Ruthenium Trispyrazolylborate Complexes. 18. Aminocarbene Ruthenium Complexes derived from Terminal Alkynes and 2-Amino-pyridines

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Supporting Information

Table S1. Crystal data and structure refinement for [RuTp(=CC_6H_9mapy)Cl·$O(C_2H_5)_2$ (**3c**·$O(C_2H_5)_2$).

Empirical formula	C27 H38 B Cl N8 O Ru
Formula weight	637.98
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1 (no. 2)
Unit cell dimensions	a = 11.1834(14) Å α = 112.451(2) deg.
	b = 11.2476(15) Å β = 95.864(2) deg.
	c = 13.0811(17) Å γ = 101.221(2) deg.
Volume	1463.1(3) $Å^3$
Z, Calculated density	2, 1.448 Mg/m^3
Absorption coefficient	0.663 mm^{-1}
F(000)	660
Crystal size	0.60 x 0.40 x 0.30 mm, redbrown prism
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 8 sec. per frame full sphere data collection, 4 x 606 frames
Theta range for data collection	2.03 to 30.00 deg.
Index ranges	-15<=h<=15, -15<=k<=15, -18<=l<=18
Reflections collected / unique	21100 / 8259 [R(int) = 0.0141]
Completeness to theta = 30.00	96.8%
Absorption correction	Semi-empirical from equivalents (prg. SADABS)
Max. and min. rel. transmission	1.00 and 0.92
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	8259 / 0 / 353
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0725
R indices (all data)	R1 = 0.0294, wR2 = 0.0743
Largest diff. peak and hole	1.143 and -0.618 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{½}$

Table S2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [$RuTp(=CC_6H_9mapy)Cl \cdot O(C_2H_5)_2$ (**3c**$\cdot O(C_2H_5)_2$). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	38842(1)	20783(1)	29402(1)	15(1)
Cl	57365(3)	34275(4)	27253(3)	21(1)
N(1)	34428(13)	-5912(13)	8910(11)	20(1)
N(2)	43711(12)	3364(13)	17433(11)	19(1)
N(3)	20913(12)	8881(13)	7446(11)	20(1)
N(4)	28612(12)	20492(13)	15179(11)	18(1)
N(5)	17435(12)	-3144(13)	19913(12)	21(1)
N(6)	24120(12)	6972(13)	29688(11)	19(1)
N(7)	48494(12)	21883(13)	44128(11)	17(1)
N(8)	39468(12)	39084(13)	51149(11)	18(1)
B	21077(16)	-4314(17)	8524(15)	21(1)
C(1)	54171(15)	-377(16)	15432(14)	23(1)
C(2)	51770(17)	-12092(17)	5675(15)	27(1)
C(3)	39180(17)	-15219(16)	1751(14)	25(1)
C(4)	27535(15)	29816(16)	11422(13)	22(1)
C(5)	18937(16)	24350(18)	1262(14)	26(1)
C(6)	14997(16)	11032(18)	-955(14)	25(1)
C(7)	19320(15)	5225(17)	38120(14)	24(1)
C(8)	9448(16)	-6108(19)	33849(17)	29(1)
C(9)	8532(15)	-11134(17)	22318(16)	26(1)
C(10)	47343(13)	31961(15)	53414(13)	18(1)
C(11)	53147(14)	34658(16)	64291(13)	21(1)
C(12)	60473(15)	26597(17)	65776(14)	24(1)
C(13)	61702(16)	16171(18)	56167(15)	26(1)
C(14)	55653(15)	14084(16)	45653(14)	23(1)
C(15)	66690(20)	28850(20)	77370(17)	36(1)
C(16)	34026(13)	35213(14)	40219(12)	17(1)
C(17)	24328(14)	42643(16)	39136(14)	21(1)
C(18)	11579(15)	35245(16)	39520(14)	23(1)
C(19)	8610(20)	36740(20)	50200(20)	39(1)
C(20)	-4170(20)	30450(30)	50830(20)	53(1)
C(21)	-10830(30)	18900(30)	40610(40)	76(1)
C(22)	-9970(20)	21280(30)	29860(20)	59(1)
C(23)	3095(19)	27050(20)	29310(20)	40(1)
O	15056(17)	35226(19)	79813(17)	51(1)
C(24)	15300(20)	48560(20)	85430(20)	45(1)
C(25)	2550(40)	50430(40)	85890(40)	88(1)
C(26)	26540(30)	32630(40)	77310(30)	69(1)
C(27)	25760(20)	19290(40)	72270(30)	63(1)

