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trans-(2,2′-Bipyridine)dichlorido[methyl 1-(phenylhydrazono)-1-(phenylimino)-acetato]ruthenium(II) dichloromethane solvate

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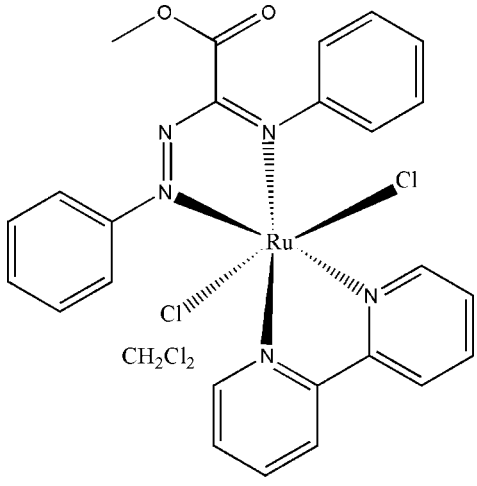
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.010 Å; disorder in main residue; R factor = 0.066; wR factor = 0.169; data-to-parameter ratio = 18.5.

The title compound, $[RuCl_2(C_{15}H_{13}N_3O_2)(C_{10}H_8N_2)]\cdot CH_2Cl_2$, has a pseudo-octahedral coordination environment made up of two *trans* chloride ligands and four N-donor atoms, two of which belong to the azoimine bidentate ligand and two to the bipyridyl molecule. The ester group is disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

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



Experimental

Crystal data

$[RuCl_2(C_{15}H_{13}N_3O_2)(C_{10}H_8N_2)]\cdot CH_2Cl_2$
M_r = 680.36
Monoclinic, $P2_1/c$
a = 12.1073 (7) Å
b = 11.4851 (5) Å
c = 20.2336 (9) Å
β = 100.858 (3)°
V = 2763.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 183 (2) K
0.05 × 0.05 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
18205 measured reflections
6319 independent reflections
3610 reflections with $I > 2\sigma(I)$
R_{int} = 0.120

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.169
S = 1.02
6319 reflections
341 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 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: BT2529).

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supplementary materials

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trans-(2,2'-Bipyridine)dichlorido[methyl 1-(phenylhydrazono)-1-(phenylimino)acetato]ruthenium(II) dichloromethane solvate

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

Comment

Ruthenium (II) complexes containing the azoimine (N=N—C=N) functional unit are light-sensitive, redox-active, and efficient colorant materials (Kaim, 2001). This function is π-acidic and has successfully been used to stabilize the low-valent metal redox state. The importance of azoimine chemistry encourages us to develop a new ligand containing an azoimine unit. The new unsymmetrical bidentate ligand, methyl-1-(phenylimino)-1-(phenylhydrazono)-acetate (*L*), lacks a twofold symmetry axis and on complexation with ruthenium (II), affords a pseudo-octahedral, *trans*-[Ru(bpy)LCl_2] complex. The five membered rings formed by the coordination of azoimine and bpy are planar and have almost equivalent coordination bite-angles N1—Ru—N2 = 75.9 (2)°, and N4—Ru—N5 = 76.6 (2)°, respectively, whereas Cl2—Ru—Cl1 angle is 169.52 (6)°. However, it is interesting to note that the bond lengths of Ru(II) and azoimine N atoms, (Ru—N1) = 2.009 (5) Å and (Ru—N2) = 1.953 (5) (4) Å are significantly shorter than those of Ru(II) and the bpy N atoms, (Ru—N4) = 2.145 (5) Å and (Ru—N5) = 2.123 (5) Å indicated preferential π-bonding of Ru(II) with the azo group.

Experimental

Trans-2,2'-bipyridinedichloromethyl-1-(phenylimino)-1-(phenylhydrazono)-acetate ruthenium(II) was prepared according to literature procedure (Al-Noaimi *et al.*,2007) and recrystallized by slowly evaporating a solution of dichloromethane.

