Supporting Information

A pH-controlled recyclable indolinooxazolidine tagged N-heterocyclic carbene Ru catalyst for olefin metathesis

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Table of contents

1. General techniques

Unless otherwise noted, all reactions were performed under an atmosphere of dry N_2 with oven-dried glassware and anhydrous solvents. Toluene was distilled from sodium/benzophenone under a N_2 atmosphere. CH_2Cl_2 was dried over CaH_2, and distilled prior to use. All other solvents were dried over 4-8 Å mesh molecular sieves (Aldrich) and were either saturated with dry argon or degassed before use. Reactions were monitored by analytical thin layer chromatography on 0.20 mm Yantai Huagong silica gel plates. Silica gel (200-300 mesh) (from Yantai Huagong Company.) was used for flash chromatography. Dienes[1-8] were synthesized and purified according to the literature procedures. Grubbs catalyst II was prepared according literature method[9]. Ligand **9** was prepared according to a literature method[10]. All other chemicals or reagents were obtained from commercial sources.

^{1}H-NMR and ^{13}C-NMR spectra were acquired in $CDCl_3$ on Varian 200 and Varian 400 spectrometers. If not otherwise noted, chemical shift values of are reported as values in ppm relative to residual $CHCl_3$ (J=7.26) for ^{1}H-NMR spectra, relative to $CDCl_3$ (77.16 ppm) for ^{13}C-NMR spectra. Multiplicities are described using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiple, br = broad. Coupling constants (J) are quoted in Hz. at 400 MHz for ^{1}H. Gas chromatography-mass spectroscopy (GC-MS) analyses were performed on a Thermo Exactive Orbitrap apparatus.

2. Absorption Spectrum of Complex 10 and 10a

In order to compare the UV absorption of the catalysts **10**, **10a** and recovery **10** under the same external conditions, dichloromethane (CH_2Cl_2) was selected as the solvent for the experiment. First, catalyst **10** (1 x 10^{-3} mmol) was dissolved in 5 mL CH_2Cl_2 (c =2.0 x 10^{-4} M). The absorption spectrum of the resulting solution was then measured and the results are shown in Figure 2 (solid line). Next, HCl (2 x 10^{-3} mmol) were added and the solution was shaken by hand, at which complex **10a** was formed. The absorption spectrum of the resulting solution was then measured and the results are shown in Figure 2 (short dashed line). Finally, the pH of the above solution was adjusted to 7.0 with Et_3N and tested immediately. The absorption spectrum of that solution is shown in Figure 2 (long dashed line).

3. Monitoring the Transformation of Ruthenium Carbene Complex 10 by UV-vis Spectroscopy

We only tested the UV-vis of the upper solution containing the original catalyst for monitoring the transformation of complex **10**. First, the original complex **10** (1 x 10^{-3} mmol) was dispensed into a bi-phase system containing a mixture of 5 mL cyclohexane with three drops of dichloromethane and 5 mL of glycol, HCl (2 equivalents) was added the bi-phase system to transfer the original catalyst **10** from the upper solvent to the lower solvent, then, triethylamine (2 equivalents) was added with aiming to return the complex **10a** to the upper non-polar solvent, again, and to measure UV absorption of the recovered **10**. Repeated the above steps for five times the results were shown in Figure 4.

4. General procedure for the catalytic activities for the RCM and CM reaction

The N-protected substrate **13** (0.1 M), catalyst **10** (1 mol%), a mount of CH_2Cl_2 was introduced to a Schlenk tube and stirred at 40^{o}C until the reaction was completed. The volatiles were evaporated. The conversion was determined by ^{1}H NMR and we got the yield after the product was purified. The method for N-protected substrates (**15**, **19, 21** and **27**)(0.1 M), **17** (1M), the oxygen-containing substrates (**23** and **25**)(0.1 M), the diethyldiallylmalonate (0.1 M) **11** and substrate of CM reaction **29**(0.1 M) and **30**(0.2 M) were deal with the same as substrate **13.** The both the amount of substrate and the amount of catalyst are reference Table 2.

5. Separated catalyst after catalytic reaction

In the process of recovering the catalyst, it is worthy to note that the cyclohexane (with three drops of CH_2Cl_2) cannot completely extract the product. In order to extract completely, an equal volume of toluene was added after separation of part of the product in cyclohexane. After the two parts of the product were combined, the residual amount of ruthenium was tested. The other should follow the steps of the text. The result was shown in Figure 5.