Table S3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [RuTp(=CC_6H_9mapy)Cl·$O(C_2H_5)_2$ (**3c**·$O(C_2H_5)_2$).

	x	y	z	U_{eq}
H(8)	3802	4589	5659	22
H(0B)	1521	-1203	209	26
H(1)	6216	431	2003	27
H(2)	5756	-1686	245	32
H(3)	3460	-2266	-487	30
H(4)	3200	3890	1514	26
H(5)	1638	2879	-313	31
H(6)	910	448	-733	29
H(7)	2223	1089	4589	28
H(8)	443	-962	3799	34
H(9)	264	-1890	1696	31
H(11)	5210	4191	7059	25
H(13)	6671	1050	5686	31
H(14)	5656	687	3923	27
H(15A)	7484	2690	7705	54
H(15B)	6153	2299	8004	54
H(15C)	6774	3814	8256	54
H(17A)	2399	4365	3192	25
H(17B)	2671	5165	4536	25
H(19)	1472	4174	5690	47
H(19A)	1432	3339	5367	47
H(19B)	1026	4610	5478	47
H(20A)	-359	2772	5718	63
H(20B)	-906	3718	5252	63
H(21A)	-1968	1655	4113	91
H(21B)	-739	1126	4007	91
H(22A)	-1341	1273	2320	70
H(22B)	-1513	2741	2955	70
H(23)	561	2529	2226	48
H(23A)	273	3219	2492	48
H(23B)	648	1980	2524	48
H(24A)	1950	5366	8153	54
H(24B)	2014	5205	9320	54
H(25A)	303	5985	9025	133
H(25B)	-172	4512	8951	133
H(25C)	-207	4756	7822	133
H(26A)	2931	3682	7225	83
H(26B)	3286	3671	8437	83
H(27A)	3374	1796	7023	94
H(27B)	1924	1513	6545	94
H(27C)	2373	1523	7751	94

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had U_{iso} = U_{eq} x 1.2 (x 1.5 for CH_3) of their carrier atoms. Hydrogen atoms of C(19) and C(23) half occupied and defining either CH or CH_2 groups due to orientation disorder of cyclohexene ring.

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [RuTp(=CC$_6$H$_9$mapy)Cl·O(C$_2$H$_5$)$_2$ (**3c**·O(C$_2$H$_5$)$_2$). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	14(1)	16(1)	15(1)	5(1)	3(1)	5(1)
Cl	20(1)	18(1)	21(1)	4(1)	7(1)	2(1)
N(1)	22(1)	17(1)	18(1)	4(1)	3(1)	4(1)
N(2)	18(1)	18(1)	19(1)	6(1)	3(1)	4(1)
N(3)	19(1)	21(1)	18(1)	7(1)	0(1)	4(1)
N(4)	18(1)	19(1)	17(1)	6(1)	3(1)	5(1)
N(5)	17(1)	20(1)	24(1)	9(1)	2(1)	2(1)
N(6)	17(1)	19(1)	20(1)	9(1)	3(1)	5(1)
N(7)	15(1)	19(1)	19(1)	8(1)	3(1)	4(1)
N(8)	18(1)	18(1)	18(1)	5(1)	3(1)	6(1)
B	20(1)	19(1)	21(1)	6(1)	0(1)	3(1)
C(1)	21(1)	24(1)	26(1)	11(1)	8(1)	8(1)
C(2)	32(1)	24(1)	28(1)	10(1)	14(1)	13(1)
C(3)	34(1)	18(1)	21(1)	6(1)	8(1)	8(1)
C(4)	22(1)	23(1)	22(1)	10(1)	5(1)	8(1)
C(5)	26(1)	30(1)	24(1)	14(1)	2(1)	9(1)
C(6)	22(1)	30(1)	20(1)	10(1)	0(1)	6(1)
C(7)	23(1)	28(1)	27(1)	16(1)	9(1)	9(1)
C(8)	23(1)	32(1)	39(1)	22(1)	10(1)	6(1)
C(9)	18(1)	25(1)	37(1)	17(1)	2(1)	2(1)
C(10)	15(1)	18(1)	19(1)	8(1)	3(1)	3(1)
C(11)	20(1)	24(1)	18(1)	9(1)	2(1)	3(1)
C(12)	21(1)	29(1)	23(1)	15(1)	2(1)	4(1)
C(13)	23(1)	29(1)	29(1)	16(1)	2(1)	10(1)
C(14)	22(1)	24(1)	26(1)	11(1)	5(1)	9(1)
C(15)	39(1)	47(1)	28(1)	20(1)	-1(1)	15(1)
C(16)	15(1)	17(1)	19(1)	8(1)	4(1)	4(1)
C(17)	20(1)	22(1)	23(1)	10(1)	6(1)	8(1)
C(18)	20(1)	24(1)	29(1)	11(1)	7(1)	10(1)
C(19)	32(1)	39(1)	43(1)	10(1)	18(1)	9(1)
C(20)	39(1)	72(2)	63(2)	44(2)	21(1)	10(1)
C(21)	48(2)	53(2)	117(3)	21(2)	43(2)	6(1)
C(22)	24(1)	64(2)	62(2)	5(1)	3(1)	-1(1)
C(23)	23(1)	47(1)	45(1)	18(1)	1(1)	5(1)
O	46(1)	50(1)	60(1)	28(1)	12(1)	4(1)
C(24)	41(1)	31(1)	68(2)	25(1)	21(1)	6(1)
C(25)	107(3)	59(2)	111(3)	37(2)	39(3)	34(2)
C(26)	48(2)	95(3)	94(2)	66(2)	34(2)	20(2)
C(27)	36(1)	112(3)	55(2)	50(2)	18(1)	16(1)

