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trans-(2,2′-Bipyridine)dichlorido-[1-(4-methylphenylimino)-1-(phenylhydrazono)propan-2-one]ruthenium(II) dichloromethane solvate

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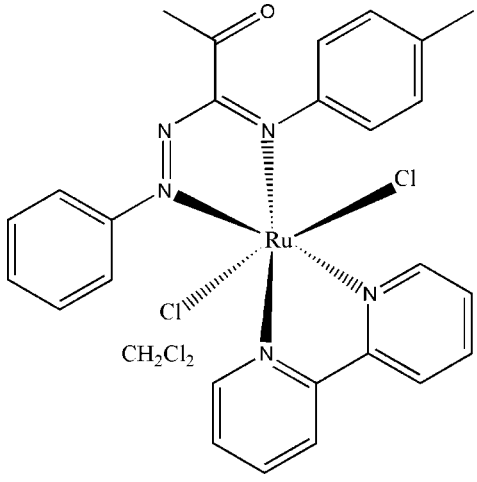
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.060; wR factor = 0.142; data-to-parameter ratio = 17.6.

The title compound, $[RuCl_2(C_{10}H_8N_2)(C_{16}H_{15}N_3O)]\cdot CH_2Cl_2$, has a pseudo-octahedral coordination environment made up of two *trans* chloride ligands and four N-donor atoms, two of which are from the strong π-acceptor azoimine bidentate ligand. The two Cl atoms of the solvent molecule are disordered over two positions in an approximately 0.7:0.3 ratio.

Related literature

For related literature, see: Al-Noaimi *et al.* (2007); Kaim (2001).



Experimental

Crystal data

$[RuCl_2(C_{10}H_8N_2)(C_{16}H_{15}N_3O)]\cdot CH_2Cl_2$
M_r = 678.39
Triclinic, $P\overline{1}$
a = 8.9994 (4) Å
b = 11.3852 (9) Å
c = 15.0563 (12) Å
α = 106.387 (3)°
β = 104.123 (4)°
γ = 99.231 (5)°
V = 1391.01 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 183 (2) K
0.04 × 0.04 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
9663 measured reflections
6311 independent reflections
3840 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.142
S = 1.00
6311 reflections
359 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2238).

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supplementary materials

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trans-(2,2'-Bipyridine)dichlorido[1-(4-methylphenylimino)-1-(phenylhydrazono)propan-2-one]ruthenium(II) dichloromethane solvate

M. Al-Noaimi, M. El-khateeb and H. Görls

Comment

The chemistry of ruthenium (II) complexes containing azoimine (N=N—C=N) functional unit has been reported elsewhere (Kaim, 2001). This function is pi-acidic in character and has a strong ability to stabilize low valent metal redox states, such as Ru(II), Os(II),*etc*. The chemistry of azoimine functionalized ligand complexes encourages us to develop a new ligand containing an azoimine unit. The new unsymmetrical bidentate ligand, 1-(4-methylphenylimino)-1-(phenylhydrazono)propan-2-one (*L*), lacks a twofold symmetry axis and on complexation with ruthenium (II), affords pseudo-octahedral, *trans*-[Ru(bpy)LCl_2] complex **1**. This compound is published in literature (Al-Noaimi *et al.*, 2007) but no structural data have been published.

The compound, **1**, posseses a pseudo octahedral coordination sphere made up of two *trans* chloride ligands and four nitrogen donor atoms. Two of them are coresponding to the strong pi-acceptor azoimine bidentate ligand (Fig. 1). The five membered rings formed by the coordination of azoimine and bpy have almost equivalent coordination bite-angles N1—Ru—N2 = 76.56 (16)° and N4—Ru—N5 = 77.06 (16)°, respectively). However, it is interesting to note that the bond lengths of Ru(II) and azoimine N atoms, d(Ru—N1) = 1.997 (4) Å and d(Ru—N2) = 1.968 (4) Å are significantly shorter than those of Ru(II) and the bpy N atoms, d(Ru—N4) = 2.139 (4) Å and d(Ru—N5) = 2.110 (4) Å indicated preferential pi bonding of Ru(II) with the azo group.