6. Kinetic Study of 10

Under a nitrogen atmosphere, the solution of catalyst **10** (8.75mg, 0.01 mmol, 5 ml) in dichloromethane was added to the substrate **11** (240mg, 1.0 mmol, 5 ml) in dichloromethane at 30°C. During the course of the reaction, 1 ml of the solution was taken at an appropriate time using a syringe and immediately passed through a chromatographic silica gel column using dichloromethane as eluent. The solvent was then evaporated under vacuum. The conversion ratio for **12** was determined by comparing the ratio of the integrals of the methylene protons in the starting material **11**. The results are shown in Figure. S1.

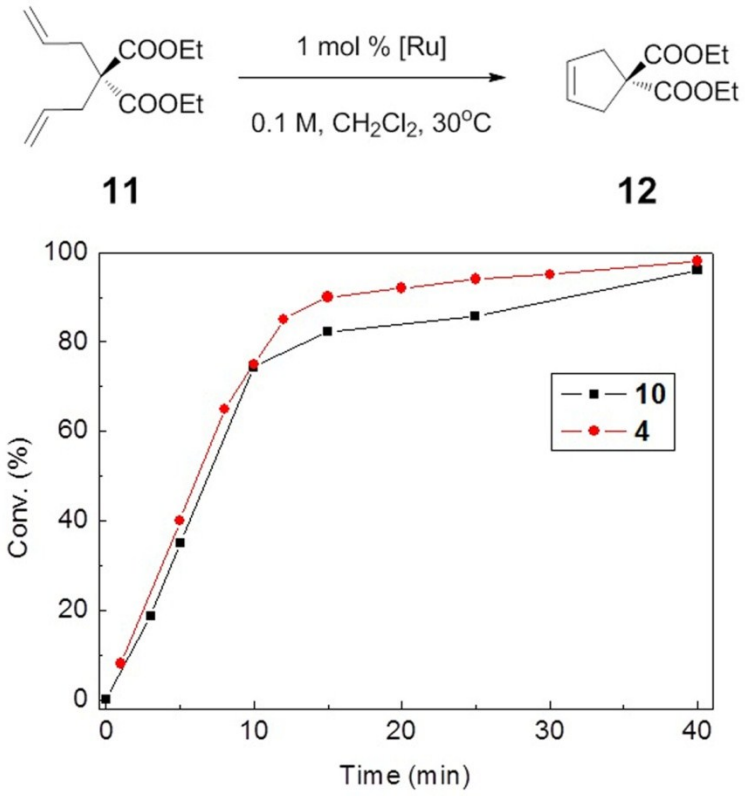


Figure. S1 Relative conversion rates of **10** and **4** at the same condition

7. Kinetics study of recycled catalyst

The catalytic activity and the initiation rate of the original catalyst **10** and the recovered catalyst **10** were compared at 18°C. After the recovery of the catalyst followed the conditions in manuscript (the recovery process was shown in Fig.5), the recovered catalyst **10** was further purified and weighed, followed by the kinetic study. The conversion monitored by ^{1}H NMR (Figure. S2).