Table S5. Bond lengths [Å] and angles [deg] for [RuTp(=CC_6H_9mapy)Cl·$O(C_2H_5)_2$ (**3c**·$O(C_2H_5)_2$).

Bond distances	
Ru-C(16)	1.9153(15)
Ru-N(6)	2.0462(13)
Ru-N(7)	2.0572(13)
Ru-N(4)	2.0678(13)
Ru-N(2)	2.1983(13)
Ru-Cl	2.4278(4)
N(1)-C(3)	1.351(2)
N(1)-N(2)	1.3648(18)
N(1)-B	1.536(2)
N(2)-C(1)	1.336(2)
N(3)-C(6)	1.349(2)
N(3)-N(4)	1.3585(18)
N(3)-B	1.547(2)
N(4)-C(4)	1.337(2)
N(5)-C(9)	1.353(2)
N(5)-N(6)	1.3604(18)
N(5)-B	1.549(2)
N(6)-C(7)	1.338(2)
N(7)-C(10)	1.3469(19)
N(7)-C(14)	1.3507(19)
N(8)-C(16)	1.3594(19)
N(8)-C(10)	1.3812(19)
C(1)-C(2)	1.395(2)
C(2)-C(3)	1.375(3)
C(4)-C(5)	1.398(2)
C(5)-C(6)	1.381(2)
C(7)-C(8)	1.392(2)
C(8)-C(9)	1.378(3)
C(10)-C(11)	1.394(2)
C(11)-C(12)	1.386(2)
C(12)-C(13)	1.395(3)
C(12)-C(15)	1.507(2)
C(13)-C(14)	1.380(2)
C(16)-C(17)	1.519(2)
C(17)-C(18)	1.521(2)
C(18)-C(23)	1.412(3)
C(18)-C(19)	1.424(3)
C(19)-C(20)	1.492(3)
C(20)-C(21)	1.457(5)
C(21)-C(22)	1.537(5)
C(22)-C(23)	1.500(3)
O-C(24)	1.388(3)
O-C(26)	1.415(4)
C(24)-C(25)	1.486(5)
C(26)-C(27)	1.370(5)