Refinement

The methylyester group has a 0.591 (18):0.409 (18) occupancy disorder over two positions. The disordered atoms were refined isotropically. The O2A—C3A distance was restrained to 1.433 (9) Å. All hydrogen atoms were set to idealized positions and were refined with 1.2 times (1.5 for the methyl group) the isotropic displacement parameter of the corresponding carbon atom.

Figures

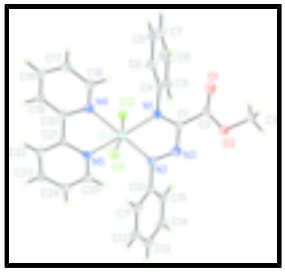


Fig. 1. The molecular structure of the title compound, showing 40% prabability displacement ellipsoides and the atom-numbering scheme. Solvente molecule and one of the disordered parts of the methylester group have been omitted for clarity.

trans-(2,2'-bipyridine)dichlorido[methyl 1-(phenylhydrazono)-1-(phenylimino)acetato]ruthenium(II) dichloromethane solvate

Crystal data

$[RuCl_2(C_{15}H_{13}N_3O_2)(C_{10}H_8N_2)]\cdot CH_2Cl_2$	F_{000} = 1368
M_r = 680.36	D_x = 1.635 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 18205 reflections
a = 12.1073 (7) Å	θ = 2.5–27.5º
b = 11.4851 (5) Å	μ = 0.99 mm^{-1}
c = 20.2336 (9) Å	T = 183 (2) K
β = 100.858 (3)º	Prism, red-brown
V = 2763.2 (2) Å^3	0.05 × 0.05 × 0.04 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	3610 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.120
Monochromator: graphite	θ_{max} = 27.5º
T = 183(2) K	θ_{min} = 2.5º
φ and ω scans	h = −15→15
Absorption correction: none	k = −14→14
18205 measured reflections	l = −26→24
6319 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
$R[F^2 > 2\sigma(F^2)]$ = 0.066	H-atom parameters constrained
$wR(F^2)$ = 0.169	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 2.7651P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.002
6319 reflections	$\Delta\rho_{max}$ = 2.18 e Å^{-3}
341 parameters	$\Delta\rho_{min}$ = −0.94 e Å^{-3}
1 restraint	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 $F^2 > 2\text{sigma}(F^2)$ 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	0.80699 (4)	0.05555 (4)	0.84888 (3)	0.02344 (17)	
Cl1	0.79947 (13)	0.00091 (14)	0.73396 (8)	0.0302 (4)	
Cl2	0.81852 (13)	0.14379 (14)	0.95461 (8)	0.0314 (4)	
O1	0.4366 (8)	−0.0154 (8)	0.9012 (6)	0.031 (3)*	0.591 (18)
O2	0.5162 (8)	−0.1884 (7)	0.9350 (5)	0.028 (2)*	0.591 (18)
C3	0.4083 (9)	−0.2204 (9)	0.9550 (6)	0.026 (3)*	0.591 (18)
H3A	0.4151	−0.2980	0.9756	0.039*	0.591 (18)
H3B	0.3481	−0.2209	0.9152	0.039*	0.591 (18)
H3C	0.3906	−0.1635	0.9876	0.039*	0.591 (18)
O1A	0.4517 (12)	0.0003 (12)	0.9250 (9)	0.035 (4)*	0.409 (18)
O2A	0.4811 (12)	−0.1968 (10)	0.9050 (9)	0.035 (4)*	0.409 (18)
C3A	0.3700 (15)	−0.244 (2)	0.9125 (15)	0.075 (8)*	0.409 (18)
H3AA	0.3713	−0.3289	0.9097	0.113*	0.409 (18)
H3AB	0.3117	−0.2130	0.8765	0.113*	0.409 (18)
H3AC	0.3538	−0.2203	0.9563	0.113*	0.409 (18)
N1	0.6430 (4)	0.0329 (4)	0.8503 (3)	0.0234 (11)	
N2	0.7989 (4)	−0.1010 (4)	0.8852 (3)	0.0253 (12)	
N3	0.7061 (4)	−0.1351 (4)	0.9053 (3)	0.0300 (13)	
N4	0.8169 (4)	0.2264 (4)	0.8076 (3)	0.0267 (12)	
N5	0.9826 (4)	0.0887 (4)	0.8655 (3)	0.0258 (12)	
C1	0.6232 (5)	−0.0568 (6)	0.8861 (3)	0.0286 (14)	
C2	0.5114 (5)	−0.0823 (6)	0.9070 (4)	0.0332 (16)	
C4	0.5537 (5)	0.1105 (5)	0.8210 (3)	0.0230 (14)	
C5	0.4923 (6)	0.0882 (6)	0.7574 (4)	0.0384 (18)	
H5A	0.5069	0.0200	0.7338	0.046*	
C6	0.4104 (6)	0.1649 (7)	0.7284 (4)	0.050 (2)	
H6A	0.3679	0.1490	0.6849	0.060*	
C7	0.3891 (6)	0.2648 (6)	0.7615 (4)	0.0382 (17)	
H7A	0.3316	0.3171	0.7415	0.046*	
C8	0.4516 (6)	0.2874 (6)	0.8234 (4)	0.0383 (18)	
H8A	0.4374	0.3563	0.8464	0.046*	
C9	0.5349 (6)	0.2124 (5)	0.8534 (4)	0.0344 (16)	
H9A	0.5791	0.2306	0.8961	0.041*	