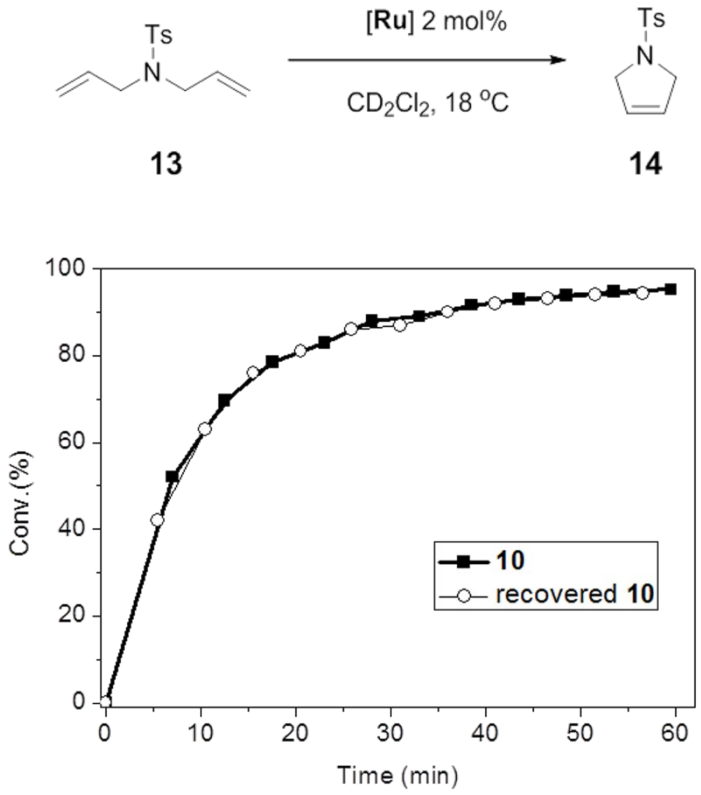


Figure. S2 Kinetic study for the RCM of **13** in a CD_2Cl_2 (0.1M) at 18°C with complex **10** and the recovered catalyst **10**. Conversion monitored by ^1H NMR