Experimental

trans-2,2'-bipyridinedichloro1-(4-methylphenylimino)-1-(phenylhydrazono)- propan-2-one ruthenium(II) was prepared according to literature procedure (Al-Noaimi *et al.*,2007) and recrystallized by slowly evaporating solution of dichloromethane.

Refinement

Both chlorine atoms of the methylene chloride solvent molecule show a 72:28 occupancy disorder over two positions. All hydrogen atoms were set to idealized positions and were refined with 1.2 times (1.5 for methyl groups) the isotropic displacement parameter of the corresponding carbon atom. The methyl groups were allowed to rotate but not to tip.

Figures

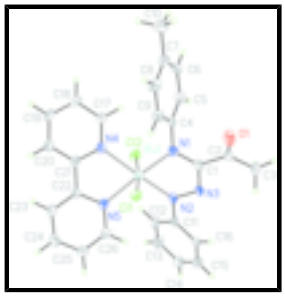


Fig. 1. The molecular structure of **I**, showing 40% prabability displacement ellipsoides and the atom-numbering scheme. H atoms have been omitted for clarity.

trans-(2,2'-Bipyridine)dichlorido[1-(4-methylphenylimino)-1- (phenylhydrazono)propan-2-one]ruthenium(II) dichloromethane solvate

Crystal data

$[RuCl_2(C_{10}H_8N_2)(C_{16}H_{15}N_3O)]\cdot CH_2Cl_2$	$Z = 2$
$M_r = 678.39$	$F_{000} = 684$
Triclinic, $P\overline{1}$	$D_x = 1.620$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9994$ (4) Å	Cell parameters from 9663 reflections
$b = 11.3852$ (9) Å	$\theta = 2.7$–27.6º
$c = 15.0563$ (12) Å	$\mu = 0.98$ mm^{-1}
$\alpha = 106.387$ (3)º	$T = 183$ (2) K
$\beta = 104.123$ (4)º	Prism, red–brown
$\gamma = 99.231$ (5)º	0.04 × 0.04 × 0.04 mm
$V = 1391.01$ (17) Å^3	

Data collection

Nonius KappaCCD diffractometer	3840 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.053$
Monochromator: graphite	$\theta_{max} = 27.6$º
$T = 183(2)$ K	$\theta_{min} = 2.7$º
φ and ω scans	$h = -10\rightarrow11$
Absorption correction: none	$k = -14\rightarrow13$
9663 measured reflections	$l = -15\rightarrow19$
6311 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained

$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.6048P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
6311 reflections	$\Delta\rho_{max} = 1.00$ e Å^{-3}
359 parameters	$\Delta\rho_{min} = -0.78$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Ru1	0.09028 (5)	0.45222 (4)	0.24154 (3)	0.02556 (15)	
Cl1	0.28449 (13)	0.59316 (13)	0.38662 (10)	0.0307 (3)	
Cl2	−0.12615 (14)	0.31457 (14)	0.10849 (10)	0.0373 (3)	
O1	0.3430 (5)	0.7905 (4)	0.1562 (3)	0.0488 (11)	
N1	0.1385 (4)	0.5860 (4)	0.1838 (3)	0.0265 (10)	
N2	0.2432 (4)	0.3980 (4)	0.1750 (3)	0.0239 (9)	
N3	0.3159 (4)	0.4750 (4)	0.1385 (3)	0.0240 (9)	
N4	−0.0968 (4)	0.4968 (4)	0.2988 (3)	0.0258 (10)	
N5	0.0763 (5)	0.3358 (4)	0.3277 (3)	0.0275 (10)	
C1	0.2587 (6)	0.5804 (5)	0.1489 (4)	0.0280 (12)	
C2	0.3486 (6)	0.6820 (5)	0.1223 (4)	0.0307 (12)	
C3	0.4458 (6)	0.6447 (6)	0.0579 (5)	0.0419 (15)	
H3A	0.4870	0.7168	0.0400	0.063*	
H3B	0.3807	0.5749	−0.0010	0.063*	
H3C	0.5342	0.6175	0.0920	0.063*	
C4	0.0646 (6)	0.6901 (5)	0.1861 (4)	0.0284 (12)	
C5	−0.0400 (6)	0.6902 (6)	0.1015 (4)	0.0352 (13)	
H5A	−0.0567	0.6259	0.0414	0.042*	
C6	−0.1193 (6)	0.7840 (6)	0.1057 (4)	0.0359 (14)	
H6A	−0.1914	0.7829	0.0476	0.043*	
C7	−0.0984 (6)	0.8796 (5)	0.1909 (5)	0.0366 (14)	
C8	0.0069 (6)	0.8776 (5)	0.2750 (5)	0.0380 (14)	
H8A	0.0241	0.9426	0.3349	0.046*	
C9	0.0867 (6)	0.7839 (5)	0.2735 (4)	0.0340 (13)	
H9A	0.1564	0.7834	0.3319	0.041*	

