Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-benzyliminomethyl-5-methylphenyl-κ^2C^1,N)dicarbonylruthenium(II)

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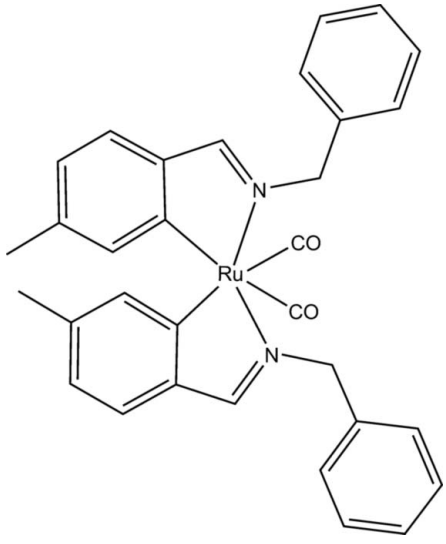
Received 11 April 2007; accepted 14 April 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.084; data-to-parameter ratio = 18.7.

The title compound, $[Ru(C_{15}H_{14}N)_2(CO)_2]$, has been prepared by the reaction of $Ru_3(CO)_{12}$ with *N*-(4-methylbenzylidene)-1-phenylmethanamine in toluene under a nitrogen atmosphere. In the complex, the Ru atom is coordinated by two N atoms, two C atoms of two benzene rings, and two carbonyl ligands, forming an octahedral arrangement with Ru—C distances of 1.850 (3), 1.921 (3), 2.066 (2) and 2.110 (2) Å and Ru—N distances of 2.1583 (18) and 2.1763 (19) Å.

Related literature

For related literature, see: Cabeza *et al.* (2001); Crabtree (1985); Kakiuchi *et al.* (2001); Kleiman & Dubeck (1963); Murai *et al.* (1993).



Experimental

Crystal data

$[Ru(C_{15}H_{14}N)_2(CO)_2]$
M_r = 573.63
Monoclinic, $P2_1/c$
a = 9.685 (3) Å
b = 16.813 (4) Å
c = 17.126 (4) Å
β = 99.156 (5)°
V = 2753.3 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 293 (2) K
0.33 × 0.20 × 0.16 mm

Data collection

Rigaku Saturn70 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2004)
T_{min} = 0.827, T_{max} = 0.910
21246 measured reflections
6290 independent reflections
5347 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.084
S = 1.09
6290 reflections
336 parameters
66 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of China (grant Nos. 20325106 and 20333070) and the 'One Hundred Talent' Projects from the Chinese Academy of Sciences.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG3035).

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 doi:10.1107/S1600536807018673

supplementary materials

Acta Cryst. (2007). E**63**, m1421 [**doi:10.1107/S1600536807018673**]

Bis(2-benzyliminomethyl-5-methylphenyl-κ^2C^1,N)dicarbonylruthenium(II)

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Comment

Transition metal catalyzed organic transformations involving C—H bond activation have been sought after for decades (Kleiman & Dubeck 1963; Crabtree, 1985; Murai *et al.*, 1993). In this context, Ru and Pd complexes are most often used as catalysts, and substrates for these reactions usually contain directing groups. The proposed mechanism for these reactions involves cleavage of a C—H bond *ortho* to a directing group and formation of a cyclometalated intermediate (Kakiuchi *et al.*, 2001). However, very few examples have been reported of these intermediates. Herein, we wish to report the structure of a Ru(II) complex derived from the cleavage of a C—H bond in *p*-methylbenzylidenebenzylamine with $Ru_3(CO)_{12}$, $Ru(\eta^2\text{-}(C,N)\text{-}p\text{-}MeC_6H_3CH{=}NCH_2Ph)_2(CO)_2$ (I).