8. NMR-spectra of compounds of 9 and 10

Figure S3: ^{1}H NMR spectrum of compound **10** in $CDCl_3$

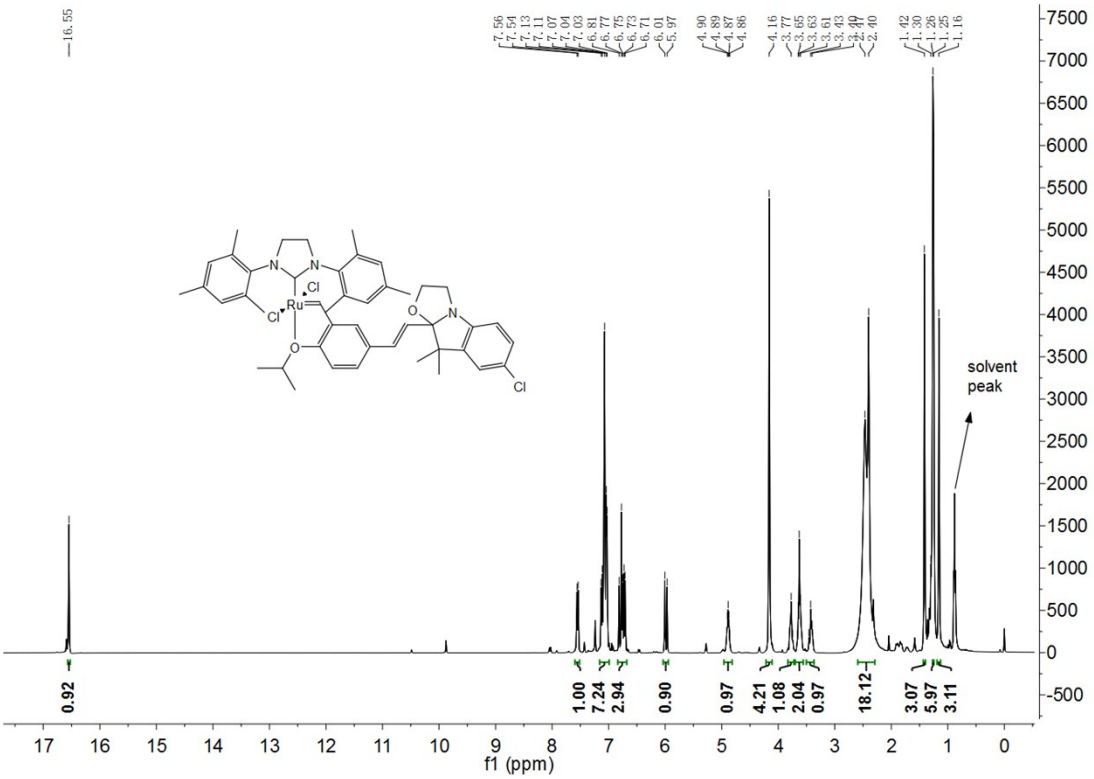


Figure S4: ^{13}C NMR spectrum of compound **10** in $CDCl_3$