Bond angles	
C(16)-Ru-N(6)	92.46(6)
C(16)-Ru-N(7)	79.68(6)
N(6)-Ru-N(7)	90.96(5)
C(16)-Ru-N(4)	96.93(6)
N(6)-Ru-N(4)	88.69(5)
N(7)-Ru-N(4)	176.57(5)
C(16)-Ru-N(2)	176.26(5)
N(6)-Ru-N(2)	84.14(5)
N(7)-Ru-N(2)	98.79(5)
N(4)-Ru-N(2)	84.57(5)
C(16)-Ru-Cl	96.25(4)
N(6)-Ru-Cl	171.23(4)
N(7)-Ru-Cl	89.61(4)
N(4)-Ru-Cl	91.25(4)
N(2)-Ru-Cl	87.12(4)
C(3)-N(1)-N(2)	109.76(13)
C(3)-N(1)-B	130.69(14)
N(2)-N(1)-B	119.52(12)
C(1)-N(2)-N(1)	106.21(13)
C(1)-N(2)-Ru	136.11(11)
N(1)-N(2)-Ru	117.32(10)
C(6)-N(3)-N(4)	109.71(13)
C(6)-N(3)-B	130.02(14)
N(4)-N(3)-B	119.89(12)
C(4)-N(4)-N(3)	106.62(13)
C(4)-N(4)-Ru	133.70(11)
N(3)-N(4)-Ru	119.68(10)
C(9)-N(5)-N(6)	109.20(14)
C(9)-N(5)-B	130.86(14)
N(6)-N(5)-B	119.86(12)
C(7)-N(6)-N(5)	107.11(13)
C(7)-N(6)-Ru	132.52(12)
N(5)-N(6)-Ru	120.33(10)
C(10)-N(7)-C(14)	117.14(13)
C(10)-N(7)-Ru	113.53(10)
C(14)-N(7)-Ru	129.33(11)
C(16)-N(8)-C(10)	117.68(13)
N(1)-B-N(3)	108.39(13)
N(1)-B-N(5)	107.98(13)
N(3)-B-N(5)	107.73(13)
N(2)-C(1)-C(2)	110.78(15)
C(3)-C(2)-C(1)	104.80(14)
N(1)-C(3)-C(2)	108.44(15)
N(4)-C(4)-C(5)	110.63(15)
C(6)-C(5)-C(4)	104.41(14)
N(3)-C(6)-C(5)	108.63(14)
N(6)-C(7)-C(8)	110.11(16)
C(9)-C(8)-C(7)	105.06(15)
N(5)-C(9)-C(8)	108.51(15)
N(7)-C(10)-N(8)	113.37(13)
N(7)-C(10)-C(11)	123.43(14)
N(8)-C(10)-C(11)	123.15(14)
C(12)-C(11)-C(10)	119.03(15)
C(11)-C(12)-C(13)	117.63(15)
C(11)-C(12)-C(15)	121.20(16)
C(13)-C(12)-C(15)	121.16(16)
C(14)-C(13)-C(12)	120.13(15)
N(7)-C(14)-C(13)	122.63(15)
N(8)-C(16)-C(17)	111.94(13)
N(8)-C(16)-Ru	115.59(10)
C(17)-C(16)-Ru	132.24(11)
C(16)-C(17)-C(18)	110.90(13)
C(23)-C(18)-C(19)	122.07(18)
C(23)-C(18)-C(17)	119.17(16)
C(19)-C(18)-C(17)	118.76(16)
C(18)-C(19)-C(20)	119.6(2)
C(21)-C(20)-C(19)	114.5(2)
C(20)-C(21)-C(22)	112.8(2)
C(23)-C(22)-C(21)	112.8(2)
C(18)-C(23)-C(22)	118.4(2)
C(24)-O-C(26)	115.4(2)
O-C(24)-C(25)	111.3(2)
C(27)-C(26)-O	112.3(3)

Hydrogen-bond	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(8)-H(8)...Cl#1	0.88	2.33	3.1627(14)	157.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table S6. Crystal data and structure refinement for $[RuTp(\mu\text{-mapy})Cl]_2 \cdot 2O(C_2H_5)_2$ (**5b**$\cdot 2O(C_2H_5)_2$).

Empirical formula	C38 H56 B2 Cl2 N16 O2 Ru2
Formula weight	1063.64
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbca (no. 61)
Unit cell dimensions	a = 15.674(4) Å α = 90 deg.
	b = 16.711(4) Å β = 90 deg.
	c = 17.955(4) Å γ = 90 deg.
Volume	4702.9(19) $Å^3$
Z, Calculated density	4, 1.502 Mg/m^3
Absorption coefficient	0.808 mm^{-1}
F(000)	2176
Crystal size	0.50 x 0.30 x 0.25 mm, yellow prism
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / $\Delta\omega$ = 0.3° / 20 sec. per frame full sphere data collection, 4 x 606 frames
Theta range for data collection	2.11 to 30.00 deg.
Index ranges	-21<=h<=21, -23<=k<=23, -24<=l<=24
Reflections collected / unique	73636 / 6701 [R(int) = 0.0726]
Completeness to theta = 30.00	97.8%
Absorption correction	Semi-empirical from equivalents (prg. SADABS)
Max. and min. rel. transmission	1.00 and 0.86
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	6701 / 4 / 291
Goodness-of-fit on F^2	1.093
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0846 (4586 data)
R indices (all data)	R1 = 0.0701, wR2 = 0.1041 (6701 data)
Extinction coefficient	0.00003(6)
Largest diff. peak and hole	1.262 and -1.125 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{½}$

