
C6—C7—C8—C9	179.4 (6)	C1—C2—N1—C6	13.7 (7)
C7—C8—C9—C10	2.9 (11)	C3—C2—N1—C6	−108.3 (7)
C8—C9—C10—C11	−3.0 (13)	C1—C2—N1—Ru1	−166.5 (4)
C9—C10—C11—C12	1.1 (13)	C3—C2—N1—Ru1	71.5 (7)
C10—C11—C12—O1	−179.3 (7)	C11—C12—O1—Ru1	171.7 (4)
C10—C11—C12—C7	0.9 (10)	C7—C12—O1—Ru1	−8.6 (10)
C8—C7—C12—O1	179.3 (6)	N1—C6—O2—C1	−5.9 (8)
C6—C7—C12—O1	−1.1 (10)	C7—C6—O2—C1	174.8 (6)
C8—C7—C12—C11	−1.0 (9)	C2—C1—O2—C6	14.2 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.93	2.38	2.725 (9)	102
C17—H17···Cl1^{i}	0.93	2.80	3.440 (8)	127
C18—H18···O1^{i}	0.93	2.54	3.405 (8)	156

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