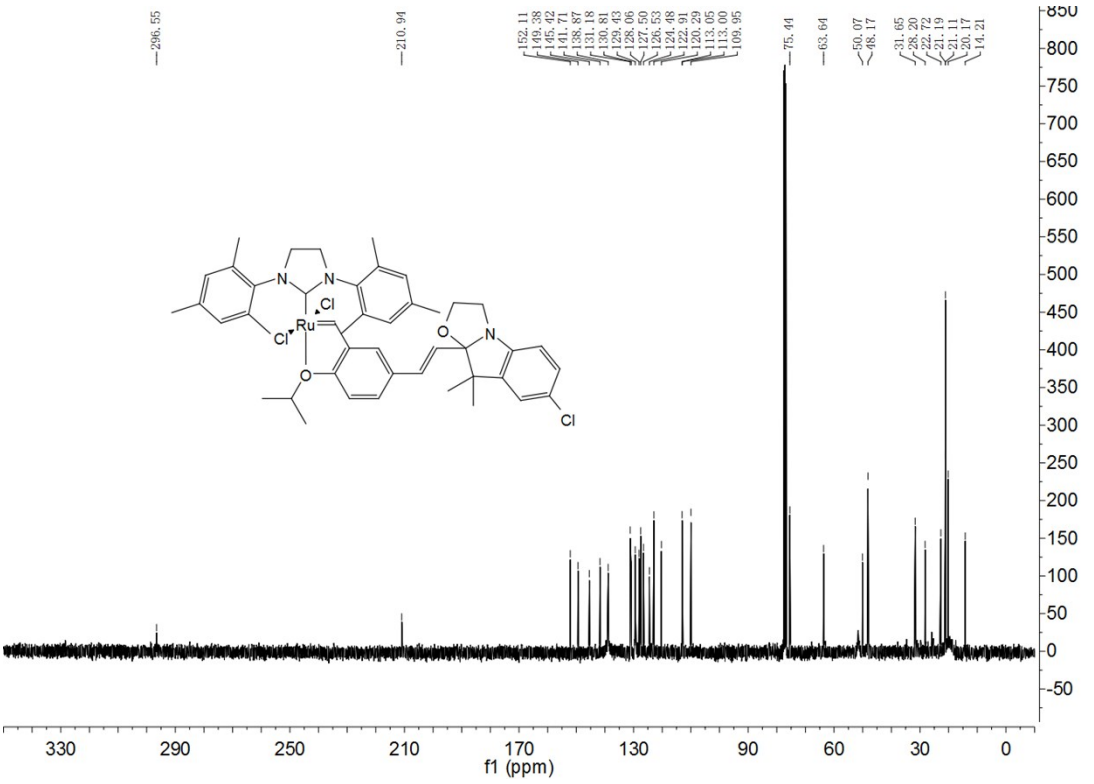


Figure S5: ^{1}H NMR spectrum of compound **10a** in $CDCl_3$

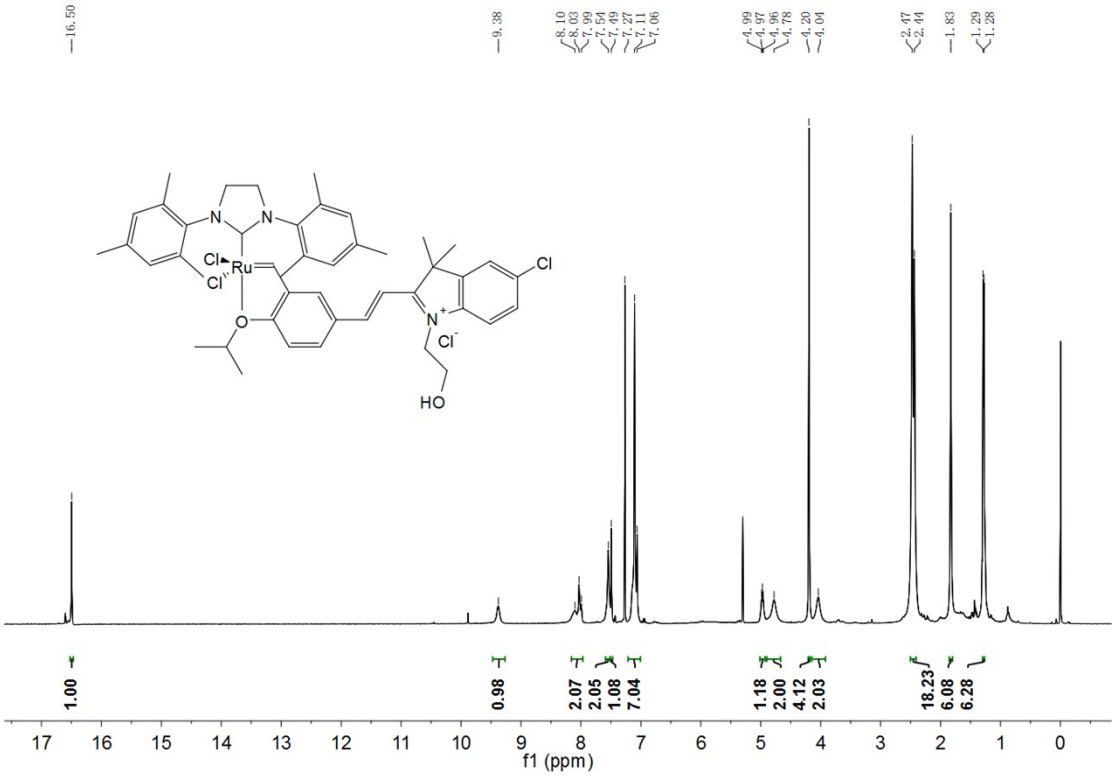


Figure S6: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

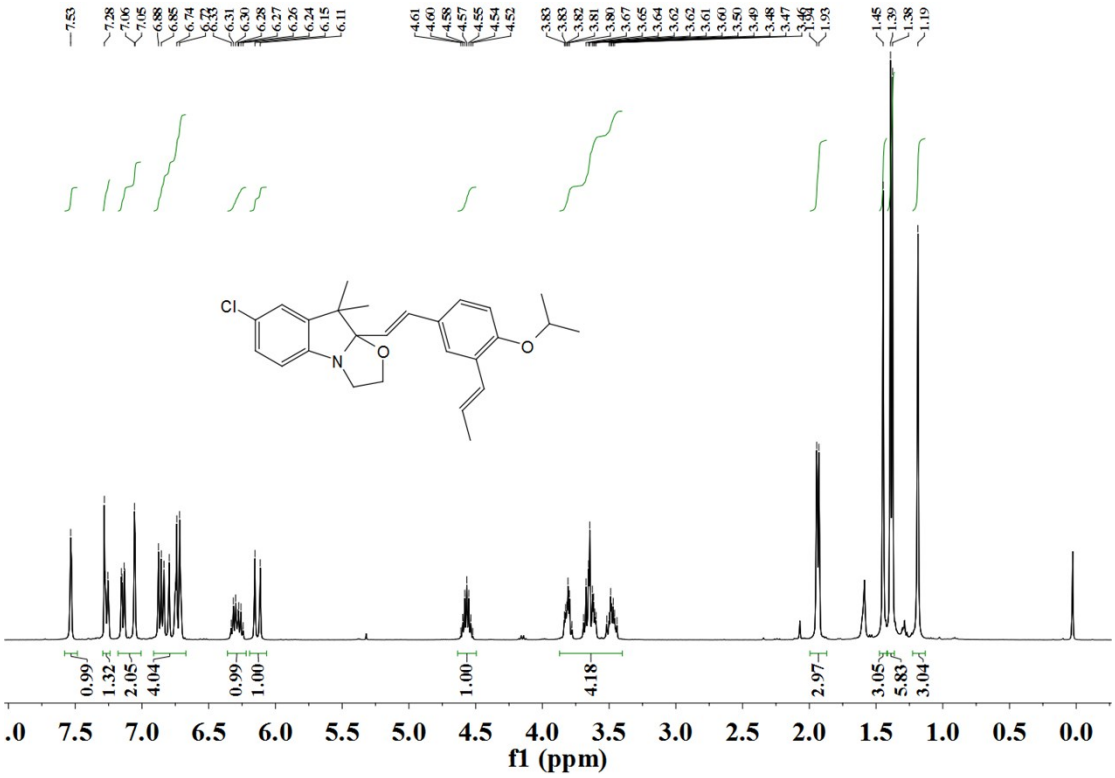