As shown in Fig. 1 the Ru coordination polyhedron adopts in (I) a distorted octahedral geometry by coordination of two N atoms and two C atoms from two Schiff base molecules, and two *cis*-disposed carbonyl ligands. The N atoms from the Schiff bases are respectively *trans* to a carbonyl ligand and an aryl C atom. The Ru—N bond distances are 2.1556 (19)Å and 2.176 (2) Å, respectively, somewhat longer than those of other similar Ru(II) complexes (Cabeza *et al.*, 2001), while Ru—C distances involving carbonyl ligands are normal. The remaining Ru—C bond distances are 2.067 (2)Å and 2.111 (2) Å. Bond angles involving the ruthenium center fall in the range 78.12 (9) (C4—Ru(1)—N(1)) to 167.99 (11)° (C31—Ru(1)—N(2)). The configurations of the two Schiff base molecules are significantly different, with dihedral angles between aromatic ring planes being 73.3 (1)° (for C1 → C6 and C10 → C15) and 86.4 (1)° (C17 → C22 and C25 → C30), respectively.

Experimental

The title compound was obtained by refluxing a mixture of $Ru_3(CO)_{12}$ (0.02 mmol) with imine (0.5 mmol) in toluene (2 ml) under a nitrogen atmosphere for 48 h. The product was isolated and purified by silica gel column chromatography. Green block-shaped crystals suitable for X-ray diffraction were grown from hexane.

Refinement

H atoms were placed in calculated positions and made to ride on their parent atoms, with C—H = 0.95Å for aromatic, 0.99Å for methylene and 0.98Å for methyl H atoms. The latter ones were allowed to rotate around the C—C bond. In all cases, $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

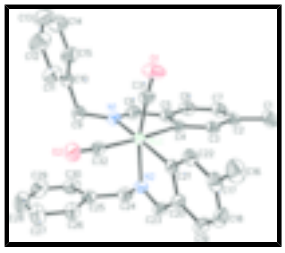


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

Bis(2-benzyliminomethyl-5-methylphenyl-κ^2*C*^{1},*N*)dicarbonylruthenium(II)

Crystal data

$[Ru(C_{15}H_{14}N_1)_2(C_1O_1)_2]$	F_{000} = 1176
M_r = 573.63	D_x = 1.384 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6859 reflections
a = 9.685 (3) Å	θ = 2.5–27.5º
b = 16.813 (4) Å	μ = 0.60 mm^{-1}
c = 17.126 (4) Å	T = 293 (2) K
β = 99.156 (5)º	Block, green
V = 2753.3 (12) Å^3	0.33 × 0.20 × 0.16 mm
Z = 4	

Data collection

Rigaku Saturn70 CCD diffractometer	6290 independent reflections
Radiation source: fine-focus sealed tube	5347 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
Detector resolution: 28.5714 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 2.5º
CCD_Profile_fitting scans	h = −12→12
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2004)	k = −21→21
T_{min} = 0.827, T_{max} = 0.910	l = −18→22
21246 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.084	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.4314P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
6290 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
336 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
66 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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	0.666953 (16)	0.543113 (10)	0.211497 (9)	0.03961 (7)
O1	0.6571 (2)	0.66359 (15)	0.33920 (13)	0.0899 (7)
O2	0.97164 (18)	0.50689 (15)	0.28032 (12)	0.0752 (6)
N1	0.5711 (2)	0.44267 (12)	0.26255 (11)	0.0491 (5)
N2	0.65760 (18)	0.47949 (12)	0.10133 (10)	0.0443 (4)
C1	0.1693 (3)	0.70533 (19)	0.07321 (18)	0.0735 (8)
H1A	0.0858	0.6897	0.0363	0.088*
H1B	0.2349	0.7325	0.0442	0.088*
H1C	0.1424	0.7413	0.1132	0.088*
C2	0.2378 (2)	0.63257 (16)	0.11296 (14)	0.0539 (6)
C3	0.3838 (2)	0.62912 (15)	0.13376 (13)	0.0467 (5)
H3A	0.4382	0.6721	0.1194	0.056*
C4	0.4520 (2)	0.56516 (14)	0.17458 (13)	0.0441 (5)
C5	0.3664 (2)	0.50282 (16)	0.19466 (14)	0.0502 (5)
C6	0.2212 (3)	0.50428 (19)	0.17314 (16)	0.0627 (7)
H6A	0.1661	0.4611	0.1863	0.075*
C7	0.1583 (3)	0.56926 (19)	0.13246 (17)	0.0640 (7)
H7A	0.0596	0.5705	0.1177	0.077*
C8	0.4383 (3)	0.43938 (16)	0.24164 (15)	0.0556 (6)
H8A	0.3871	0.3954	0.2569	0.067*
C9	0.6414 (3)	0.37917 (15)	0.31463 (14)	0.0581 (6)
H9A	0.7336	0.3676	0.2992	0.070*
H9B	0.5846	0.3300	0.3070	0.070*
C10	0.6618 (3)	0.40231 (15)	0.40034 (14)	0.0568 (6)
C11	0.7827 (4)	0.4365 (2)	0.43649 (19)	0.0815 (9)