Note: Compound is a stoichiometric diethylether solvate. The Ru complex forms also a dichloromethane / diethylether solvate of monoclinic symmetry, space group C2/c.

Table S7. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[RuTp(\mu\text{-mapy})Cl]_2 \cdot 2O(C_2H_5)_2$ (**5b**$\cdot 2O(C_2H_5)_2$). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	37698(1)	55329(1)	54824(1)	19(1)
Cl	37573(5)	40878(4)	57288(4)	26(1)
N(1)	19980(16)	61314(16)	55649(16)	28(1)
N(2)	24869(16)	55266(16)	52805(14)	25(1)
N(3)	28215(18)	62431(18)	67422(16)	32(1)
N(4)	34200(16)	56768(16)	65861(14)	27(1)
N(5)	31277(16)	71847(16)	56909(16)	27(1)
N(6)	37767(15)	67570(15)	53785(14)	22(1)
N(7)	39429(15)	54545(14)	43093(14)	20(1)
N(8)	48619(16)	43230(15)	43024(15)	22(1)
B	24130(20)	67380(20)	61120(20)	31(1)
C(1)	19740(20)	50710(20)	48670(18)	29(1)
C(2)	11450(20)	53870(20)	48730(20)	36(1)
C(3)	11890(20)	60480(20)	53200(20)	34(1)
C(4)	35640(20)	52710(20)	72206(19)	35(1)
C(5)	30630(30)	55870(30)	77870(20)	47(1)
C(6)	26010(30)	61930(30)	74690(20)	43(1)
C(7)	42990(20)	72818(19)	50520(18)	28(1)
C(8)	39860(20)	80610(20)	51500(20)	38(1)
C(9)	32430(20)	79720(20)	55500(20)	34(1)
C(10)	43757(18)	48964(17)	39053(16)	21(1)
C(11)	43550(20)	48540(19)	31304(17)	26(1)
C(12)	38890(20)	54050(20)	27157(18)	29(1)
C(13)	34610(20)	59910(20)	31218(19)	31(1)
C(14)	35000(20)	59961(19)	38853(18)	26(1)
C(15)	38370(30)	53520(20)	18824(19)	42(1)
O	44450(30)	28460(20)	32340(20)	89(2)
C(16)	51020(80)	25610(60)	27360(50)	191(6)
C(17)	50660(40)	27900(50)	20360(30)	93(2)
C(18)	39140(40)	22640(30)	35200(30)	70(2)
C(19)	33050(30)	26390(30)	40810(30)	64(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [RuTp(μ-mapy)Cl]$_2$·2O(C_2H_5)$_2$ (**5b**·2O(C_2H_5)$_2$).

	x	y	z	U_{eq}
H(8NB)	4810(20)	3871(17)	4084(19)	26
H(8NA)	4600(20)	4260(20)	4715(16)	26
H(0B)	1954(17)	7137(15)	6318(8)	37
H(1)	2144	4603	4607	35
H(2)	658	5185	4621	43
H(3)	726	6392	5439	41
H(4)	3949	4836	7273	41
H(5)	3044	5418	8292	57
H(6)	2195	6521	7716	52
H(7)	4807	7147	4792	33
H(8)	4233	8546	4977	45
H(9)	2873	8392	5701	41
H(11)	4664	4444	2882	31
H(13)	3141	6389	2869	37
H(14)	3198	6406	4139	31
H(15A)	3241	5412	1725	63
H(15B)	4052	4830	1719	63
H(15C)	4182	5778	1660	63
H(16A)	5661	2731	2939	229
H(16B)	5092	1968	2745	229
H(17A)	5559	2575	1766	140
H(17B)	5074	3375	2012	140
H(17C)	4539	2589	1810	140
H(18A)	4258	1843	3767	84
H(18B)	3585	2012	3112	84
H(19A)	2933	2224	4288	96
H(19B)	2957	3046	3832	96
H(19C)	3634	2888	4483	96