C10	−0.1859 (7)	0.9824 (6)	0.1920 (5)	0.0506 (17)	
H10A	−0.1765	1.0150	0.1394	0.076*	
H10B	−0.1402	1.0511	0.2545	0.076*	
H10C	−0.2977	0.9478	0.1827	0.076*	
C11	0.2867 (6)	0.2792 (5)	0.1525 (4)	0.0283 (12)	
C12	0.1745 (6)	0.1680 (5)	0.1340 (4)	0.0368 (14)	
H12A	0.0729	0.1715	0.1407	0.044*	
C13	0.2120 (7)	0.0530 (6)	0.1060 (5)	0.0424 (15)	
H13A	0.1354	−0.0228	0.0923	0.051*	
C14	0.3628 (7)	0.0476 (6)	0.0976 (4)	0.0398 (14)	
H14A	0.3885	−0.0317	0.0786	0.048*	
C15	0.4728 (6)	0.1568 (5)	0.1168 (5)	0.0385 (14)	
H15A	0.5754	0.1529	0.1121	0.046*	
C16	0.4365 (6)	0.2730 (5)	0.1430 (4)	0.0313 (13)	
H16A	0.5129	0.3480	0.1546	0.038*	
C17	−0.1920 (6)	0.5704 (5)	0.2732 (4)	0.0313 (13)	
H17A	−0.1689	0.6150	0.2317	0.038*	
C18	−0.3216 (6)	0.5827 (6)	0.3056 (4)	0.0369 (14)	
H18A	−0.3852	0.6361	0.2873	0.044*	
C19	−0.3579 (6)	0.5172 (6)	0.3645 (4)	0.0398 (15)	
H19A	−0.4460	0.5253	0.3878	0.048*	
C20	−0.2646 (6)	0.4394 (6)	0.3892 (4)	0.0340 (13)	
H20A	−0.2884	0.3926	0.4293	0.041*	
C21	−0.1353 (5)	0.4301 (5)	0.3549 (4)	0.0261 (12)	
C22	−0.0323 (5)	0.3476 (5)	0.3770 (4)	0.0261 (12)	
C23	−0.0384 (6)	0.2906 (5)	0.4462 (4)	0.0318 (13)	
H23A	−0.1160	0.2995	0.4789	0.038*	
C24	0.0683 (6)	0.2207 (6)	0.4677 (4)	0.0377 (14)	
H24A	0.0633	0.1785	0.5135	0.045*	
C25	0.1826 (6)	0.2134 (6)	0.4211 (4)	0.0395 (14)	
H25A	0.2595	0.1678	0.4359	0.047*	
C26	0.1849 (6)	0.2717 (5)	0.3536 (4)	0.0355 (13)	
H26A	0.2660	0.2673	0.3234	0.043*	
Cl2M	0.4359 (3)	0.8672 (3)	0.5625 (3)	0.0807 (15)	0.721 (6)
Cl1M	0.3443 (5)	1.0975 (4)	0.6269 (3)	0.0966 (14)	0.721 (6)
Cl2A	0.4700 (8)	0.8732 (8)	0.6501 (8)	0.070 (3)	0.279 (6)
Cl1A	0.2880 (11)	1.0169 (11)	0.5604 (9)	0.097 (3)*	0.279 (6)
C1M	0.4867 (9)	1.0152 (8)	0.6452 (8)	0.101 (4)	
H1MA	0.5864	1.0628	0.6420	0.122*	0.721 (6)
H1MB	0.5066	1.0092	0.7112	0.122*	0.721 (6)
H1MC	0.5742	1.0375	0.6192	0.122*	0.279 (6)
H1MD	0.5090	1.0771	0.7109	0.122*	0.279 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.0246 (2)	0.0314 (3)	0.0262 (3)	0.00902 (17)	0.01277 (17)	0.0126 (2)
Cl1	0.0263 (6)	0.0389 (8)	0.0283 (7)	0.0104 (5)	0.0091 (5)	0.0116 (6)