H11A	0.8547	0.4477	0.4063	0.098*
C12	0.8031 (6)	0.4554 (2)	0.5160 (2)	0.1053 (13)
H12A	0.8890	0.4783	0.5401	0.126*
C13	0.7030 (7)	0.4417 (2)	0.5583 (2)	0.1127 (15)
H13A	0.7167	0.4566	0.6125	0.135*
C14	0.5816 (6)	0.4068 (3)	0.5261 (3)	0.1253 (17)
H14A	0.5114	0.3966	0.5578	0.150*
C15	0.5590 (4)	0.3853 (3)	0.4445 (2)	0.0976 (12)
H15A	0.4748	0.3599	0.4213	0.117*
C16	0.8430 (4)	0.84485 (18)	0.1159 (2)	0.0879 (10)
H16A	0.8169	0.8794	0.0698	0.106*
H16B	0.9448	0.8455	0.1316	0.106*
H16C	0.7983	0.8641	0.1597	0.106*
C17	0.7953 (3)	0.76125 (16)	0.09517 (18)	0.0620 (7)
C18	0.7899 (3)	0.73321 (19)	0.01830 (18)	0.0692 (8)
H18A	0.8117	0.7679	−0.0218	0.083*
C19	0.7533 (3)	0.65603 (19)	0.00026 (15)	0.0632 (7)
H19A	0.7491	0.6372	−0.0524	0.076*
C20	0.7220 (2)	0.60473 (15)	0.05940 (13)	0.0484 (5)
C21	0.7236 (2)	0.63084 (14)	0.13826 (13)	0.0428 (5)
C22	0.7614 (2)	0.70990 (15)	0.15326 (15)	0.0512 (5)
H22A	0.7643	0.7298	0.2054	0.061*
C23	0.6840 (2)	0.52299 (15)	0.04390 (13)	0.0505 (5)
H23A	0.6785	0.5016	−0.0078	0.061*
C24	0.6183 (3)	0.39617 (15)	0.08596 (14)	0.0542 (6)
H24A	0.6056	0.3865	0.0282	0.065*
H24B	0.5276	0.3862	0.1038	0.065*
C25	0.7248 (3)	0.33834 (15)	0.12673 (14)	0.0533 (6)
C26	0.8671 (3)	0.35274 (18)	0.13351 (17)	0.0670 (7)
H26A	0.8993	0.4011	0.1142	0.080*
C27	0.9623 (4)	0.2969 (2)	0.1684 (2)	0.0945 (11)
H27A	1.0598	0.3064	0.1718	0.113*
C28	0.9154 (5)	0.2271 (2)	0.1983 (2)	0.1035 (13)
H28A	0.9808	0.1893	0.2235	0.124*
C29	0.7769 (5)	0.2127 (2)	0.19186 (19)	0.0909 (11)
H29A	0.7451	0.1645	0.2120	0.109*
C30	0.6814 (4)	0.26767 (17)	0.15608 (17)	0.0722 (8)
H30A	0.5842	0.2567	0.1516	0.087*
C31	0.6608 (3)	0.61511 (17)	0.29255 (14)	0.0560 (6)
C32	0.8588 (2)	0.51820 (15)	0.25146 (13)	0.0490 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.03367 (10)	0.04795 (12)	0.03712 (11)	−0.00101 (7)	0.00534 (7)	−0.00166 (7)
O1	0.0984 (16)	0.1024 (18)	0.0723 (13)	−0.0069 (13)	0.0236 (12)	−0.0440 (13)
O2	0.0395 (10)	0.1078 (17)	0.0765 (13)	0.0074 (10)	0.0033 (9)	0.0094 (12)
N1	0.0520 (12)	0.0533 (12)	0.0433 (10)	−0.0021 (9)	0.0112 (9)	0.0027 (8)