C10	0.8811 (5)	−0.1937 (5)	0.8949 (3)	0.0248 (14)
C11	0.9375 (6)	−0.2197 (6)	0.8435 (4)	0.0342 (16)
H11A	0.9222	−0.1771	0.8026	0.041*
C12	1.0165 (6)	−0.3083 (6)	0.8520 (4)	0.0415 (18)
H12A	1.0540	−0.3284	0.8163	0.050*
C13	1.0405 (6)	−0.3671 (6)	0.9123 (4)	0.0419 (19)
H13A	1.0970	−0.4256	0.9189	0.050*
C14	0.9829 (6)	−0.3416 (6)	0.9634 (4)	0.0363 (17)
H14A	0.9979	−0.3848	1.0041	0.044*
C15	0.9035 (5)	−0.2534 (6)	0.9554 (3)	0.0331 (16)
H15A	0.8651	−0.2343	0.9908	0.040*
C16	0.7321 (5)	0.2876 (6)	0.7724 (3)	0.0345 (16)
H16A	0.6594	0.2534	0.7630	0.041*
C17	0.7458 (6)	0.3988 (6)	0.7490 (4)	0.0386 (18)
H17A	0.6835	0.4396	0.7239	0.046*
C18	0.8492 (6)	0.4493 (6)	0.7624 (3)	0.0337 (16)
H18A	0.8598	0.5271	0.7490	0.040*
C19	0.9369 (5)	0.3855 (5)	0.7953 (3)	0.0298 (15)
H19A	1.0100	0.4186	0.8041	0.036*
C20	0.9216 (5)	0.2729 (5)	0.8164 (3)	0.0270 (14)
C21	1.0138 (5)	0.1957 (5)	0.8469 (3)	0.0231 (14)
C22	1.1254 (5)	0.2272 (5)	0.8559 (3)	0.0292 (15)
H22A	1.1456	0.3011	0.8408	0.035*
C23	1.2088 (5)	0.1510 (6)	0.8871 (3)	0.0323 (16)
H23A	1.2861	0.1708	0.8920	0.039*
C24	1.1769 (5)	0.0480 (6)	0.9100 (3)	0.0292 (14)
H24A	1.2317	−0.0042	0.9333	0.035*
C25	1.0633 (5)	0.0189 (6)	0.8993 (3)	0.0314 (15)
H25A	1.0419	−0.0529	0.9166	0.038*
C1M	0.6506 (8)	−0.0735 (7)	0.4544 (5)	0.060 (2)
H1MA	0.6835	−0.1467	0.4409	0.072*
H1MB	0.5703	−0.0711	0.4324	0.072*
Cl1M	0.7200 (2)	0.0438 (2)	0.42859 (13)	0.0728 (7)
Cl2M	0.6616 (3)	−0.0711 (2)	0.54335 (14)	0.0908 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.0180 (3)	0.0213 (3)	0.0314 (3)	0.0000 (2)	0.0057 (2)	0.0029 (2)
Cl1	0.0284 (8)	0.0302 (8)	0.0333 (9)	0.0007 (7)	0.0092 (7)	−0.0002 (7)
Cl2	0.0279 (8)	0.0333 (9)	0.0321 (9)	−0.0002 (7)	0.0035 (7)	−0.0009 (7)
N1	0.019 (3)	0.025 (3)	0.026 (3)	0.000 (2)	0.003 (2)	0.004 (2)
N2	0.024 (3)	0.017 (2)	0.037 (3)	0.000 (2)	0.010 (3)	0.002 (2)
N3	0.025 (3)	0.030 (3)	0.037 (3)	0.004 (2)	0.010 (3)	0.006 (3)
N4	0.021 (3)	0.026 (3)	0.032 (3)	0.000 (2)	0.002 (2)	−0.001 (2)
N5	0.019 (3)	0.026 (3)	0.032 (3)	0.006 (2)	0.005 (2)	0.005 (2)
C1	0.022 (3)	0.033 (4)	0.032 (4)	−0.004 (3)	0.008 (3)	0.003 (3)
C2	0.018 (3)	0.040 (4)	0.042 (4)	0.005 (3)	0.007 (3)	0.007 (3)