Figure S7: ^{13}C NMR spectrum of compound **9** in $CDCl_3$

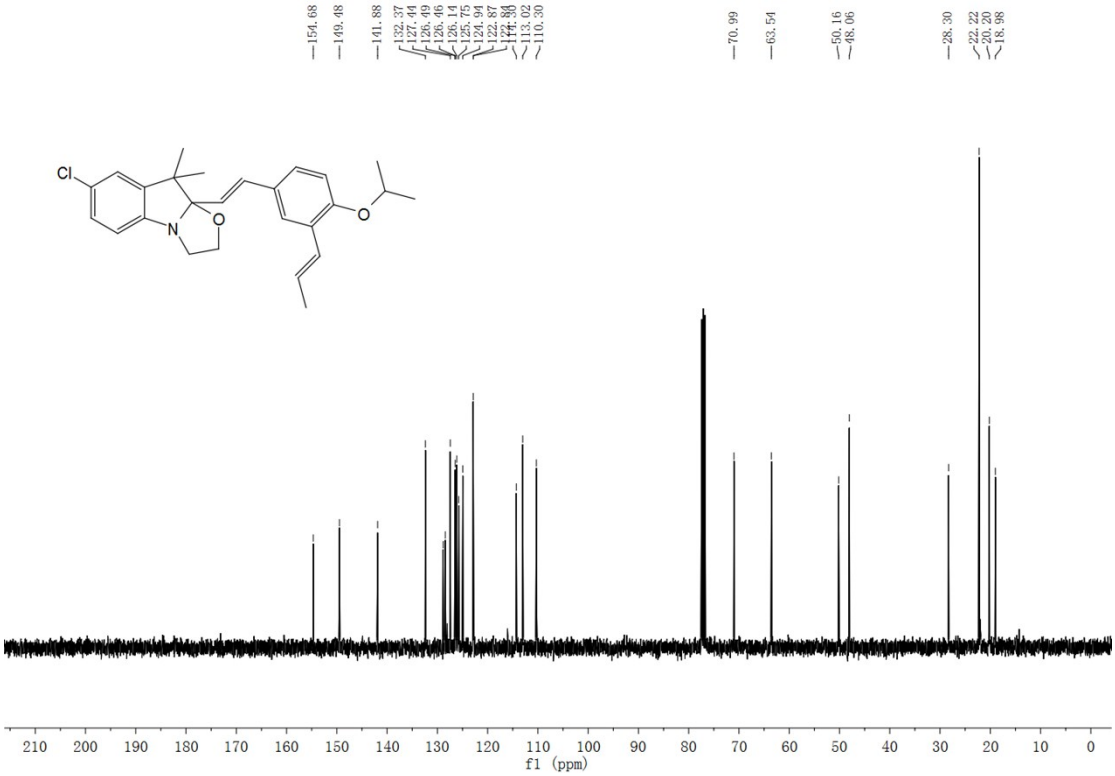


Figure S8: ^{1}H NMR spectrum of compound **7** in D_2O

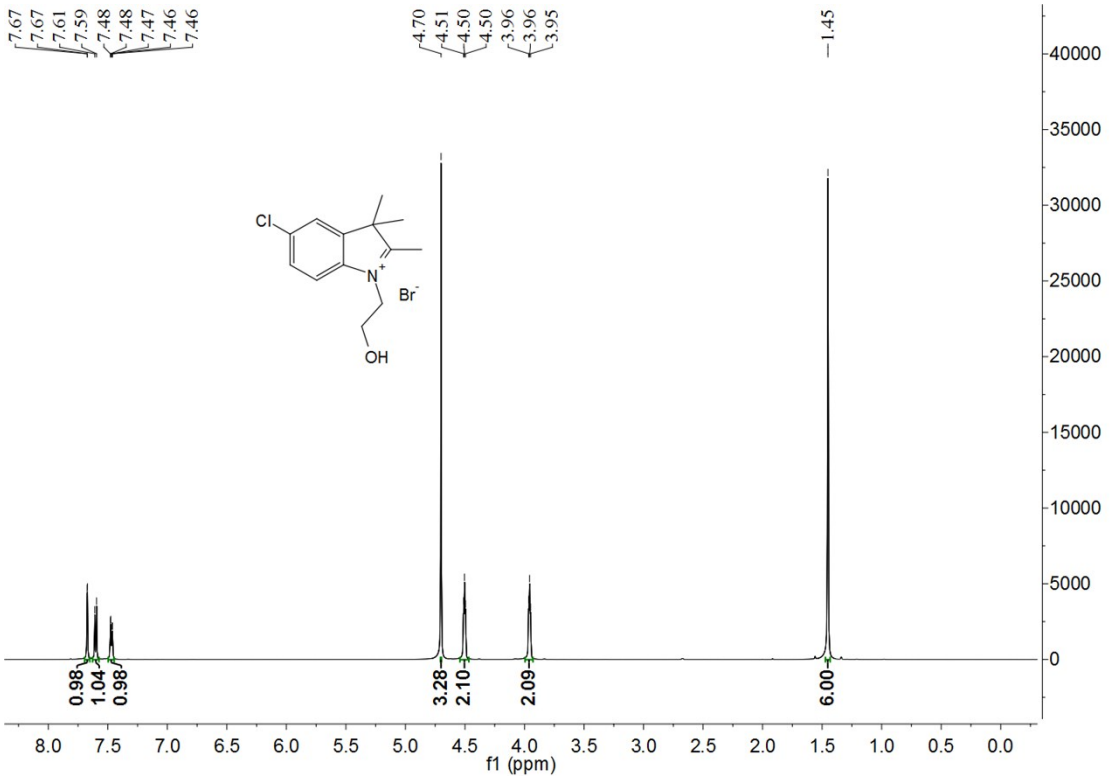