N2	0.0373 (9)	0.0542 (11)	0.0407 (10)	−0.0021 (8)	0.0044 (7)	−0.0060 (8)
C1	0.0550 (16)	0.077 (2)	0.083 (2)	0.0204 (14)	−0.0055 (14)	−0.0101 (15)
C2	0.0405 (12)	0.0696 (16)	0.0508 (13)	0.0089 (11)	0.0047 (10)	−0.0131 (11)
C3	0.0383 (11)	0.0556 (14)	0.0460 (12)	0.0013 (10)	0.0063 (9)	−0.0079 (10)
C4	0.0344 (10)	0.0577 (13)	0.0411 (11)	−0.0015 (9)	0.0088 (9)	−0.0057 (9)
C5	0.0401 (12)	0.0606 (15)	0.0518 (13)	−0.0072 (11)	0.0129 (10)	−0.0032 (11)
C6	0.0418 (13)	0.0788 (19)	0.0696 (17)	−0.0115 (13)	0.0157 (12)	−0.0039 (14)
C7	0.0327 (11)	0.086 (2)	0.0727 (17)	−0.0002 (12)	0.0074 (11)	−0.0159 (15)
C8	0.0537 (14)	0.0619 (16)	0.0539 (14)	−0.0130 (12)	0.0171 (11)	0.0017 (11)
C9	0.0686 (16)	0.0514 (15)	0.0550 (14)	0.0034 (12)	0.0125 (12)	0.0064 (11)
C10	0.0706 (16)	0.0516 (14)	0.0500 (14)	0.0111 (12)	0.0148 (12)	0.0112 (10)
C11	0.098 (2)	0.082 (2)	0.0645 (19)	−0.0137 (19)	0.0116 (17)	0.0010 (15)
C12	0.149 (4)	0.088 (3)	0.074 (2)	−0.018 (2)	0.002 (2)	−0.0047 (17)
C13	0.188 (5)	0.085 (3)	0.065 (2)	0.025 (3)	0.021 (3)	0.0027 (18)
C14	0.149 (4)	0.157 (4)	0.086 (3)	0.048 (3)	0.066 (3)	0.041 (3)
C15	0.084 (2)	0.140 (3)	0.074 (2)	0.017 (2)	0.0270 (17)	0.031 (2)
C16	0.083 (2)	0.0567 (19)	0.127 (3)	−0.0069 (16)	0.025 (2)	0.0144 (17)
C17	0.0410 (13)	0.0550 (15)	0.089 (2)	0.0005 (11)	0.0065 (12)	0.0140 (13)
C18	0.0529 (15)	0.079 (2)	0.0744 (19)	−0.0042 (14)	0.0070 (13)	0.0331 (15)
C19	0.0528 (14)	0.086 (2)	0.0499 (14)	−0.0070 (14)	0.0045 (11)	0.0145 (13)
C20	0.0350 (11)	0.0648 (15)	0.0446 (12)	−0.0007 (10)	0.0046 (9)	0.0055 (10)
C21	0.0281 (9)	0.0520 (13)	0.0477 (12)	0.0016 (9)	0.0036 (8)	0.0043 (9)
C22	0.0397 (11)	0.0519 (14)	0.0619 (14)	0.0008 (10)	0.0074 (10)	0.0018 (11)
C23	0.0430 (12)	0.0691 (16)	0.0391 (12)	−0.0019 (11)	0.0058 (9)	−0.0036 (10)
C24	0.0514 (13)	0.0592 (15)	0.0512 (13)	−0.0098 (11)	0.0055 (10)	−0.0122 (11)
C25	0.0662 (15)	0.0485 (13)	0.0455 (13)	−0.0071 (11)	0.0095 (11)	−0.0112 (10)
C26	0.0646 (16)	0.0587 (17)	0.0748 (18)	−0.0008 (13)	0.0023 (13)	−0.0020 (13)
C27	0.084 (2)	0.076 (2)	0.114 (3)	0.0108 (18)	−0.0137 (19)	−0.0072 (19)
C28	0.141 (4)	0.061 (2)	0.096 (3)	0.021 (2)	−0.022 (2)	−0.0041 (17)
C29	0.143 (3)	0.0514 (18)	0.073 (2)	−0.011 (2)	0.001 (2)	−0.0029 (14)
C30	0.095 (2)	0.0563 (17)	0.0665 (17)	−0.0171 (15)	0.0172 (15)	−0.0121 (13)
C31	0.0477 (13)	0.0719 (17)	0.0490 (14)	−0.0028 (12)	0.0093 (10)	−0.0050 (12)
C32	0.0418 (12)	0.0614 (15)	0.0446 (12)	−0.0001 (10)	0.0089 (10)	0.0025 (10)