C4	0.017 (3)	0.018 (3)	0.035 (4)	−0.004 (2)	0.007 (3)	−0.003 (3)
C5	0.028 (4)	0.032 (4)	0.051 (5)	0.007 (3)	−0.003 (3)	−0.003 (3)
C6	0.039 (4)	0.057 (5)	0.045 (5)	0.012 (4)	−0.012 (4)	−0.005 (4)
C7	0.036 (4)	0.030 (4)	0.050 (5)	0.009 (3)	0.011 (4)	0.008 (4)
C8	0.048 (4)	0.028 (4)	0.044 (5)	0.012 (3)	0.022 (4)	0.000 (3)
C9	0.040 (4)	0.025 (3)	0.035 (4)	0.008 (3)	0.000 (3)	0.002 (3)
C10	0.015 (3)	0.020 (3)	0.039 (4)	0.002 (2)	0.005 (3)	0.004 (3)
C11	0.040 (4)	0.030 (4)	0.035 (4)	0.007 (3)	0.010 (3)	0.003 (3)
C12	0.036 (4)	0.039 (4)	0.050 (5)	0.014 (3)	0.011 (4)	0.003 (4)
C13	0.033 (4)	0.028 (4)	0.063 (5)	0.008 (3)	0.005 (4)	−0.001 (4)
C14	0.038 (4)	0.025 (3)	0.041 (4)	0.006 (3)	−0.006 (3)	0.002 (3)
C15	0.027 (4)	0.037 (4)	0.034 (4)	−0.001 (3)	0.001 (3)	0.001 (3)
C16	0.024 (4)	0.040 (4)	0.040 (4)	0.001 (3)	0.007 (3)	0.009 (3)
C17	0.033 (4)	0.037 (4)	0.046 (5)	0.004 (3)	0.008 (3)	0.022 (4)
C18	0.039 (4)	0.026 (3)	0.038 (4)	−0.002 (3)	0.013 (3)	0.008 (3)
C19	0.028 (4)	0.028 (3)	0.033 (4)	−0.005 (3)	0.004 (3)	0.002 (3)
C20	0.022 (3)	0.028 (3)	0.031 (4)	0.000 (3)	0.006 (3)	0.002 (3)
C21	0.018 (3)	0.024 (3)	0.029 (4)	0.002 (3)	0.009 (3)	0.008 (3)
C22	0.029 (4)	0.020 (3)	0.038 (4)	−0.003 (3)	0.006 (3)	0.007 (3)
C23	0.022 (3)	0.037 (4)	0.038 (4)	−0.005 (3)	0.005 (3)	0.007 (3)
C24	0.024 (3)	0.029 (3)	0.034 (4)	0.005 (3)	0.004 (3)	0.002 (3)
C25	0.019 (3)	0.031 (4)	0.041 (4)	0.002 (3)	−0.002 (3)	0.007 (3)
C1M	0.068 (6)	0.047 (5)	0.064 (6)	0.000 (4)	0.010 (5)	0.000 (4)
Cl1M	0.0828 (17)	0.0619 (14)	0.0747 (17)	−0.0055 (13)	0.0173 (14)	0.0212 (13)
Cl2M	0.129 (3)	0.0800 (19)	0.0746 (18)	0.0223 (17)	0.0474 (18)	0.0275 (14)