Cl2	0.0298 (7)	0.0436 (9)	0.0334 (8)	0.0051 (6)	0.0089 (6)	0.0080 (7)
O1	0.063 (3)	0.034 (3)	0.061 (3)	0.009 (2)	0.039 (2)	0.018 (2)
N1	0.026 (2)	0.028 (3)	0.026 (3)	0.0085 (18)	0.0083 (18)	0.008 (2)
N2	0.028 (2)	0.021 (2)	0.025 (2)	0.0030 (17)	0.0121 (18)	0.009 (2)
N3	0.031 (2)	0.022 (2)	0.025 (2)	0.0068 (18)	0.0133 (18)	0.012 (2)
N4	0.026 (2)	0.029 (3)	0.023 (2)	0.0045 (18)	0.0095 (18)	0.009 (2)
N5	0.030 (2)	0.029 (3)	0.028 (3)	0.0102 (19)	0.0126 (19)	0.009 (2)
C1	0.032 (3)	0.027 (3)	0.027 (3)	0.008 (2)	0.011 (2)	0.010 (3)
C2	0.032 (3)	0.034 (4)	0.031 (3)	0.008 (2)	0.012 (2)	0.015 (3)
C3	0.041 (3)	0.046 (4)	0.055 (4)	0.015 (3)	0.030 (3)	0.027 (3)
C4	0.029 (3)	0.033 (3)	0.034 (3)	0.009 (2)	0.014 (2)	0.022 (3)
C5	0.037 (3)	0.039 (4)	0.035 (3)	0.011 (3)	0.013 (3)	0.019 (3)
C6	0.035 (3)	0.046 (4)	0.038 (4)	0.015 (3)	0.013 (3)	0.027 (3)
C7	0.037 (3)	0.032 (3)	0.051 (4)	0.014 (2)	0.023 (3)	0.019 (3)
C8	0.039 (3)	0.026 (3)	0.042 (4)	0.007 (2)	0.014 (3)	0.000 (3)
C9	0.032 (3)	0.035 (3)	0.035 (3)	0.010 (2)	0.010 (2)	0.013 (3)
C10	0.048 (4)	0.050 (4)	0.067 (5)	0.022 (3)	0.022 (3)	0.030 (4)
C11	0.038 (3)	0.030 (3)	0.025 (3)	0.013 (2)	0.019 (2)	0.011 (2)
C12	0.038 (3)	0.034 (3)	0.047 (4)	0.008 (3)	0.026 (3)	0.016 (3)
C13	0.047 (3)	0.033 (4)	0.052 (4)	0.005 (3)	0.025 (3)	0.014 (3)
C14	0.053 (4)	0.031 (3)	0.046 (4)	0.017 (3)	0.027 (3)	0.015 (3)
C15	0.038 (3)	0.037 (4)	0.055 (4)	0.020 (3)	0.026 (3)	0.023 (3)
C16	0.031 (3)	0.034 (3)	0.035 (3)	0.008 (2)	0.013 (2)	0.019 (3)
C17	0.033 (3)	0.037 (3)	0.032 (3)	0.014 (2)	0.016 (2)	0.016 (3)
C18	0.028 (3)	0.043 (4)	0.043 (4)	0.017 (2)	0.014 (3)	0.012 (3)
C19	0.030 (3)	0.055 (4)	0.039 (4)	0.018 (3)	0.018 (3)	0.010 (3)
C20	0.030 (3)	0.046 (4)	0.030 (3)	0.010 (2)	0.013 (2)	0.016 (3)
C21	0.020 (2)	0.032 (3)	0.024 (3)	0.004 (2)	0.008 (2)	0.006 (2)
C22	0.026 (3)	0.031 (3)	0.025 (3)	0.005 (2)	0.010 (2)	0.013 (2)
C23	0.030 (3)	0.037 (3)	0.029 (3)	0.005 (2)	0.013 (2)	0.009 (3)
C24	0.048 (3)	0.039 (4)	0.032 (3)	0.011 (3)	0.016 (3)	0.018 (3)
C25	0.042 (3)	0.049 (4)	0.039 (4)	0.022 (3)	0.016 (3)	0.023 (3)
C26	0.034 (3)	0.042 (4)	0.037 (4)	0.015 (3)	0.018 (3)	0.016 (3)
Cl2M	0.0550 (16)	0.0580 (19)	0.108 (4)	0.0028 (12)	0.0373 (18)	−0.0087 (18)
Cl1M	0.154 (3)	0.082 (3)	0.083 (3)	0.072 (2)	0.041 (2)	0.044 (2)
Cl2A	0.067 (4)	0.071 (5)	0.092 (8)	0.033 (4)	0.024 (4)	0.049 (5)
C1M	0.051 (5)	0.085 (7)	0.129 (9)	0.012 (4)	0.023 (5)	−0.015 (6)