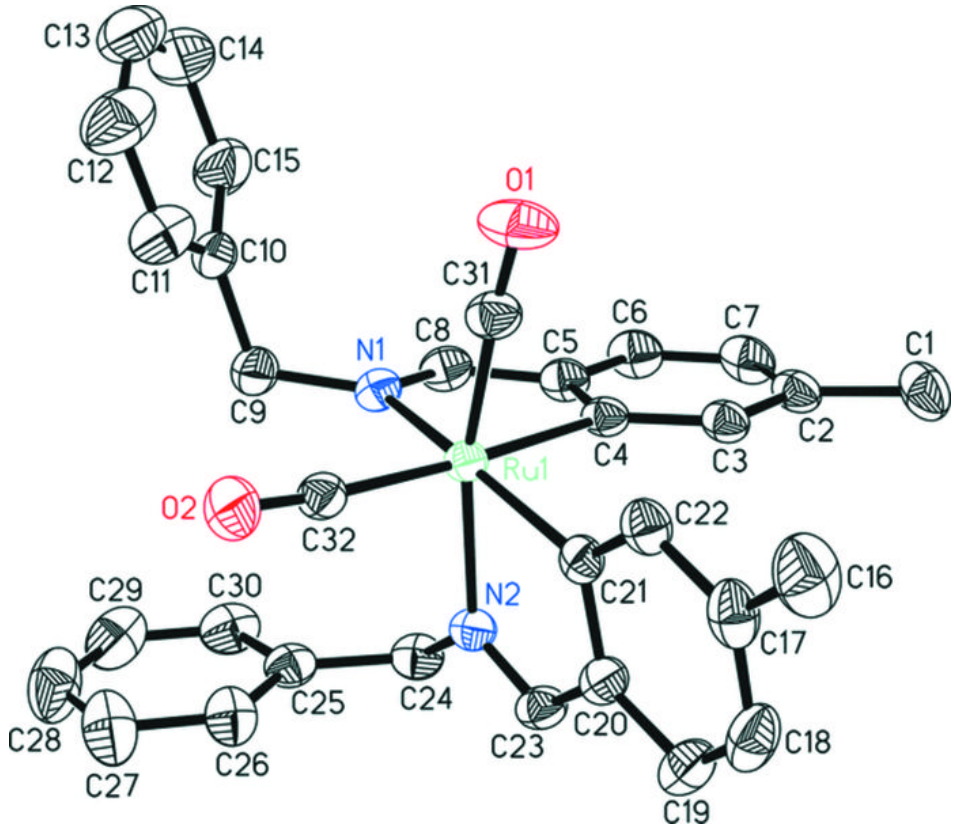
Geometric parameters (Å, °)