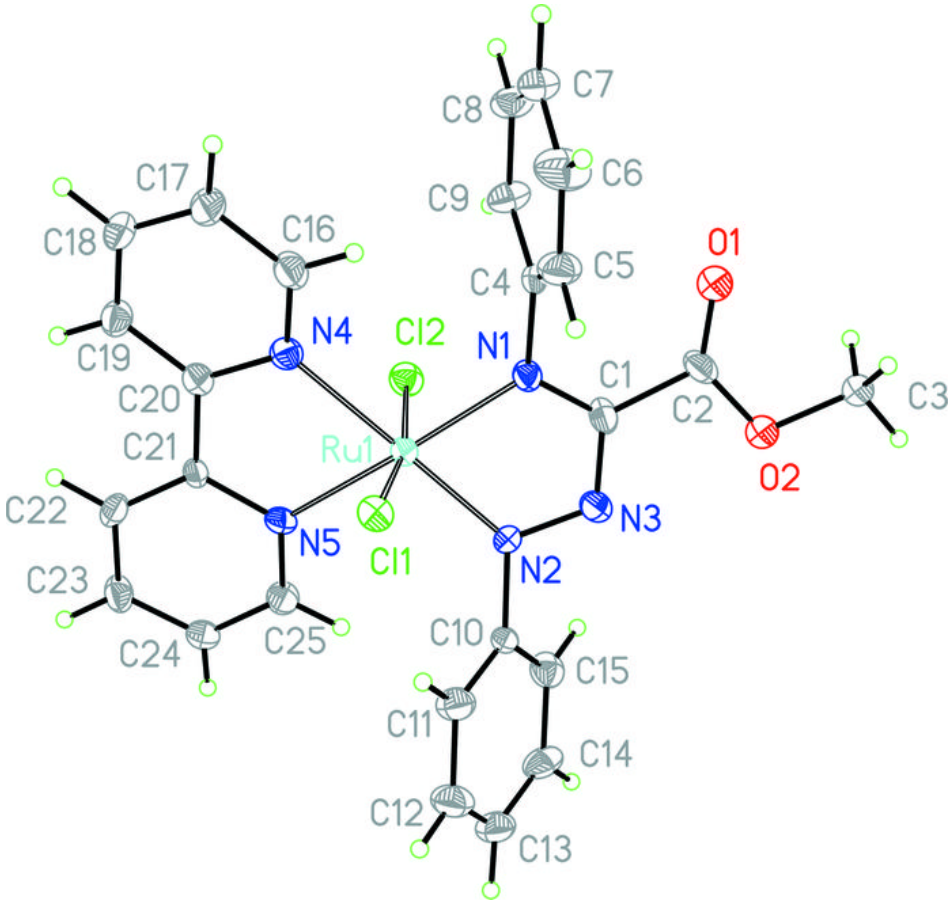
Geometric parameters (Å, °)