Hydrogen atoms H(8NA), H(8NB), and H(0B) refined in x,y,z. All other H atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had U_{iso} = U_{eq} x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[RuTp(\mu\text{-mapy})Cl]_2 \cdot 2O(C_2H_5)_2$ (**5b**$\cdot 2O(C_2H_5)_2$). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	18(1)	21(1)	18(1)	0(1)	2(1)	0(1)
Cl	29(1)	24(1)	27(1)	3(1)	3(1)	-4(1)
N(1)	20(1)	32(1)	32(1)	1(1)	3(1)	1(1)
N(2)	21(1)	29(1)	24(1)	2(1)	2(1)	0(1)
N(3)	29(1)	42(2)	24(1)	-6(1)	9(1)	0(1)
N(4)	23(1)	37(2)	21(1)	-2(1)	3(1)	-1(1)
N(5)	23(1)	26(1)	32(1)	-5(1)	4(1)	4(1)
N(6)	18(1)	24(1)	24(1)	-5(1)	3(1)	4(1)
N(7)	19(1)	20(1)	21(1)	2(1)	-4(1)	-1(1)
N(8)	22(1)	21(1)	22(1)	-1(1)	2(1)	1(1)
B	24(2)	35(2)	34(2)	-4(2)	8(1)	4(2)
C(1)	27(2)	34(2)	26(2)	3(1)	-1(1)	-5(1)
C(2)	25(2)	45(2)	37(2)	7(2)	-6(1)	-6(1)
C(3)	18(1)	42(2)	43(2)	10(2)	3(1)	3(1)
C(4)	35(2)	45(2)	24(2)	4(1)	1(1)	-6(2)
C(5)	49(2)	71(3)	22(2)	3(2)	6(2)	-6(2)
C(6)	40(2)	64(3)	26(2)	-12(2)	12(2)	-3(2)
C(7)	24(1)	24(2)	35(2)	2(1)	2(1)	1(1)
C(8)	33(2)	23(2)	57(2)	2(2)	1(2)	-1(1)
C(9)	30(2)	24(2)	48(2)	-6(2)	0(2)	6(1)
C(10)	20(1)	21(1)	22(1)	0(1)	-1(1)	-2(1)
C(11)	27(1)	27(2)	24(2)	-5(1)	1(1)	-2(1)
C(12)	34(2)	34(2)	19(1)	1(1)	-1(1)	-5(1)
C(13)	35(2)	31(2)	27(2)	5(1)	-5(1)	4(1)
C(14)	27(1)	24(2)	26(2)	1(1)	-1(1)	4(1)
C(15)	59(2)	45(2)	22(2)	0(1)	-5(2)	-1(2)
O	132(4)	55(2)	78(3)	27(2)	61(3)	40(2)
C(16)	271(13)	203(10)	99(6)	64(7)	100(8)	191(10)
C(17)	98(5)	127(6)	55(3)	6(4)	14(3)	60(4)
C(18)	95(4)	43(3)	73(3)	-2(2)	-22(3)	-2(3)
C(19)	66(3)	75(3)	49(3)	15(2)	-9(2)	-17(3)

Table S10. Bond lengths [Å] and angles [deg] for $[RuTp(\mu\text{-mapy})Cl]_2 \cdot 2O(C_2H_5)_2$ (**5b**$\cdot 2O(C_2H_5)_2$).

Bond distances

Ru-N(2)	2.043(3)
Ru-N(6)	2.054(3)
Ru-N(4)	2.070(3)
Ru-N(7)	2.128(3)
Ru-N(8)#1	2.192(3)
Ru-Cl	2.455(1)
N(1)-C(3)	1.350(4)
N(1)-N(2)	1.367(4)
N(1)-B	1.555(5)
N(2)-C(1)	1.333(4)
N(3)-C(6)	1.353(4)
N(3)-N(4)	1.362(4)
N(3)-B	1.540(5)
N(4)-C(4)	1.344(4)
N(5)-C(9)	1.352(4)
N(5)-N(6)	1.364(3)
N(5)-B	1.544(5)
N(6)-C(7)	1.335(4)
N(7)-C(10)	1.362(4)
N(7)-C(14)	1.371(4)
N(8)-C(10)	1.417(4)
N(8)-Ru#1	2.192(3)
B-H(0B)	1.05(4)
C(1)-C(2)	1.402(5)
C(2)-C(3)	1.368(6)
C(4)-C(5)	1.389(5)
C(5)-C(6)	1.368(6)
C(7)-C(8)	1.403(5)
C(8)-C(9)	1.376(5)
C(10)-C(11)	1.393(4)
C(11)-C(12)	1.393(5)
C(12)-C(13)	1.391(5)
C(12)-C(15)	1.501(5)
C(13)-C(14)	1.372(5)
O-C(18)	1.380(6)
O-C(16)	1.446(7)
C(16)-C(17)	1.314(9)
C(18)-C(19)	1.521(8)