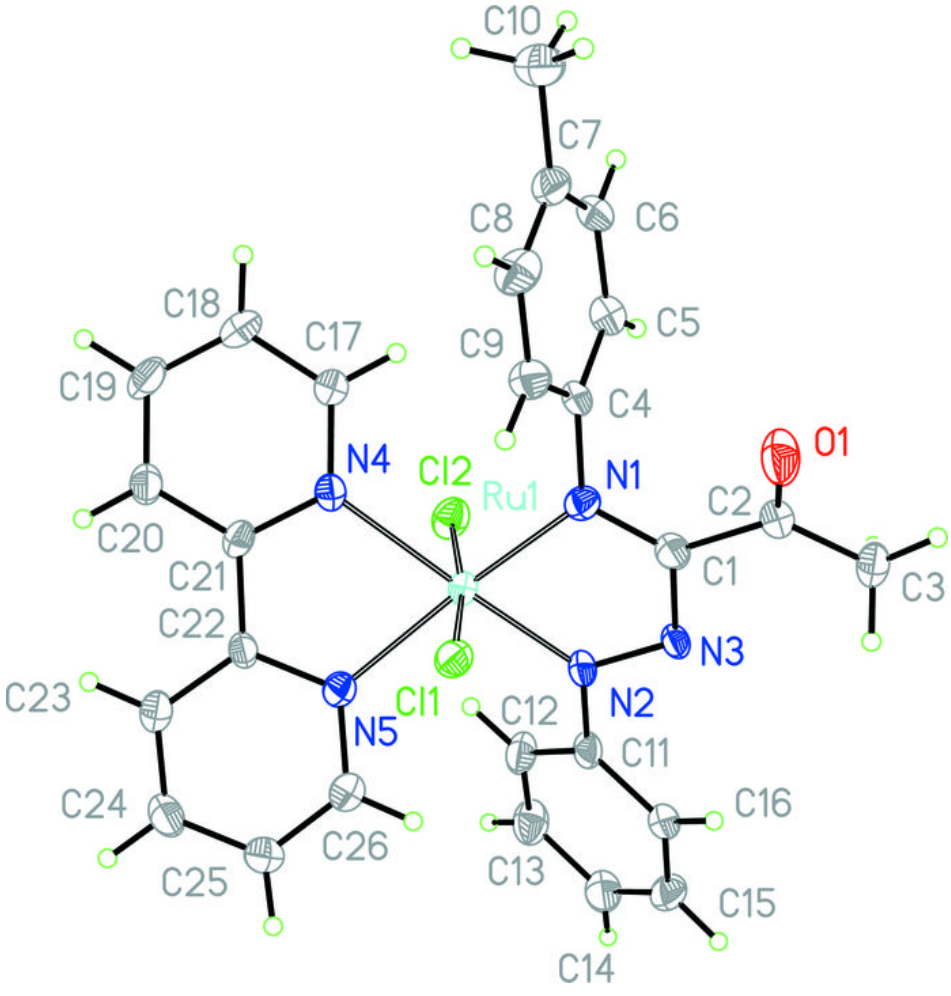
Geometric parameters (Å, °)