Ru1—N2	1.951 (5)	C8—C9	1.377 (9)
Ru1—N1	2.007 (5)	C8—H8A	0.9500
Ru1—N5	2.123 (5)	C9—H9A	0.9500
Ru1—N4	2.144 (5)	C10—C11	1.379 (8)
Ru1—Cl2	2.3475 (17)	C10—C15	1.385 (9)
Ru1—Cl1	2.3935 (17)	C11—C12	1.385 (9)
O1—C2	1.176 (10)	C11—H11A	0.9500
O2—C2	1.341 (10)	C12—C13	1.378 (10)
O2—C3	1.485 (12)	C12—H12A	0.9500
C3—H3A	0.9800	C13—C14	1.382 (10)
C3—H3B	0.9800	C13—H13A	0.9500
C3—H3C	0.9800	C14—C15	1.385 (9)
O1A—C2	1.286 (15)	C14—H14A	0.9500
O2A—C2	1.364 (13)	C15—H15A	0.9500
O2A—C3A	1.483 (9)	C16—C17	1.383 (9)
C3A—H3AA	0.9800	C16—H16A	0.9500
C3A—H3AB	0.9800	C17—C18	1.360 (9)
C3A—H3AC	0.9800	C17—H17A	0.9500
N1—C1	1.307 (8)	C18—C19	1.357 (9)
N1—C4	1.440 (8)	C18—H18A	0.9500
N2—N3	1.325 (6)	C19—C20	1.384 (9)

N2—C10	1.446 (7)	C19—H19A	0.9500
N3—C1	1.350 (8)	C20—C21	1.468 (8)
N4—C16	1.335 (8)	C21—C22	1.377 (8)
N4—C20	1.356 (7)	C22—C23	1.394 (9)
N5—C25	1.347 (8)	C22—H22A	0.9500
N5—C21	1.361 (7)	C23—C24	1.354 (9)
C1—C2	1.520 (8)	C23—H23A	0.9500
C4—C5	1.384 (9)	C24—C25	1.392 (8)
C4—C9	1.381 (9)	C24—H24A	0.9500
C5—C6	1.374 (10)	C25—H25A	0.9500
C5—H5A	0.9500	C1M—Cl1M	1.721 (8)
C6—C7	1.378 (10)	C1M—Cl2M	1.779 (9)
C6—H6A	0.9500	C1M—H1MA	0.9900
C7—C8	1.360 (10)	C1M—H1MB	0.9900
C7—H7A	0.9500		
N2—Ru1—N1	75.9 (2)	C8—C7—C6	119.0 (7)
N2—Ru1—N5	103.0 (2)	C8—C7—H7A	120.5
N1—Ru1—N5	169.8 (2)	C6—C7—H7A	120.5
N2—Ru1—N4	179.1 (2)	C7—C8—C9	121.3 (7)
N1—Ru1—N4	104.60 (19)	C7—C8—H8A	119.3
N5—Ru1—N4	76.70 (19)	C9—C8—H8A	119.3
N2—Ru1—Cl2	93.06 (16)	C8—C9—C4	119.6 (7)
N1—Ru1—Cl2	86.11 (15)	C8—C9—H9A	120.2
N5—Ru1—Cl2	83.84 (15)	C4—C9—H9A	120.2
N4—Ru1—Cl2	87.81 (14)	C11—C10—C15	121.1 (6)
N2—Ru1—Cl1	97.39 (16)	C11—C10—N2	118.9 (6)
N1—Ru1—Cl1	97.07 (15)	C15—C10—N2	120.0 (5)
N5—Ru1—Cl1	93.11 (15)	C10—C11—C12	119.7 (7)
N4—Ru1—Cl1	81.74 (14)	C10—C11—H11A	120.2
Cl2—Ru1—Cl1	169.53 (6)	C12—C11—H11A	120.2
C2—O2—C3	111.7 (7)	C13—C12—C11	119.7 (7)
O2—C3—H3A	109.5	C13—C12—H12A	120.2
O2—C3—H3B	109.5	C11—C12—H12A	120.2
H3A—C3—H3B	109.5	C12—C13—C14	120.5 (6)
O2—C3—H3C	109.5	C12—C13—H13A	119.8
H3A—C3—H3C	109.5	C14—C13—H13A	119.8
H3B—C3—H3C	109.5	C15—C14—C13	120.3 (7)
C2—O2A—C3A	126.3 (14)	C15—C14—H14A	119.9
O2A—C3A—H3AA	109.5	C13—C14—H14A	119.9
O2A—C3A—H3AB	109.5	C14—C15—C10	118.8 (6)
H3AA—C3A—H3AB	109.5	C14—C15—H15A	120.6
O2A—C3A—H3AC	109.5	C10—C15—H15A	120.6
H3AA—C3A—H3AC	109.5	N4—C16—C17	122.6 (6)
H3AB—C3A—H3AC	109.5	N4—C16—H16A	118.7
C1—N1—C4	120.9 (5)	C17—C16—H16A	118.7
C1—N1—Ru1	113.3 (4)	C18—C17—C16	119.4 (7)
C4—N1—Ru1	125.6 (4)	C18—C17—H17A	120.3
N3—N2—C10	110.0 (5)	C16—C17—H17A	120.3
N3—N2—Ru1	119.6 (4)	C19—C18—C17	118.2 (6)