Bond angles

N(2)-Ru-N(6)	89.67(10)
N(2)-Ru-N(4)	84.82(10)
N(6)-Ru-N(4)	88.43(10)
N(2)-Ru-N(7)	87.11(9)
N(6)-Ru-N(7)	88.33(9)
N(4)-Ru-N(7)	171.32(9)
N(2)-Ru-N(8)#1	173.99(10)
N(6)-Ru-N(8)#1	84.35(9)
N(4)-Ru-N(8)#1	94.45(10)
N(7)-Ru-N(8)#1	93.24(9)
N(2)-Ru-Cl	91.09(8)
N(6)-Ru-Cl	174.82(7)
N(4)-Ru-Cl	86.54(8)
N(7)-Ru-Cl	96.83(7)
N(8)#1-Ru-Cl	94.82(7)
C(3)-N(1)-N(2)	109.2(3)
C(3)-N(1)-B	131.8(3)
N(2)-N(1)-B	118.9(2)
C(1)-N(2)-N(1)	107.0(3)
C(1)-N(2)-Ru	134.1(2)
N(1)-N(2)-Ru	118.8(2)
C(6)-N(3)-N(4)	109.4(3)
C(6)-N(3)-B	129.5(3)
N(4)-N(3)-B	120.5(3)
C(4)-N(4)-N(3)	106.9(3)
C(4)-N(4)-Ru	135.1(2)
N(3)-N(4)-Ru	117.4(2)
C(9)-N(5)-N(6)	109.5(3)
C(9)-N(5)-B	131.3(3)
N(6)-N(5)-B	119.3(3)
C(7)-N(6)-N(5)	107.1(2)
C(7)-N(6)-Ru	134.2(2)
N(5)-N(6)-Ru	118.72(19)
C(10)-N(7)-C(14)	114.1(3)
C(10)-N(7)-Ru	129.25(19)
C(14)-N(7)-Ru	116.4(2)
C(10)-N(8)-Ru#1	122.73(19)
N(3)-B-N(5)	108.6(3)
N(3)-B-N(1)	106.8(3)
N(5)-B-N(1)	108.0(3)
N(3)-B-H(0B)	111.6(4)
N(5)-B-H(0B)	111.3(4)
N(1)-B-H(0B)	110.5(3)
N(2)-C(1)-C(2)	109.8(3)
C(3)-C(2)-C(1)	105.2(3)
N(1)-C(3)-C(2)	108.7(3)
N(4)-C(4)-C(5)	109.5(3)
C(6)-C(5)-C(4)	105.9(3)
N(3)-C(6)-C(5)	108.3(3)
N(6)-C(7)-C(8)	109.9(3)
C(9)-C(8)-C(7)	105.1(3)
N(5)-C(9)-C(8)	108.4(3)
N(7)-C(10)-C(11)	123.7(3)
N(7)-C(10)-N(8)	117.6(3)
C(11)-C(10)-N(8)	118.7(3)
C(12)-C(11)-C(10)	120.8(3)
C(13)-C(12)-C(11)	116.0(3)
C(13)-C(12)-C(15)	122.6(3)
C(11)-C(12)-C(15)	121.5(3)
C(14)-C(13)-C(12)	120.4(3)
N(7)-C(14)-C(13)	124.9(3)
C(18)-O-C(16)	115.3(6)
C(17)-C(16)-O	117.7(6)
O-C(18)-C(19)	109.5(4)

Hydrogen-bonds [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(8)-H(8NA)...Cl	0.86(2)	2.27(3)	3.116(3)	173(3)
N(8)-H(8NB)...O	0.86(2)	2.36(3)	3.193(5)	163(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1