Ru1—C31	1.850 (3)	C12—H12A	0.9500
Ru1—C32	1.921 (2)	C13—C14	1.351 (7)
Ru1—C21	2.066 (2)	C13—H13A	0.9500
Ru1—C4	2.110 (2)	C14—C15	1.427 (6)
Ru1—N2	2.1583 (18)	C14—H14A	0.9500
Ru1—N1	2.1763 (19)	C15—H15A	0.9500
O1—C31	1.146 (3)	C16—C17	1.504 (4)
O2—C32	1.142 (3)	C16—H16A	0.9800
N1—C8	1.280 (3)	C16—H16B	0.9800
N1—C9	1.485 (3)	C16—H16C	0.9800
N2—C23	1.284 (3)	C17—C18	1.392 (4)
N2—C24	1.464 (3)	C17—C22	1.395 (4)
C1—C2	1.502 (4)	C18—C19	1.368 (4)

C1—H1A	0.9800	C18—H18A	0.9500
C1—H1B	0.9800	C19—C20	1.400 (3)
C1—H1C	0.9800	C19—H19A	0.9500
C2—C7	1.385 (4)	C20—C21	1.418 (3)
C2—C3	1.403 (3)	C20—C23	1.437 (3)
C3—C4	1.391 (3)	C21—C22	1.392 (3)
C3—H3A	0.9500	C22—H22A	0.9500
C4—C5	1.412 (3)	C23—H23A	0.9500
C5—C6	1.396 (3)	C24—C25	1.506 (4)
C5—C8	1.446 (4)	C24—H24A	0.9900
C6—C7	1.384 (4)	C24—H24B	0.9900
C6—H6A	0.9500	C25—C30	1.382 (4)
C7—H7A	0.9500	C25—C26	1.385 (4)
C8—H8A	0.9500	C26—C27	1.384 (4)
C9—C10	1.501 (4)	C26—H26A	0.9500
C9—H9A	0.9900	C27—C28	1.386 (5)
C9—H9B	0.9900	C27—H27A	0.9500
C10—C11	1.362 (4)	C28—C29	1.350 (5)
C10—C15	1.373 (4)	C28—H28A	0.9500
C11—C12	1.381 (5)	C29—C30	1.381 (5)
C11—H11A	0.9500	C29—H29A	0.9500
C12—C13	1.319 (6)	C30—H30A	0.9500
C31—Ru1—C32	91.14 (11)	C12—C13—C14	121.3 (4)
C31—Ru1—C21	91.82 (11)	C12—C13—H13A	119.3
C32—Ru1—C21	92.11 (9)	C14—C13—H13A	119.3
C31—Ru1—C4	87.82 (10)	C13—C14—C15	119.8 (4)
C32—Ru1—C4	175.66 (9)	C13—C14—H14A	120.1
C21—Ru1—C4	92.13 (8)	C15—C14—H14A	120.1
C31—Ru1—N2	168.09 (10)	C10—C15—C14	118.4 (4)
C32—Ru1—N2	96.14 (8)	C10—C15—H15A	120.8
C21—Ru1—N2	78.54 (8)	C14—C15—H15A	120.8
C4—Ru1—N2	85.58 (8)	C17—C16—H16A	109.5
C31—Ru1—N1	98.03 (10)	C17—C16—H16B	109.5
C32—Ru1—N1	97.92 (9)	H16A—C16—H16B	109.5
C21—Ru1—N1	165.76 (8)	C17—C16—H16C	109.5
C4—Ru1—N1	78.06 (8)	H16A—C16—H16C	109.5
N2—Ru1—N1	90.31 (7)	H16B—C16—H16C	109.5
C8—N1—C9	118.8 (2)	C18—C17—C22	119.2 (3)
C8—N1—Ru1	113.26 (16)	C18—C17—C16	120.2 (3)
C9—N1—Ru1	127.94 (16)	C22—C17—C16	120.6 (3)
C23—N2—C24	119.02 (19)	C19—C18—C17	120.3 (2)
C23—N2—Ru1	113.68 (16)	C19—C18—H18A	119.8
C24—N2—Ru1	127.22 (14)	C17—C18—H18A	119.8
C2—C1—H1A	109.5	C18—C19—C20	120.0 (3)
C2—C1—H1B	109.5	C18—C19—H19A	120.0
H1A—C1—H1B	109.5	C20—C19—H19A	120.0
C2—C1—H1C	109.5	C19—C20—C21	121.9 (2)
H1A—C1—H1C	109.5	C19—C20—C23	122.3 (2)
H1B—C1—H1C	109.5	C21—C20—C23	115.8 (2)