C10—N2—Ru1	130.4 (4)	C19—C18—H18A	120.9
N2—N3—C1	110.0 (5)	C17—C18—H18A	120.9
C16—N4—C20	117.9 (5)	C18—C19—C20	121.2 (6)
C16—N4—Ru1	126.6 (4)	C18—C19—H19A	119.4
C20—N4—Ru1	115.4 (4)	C20—C19—H19A	119.4
C25—N5—C21	117.7 (5)	N4—C20—C19	120.2 (6)
C25—N5—Ru1	125.6 (4)	N4—C20—C21	115.8 (5)
C21—N5—Ru1	116.1 (4)	C19—C20—C21	123.9 (6)
N1—C1—N3	118.7 (5)	N5—C21—C22	121.2 (5)
N1—C1—C2	124.9 (6)	N5—C21—C20	115.7 (5)
N3—C1—C2	116.4 (5)	C22—C21—C20	123.2 (5)
O1—C2—O1A	23.6 (7)	C21—C22—C23	120.3 (6)
O1—C2—O2	127.4 (7)	C21—C22—H22A	119.9
O1A—C2—O2	122.2 (8)	C23—C22—H22A	119.9
O1—C2—O2A	115.4 (8)	C24—C23—C22	118.3 (6)
O1A—C2—O2A	123.9 (9)	C24—C23—H23A	120.8
O2—C2—O2A	29.1 (6)	C22—C23—H23A	120.8
O1—C2—C1	123.7 (7)	C23—C24—C25	119.6 (6)
O1A—C2—C1	120.9 (8)	C23—C24—H24A	120.2
O2—C2—C1	108.8 (6)	C25—C24—H24A	120.2
O2A—C2—C1	115.2 (7)	N5—C25—C24	122.5 (6)
C5—C4—C9	119.4 (6)	N5—C25—H25A	118.7
C5—C4—N1	119.9 (5)	C24—C25—H25A	118.7
C9—C4—N1	120.5 (6)	Cl1M—C1M—Cl2M	110.3 (5)
C6—C5—C4	119.7 (7)	Cl1M—C1M—H1MA	109.6
C6—C5—H5A	120.1	Cl2M—C1M—H1MA	109.6
C4—C5—H5A	120.1	Cl1M—C1M—H1MB	109.6
C5—C6—C7	120.9 (7)	Cl2M—C1M—H1MB	109.6
C5—C6—H6A	119.6	H1MA—C1M—H1MB	108.1
C7—C6—H6A	119.6		

Fig. 1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