Ru1—N2	1.968 (4)	C11—C16	1.400 (6)
Ru1—N1	1.996 (4)	C12—C13	1.381 (8)
Ru1—N5	2.110 (4)	C12—H12A	0.9500
Ru1—N4	2.138 (4)	C13—C14	1.402 (7)
Ru1—Cl2	2.3680 (14)	C13—H13A	0.9500
Ru1—Cl1	2.3792 (14)	C14—C15	1.368 (8)
O1—C2	1.210 (6)	C14—H14A	0.9500
N1—C1	1.315 (6)	C15—C16	1.385 (7)
N1—C4	1.446 (6)	C15—H15A	0.9500

N2—N3	1.328 (5)	C16—H16A	0.9500
N2—C11	1.440 (6)	C17—C18	1.382 (7)
N3—C1	1.364 (6)	C17—H17A	0.9500
N4—C21	1.353 (6)	C18—C19	1.373 (8)
N4—C17	1.356 (6)	C18—H18A	0.9500
N5—C22	1.365 (6)	C19—C20	1.378 (8)
N5—C26	1.358 (6)	C19—H19A	0.9500
C1—C2	1.508 (7)	C20—C21	1.391 (6)
C2—C3	1.479 (7)	C20—H20A	0.9500
C3—H3A	0.9800	C21—C22	1.469 (7)
C3—H3B	0.9800	C22—C23	1.381 (7)
C3—H3C	0.9800	C23—C24	1.378 (7)
C4—C9	1.386 (8)	C23—H23A	0.9500
C4—C5	1.387 (7)	C24—C25	1.380 (7)
C5—C6	1.372 (7)	C24—H24A	0.9500
C5—H5A	0.9500	C25—C26	1.364 (8)
C6—C7	1.376 (8)	C25—H25A	0.9500
C6—H6A	0.9500	C26—H26A	0.9500
C7—C8	1.393 (8)	Cl2M—C1M	1.700 (9)
C7—C10	1.510 (7)	Cl1M—C1M	1.719 (9)
C8—C9	1.377 (7)	Cl2A—C1M	1.624 (11)
C8—H8A	0.9500	Cl1A—C1M	1.934 (13)
C9—H9A	0.9500	C1M—H1MA	0.9900
C10—H10A	0.9800	C1M—H1MB	0.9900
C10—H10B	0.9800	C1M—H1MC	0.9900
C10—H10C	0.9800	C1M—H1MD	0.9900
C11—C12	1.398 (7)		
N2—Ru1—N1	76.58 (16)	C12—C13—C14	120.3 (5)
N2—Ru1—N5	103.79 (16)	C12—C13—H13A	119.9
N1—Ru1—N5	168.40 (16)	C14—C13—H13A	119.9
N2—Ru1—N4	173.36 (16)	C15—C14—C13	119.8 (5)
N1—Ru1—N4	103.93 (16)	C15—C14—H14A	120.1
N5—Ru1—N4	77.09 (15)	C13—C14—H14A	120.1
N2—Ru1—Cl2	91.84 (12)	C14—C15—C16	120.9 (5)
N1—Ru1—Cl2	97.65 (13)	C14—C15—H15A	119.6
N5—Ru1—Cl2	93.93 (12)	C16—C15—H15A	119.6
N4—Ru1—Cl2	81.52 (11)	C15—C16—C11	119.7 (5)
N2—Ru1—Cl1	95.22 (12)	C15—C16—H16A	120.2
N1—Ru1—Cl1	85.68 (13)	C11—C16—H16A	120.2
N5—Ru1—Cl1	82.74 (12)	N4—C17—C18	122.2 (5)
N4—Ru1—Cl1	91.42 (11)	N4—C17—H17A	118.9
Cl2—Ru1—Cl1	172.74 (5)	C18—C17—H17A	118.9
C1—N1—C4	119.8 (4)	C19—C18—C17	119.5 (5)
C1—N1—Ru1	113.9 (3)	C19—C18—H18A	120.2
C4—N1—Ru1	126.0 (3)	C17—C18—H18A	120.2
N3—N2—C11	110.7 (4)	C18—C19—C20	119.0 (5)
N3—N2—Ru1	119.3 (3)	C18—C19—H19A	120.5
C11—N2—Ru1	129.9 (3)	C20—C19—H19A	120.5
N2—N3—C1	110.3 (4)	C19—C20—C21	119.4 (5)