C7—C2—C3	118.9 (2)	C22—C21—C20	115.7 (2)
C7—C2—C1	120.8 (2)	C22—C21—Ru1	131.09 (17)
C3—C2—C1	120.2 (2)	C20—C21—Ru1	113.18 (17)
C4—C3—C2	122.6 (2)	C21—C22—C17	123.0 (2)
C4—C3—H3A	118.7	C21—C22—H22A	118.5
C2—C3—H3A	118.7	C17—C22—H22A	118.5
C3—C4—C5	116.5 (2)	N2—C23—C20	118.7 (2)
C3—C4—Ru1	130.81 (17)	N2—C23—H23A	120.7
C5—C4—Ru1	112.71 (17)	C20—C23—H23A	120.7
C6—C5—C4	121.9 (2)	N2—C24—C25	113.28 (19)
C6—C5—C8	122.4 (2)	N2—C24—H24A	108.9
C4—C5—C8	115.7 (2)	C25—C24—H24A	108.9
C7—C6—C5	119.4 (3)	N2—C24—H24B	108.9
C7—C6—H6A	120.3	C25—C24—H24B	108.9
C5—C6—H6A	120.3	H24A—C24—H24B	107.7
C6—C7—C2	120.7 (2)	C30—C25—C26	118.4 (3)
C6—C7—H7A	119.6	C30—C25—C24	119.9 (3)
C2—C7—H7A	119.6	C26—C25—C24	121.7 (2)
N1—C8—C5	119.8 (2)	C27—C26—C25	120.2 (3)
N1—C8—H8A	120.1	C27—C26—H26A	119.9
C5—C8—H8A	120.1	C25—C26—H26A	119.9
N1—C9—C10	112.2 (2)	C26—C27—C28	120.0 (4)
N1—C9—H9A	109.2	C26—C27—H27A	120.0
C10—C9—H9A	109.2	C28—C27—H27A	120.0
N1—C9—H9B	109.2	C29—C28—C27	120.1 (3)
C10—C9—H9B	109.2	C29—C28—H28A	120.0
H9A—C9—H9B	107.9	C27—C28—H28A	120.0
C11—C10—C15	118.9 (3)	C28—C29—C30	120.2 (3)
C11—C10—C9	121.6 (3)	C28—C29—H29A	119.9
C15—C10—C9	119.4 (3)	C30—C29—H29A	119.9
C10—C11—C12	121.5 (4)	C29—C30—C25	121.1 (3)
C10—C11—H11A	119.2	C29—C30—H30A	119.5
C12—C11—H11A	119.2	C25—C30—H30A	119.5
C13—C12—C11	119.9 (4)	O1—C31—Ru1	175.5 (3)
C13—C12—H12A	120.0	O2—C32—Ru1	174.6 (2)
C11—C12—H12A	120.0		

Fig. 1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