C21—N4—C17	118.0 (4)	C19—C20—H20A	120.3
C21—N4—Ru1	115.3 (3)	C21—C20—H20A	120.3
C17—N4—Ru1	126.1 (3)	N4—C21—C20	121.8 (5)
C22—N5—C26	117.1 (4)	N4—C21—C22	115.8 (4)
C22—N5—Ru1	116.1 (3)	C20—C21—C22	122.4 (5)
C26—N5—Ru1	125.3 (3)	N5—C22—C23	121.9 (4)
N1—C1—N3	118.5 (5)	N5—C22—C21	115.2 (4)
N1—C1—C2	127.0 (5)	C23—C22—C21	122.8 (4)
N3—C1—C2	114.5 (4)	C22—C23—C24	119.8 (5)
O1—C2—C3	122.6 (5)	C22—C23—H23A	120.1
O1—C2—C1	119.5 (5)	C24—C23—H23A	120.1
C3—C2—C1	117.9 (5)	C25—C24—C23	118.4 (5)
C2—C3—H3A	109.5	C25—C24—H24A	120.8
C2—C3—H3B	109.5	C23—C24—H24A	120.8
H3A—C3—H3B	109.5	C26—C25—C24	119.8 (5)
C2—C3—H3C	109.5	C26—C25—H25A	120.1
H3A—C3—H3C	109.5	C24—C25—H25A	120.1
H3B—C3—H3C	109.5	N5—C26—C25	122.8 (5)
C9—C4—C5	119.7 (5)	N5—C26—H26A	118.6
C9—C4—N1	120.5 (5)	C25—C26—H26A	118.6
C5—C4—N1	119.6 (5)	Cl2A—C1M—Cl2M	44.4 (4)
C6—C5—C4	119.3 (6)	Cl2A—C1M—Cl1M	129.7 (6)
C6—C5—H5A	120.4	Cl2M—C1M—Cl1M	113.2 (5)
C4—C5—H5A	120.4	Cl2A—C1M—Cl1A	107.0 (6)
C5—C6—C7	122.6 (5)	Cl2M—C1M—Cl1A	79.3 (5)
C5—C6—H6A	118.7	Cl1M—C1M—Cl1A	34.1 (4)
C7—C6—H6A	118.7	Cl2A—C1M—H1MA	120.6
C6—C7—C8	117.2 (5)	Cl2M—C1M—H1MA	108.9
C6—C7—C10	120.9 (6)	Cl1M—C1M—H1MA	108.9
C8—C7—C10	121.9 (6)	Cl1A—C1M—H1MA	118.9
C9—C8—C7	121.6 (6)	Cl2A—C1M—H1MB	64.6
C9—C8—H8A	119.2	Cl2M—C1M—H1MB	108.9
C7—C8—H8A	119.2	Cl1M—C1M—H1MB	108.9
C8—C9—C4	119.6 (5)	Cl1A—C1M—H1MB	127.0
C8—C9—H9A	120.2	H1MA—C1M—H1MB	107.8
C4—C9—H9A	120.2	Cl2A—C1M—H1MC	110.3
C7—C10—H10A	109.5	Cl2M—C1M—H1MC	89.0
C7—C10—H10B	109.5	Cl1M—C1M—H1MC	113.4
H10A—C10—H10B	109.5	Cl1A—C1M—H1MC	110.3
C7—C10—H10C	109.5	H1MA—C1M—H1MC	20.9
H10A—C10—H10C	109.5	H1MB—C1M—H1MC	121.8
H10B—C10—H10C	109.5	Cl2A—C1M—H1MD	110.3
C12—C11—C16	119.7 (5)	Cl2M—C1M—H1MD	154.2
C12—C11—N2	119.4 (4)	Cl1M—C1M—H1MD	77.7
C16—C11—N2	120.8 (5)	Cl1A—C1M—H1MD	110.3
C13—C12—C11	119.7 (5)	H1MA—C1M—H1MD	87.7
C13—C12—H12A	120.2	H1MB—C1M—H1MD	45.8
C11—C12—H12A	120.2	H1MC—C1M—H1MD	108.6

Fig. 1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