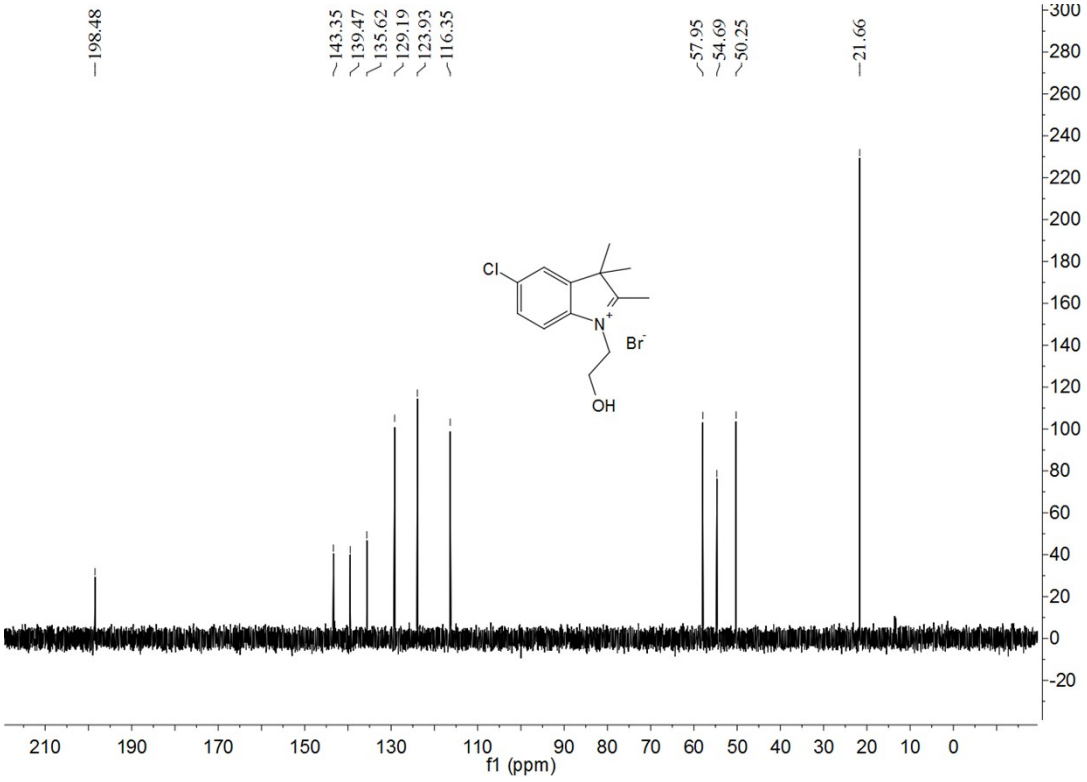


Figure S9: ^{13}C NMR spectrum of compound **7** in D_2O



9. Crystallographic details for 9 (160330A, CCDC: 1506987) and 10 (N151221A, CCDC: 1458091)

Figure S10: Crystal structure of **9**

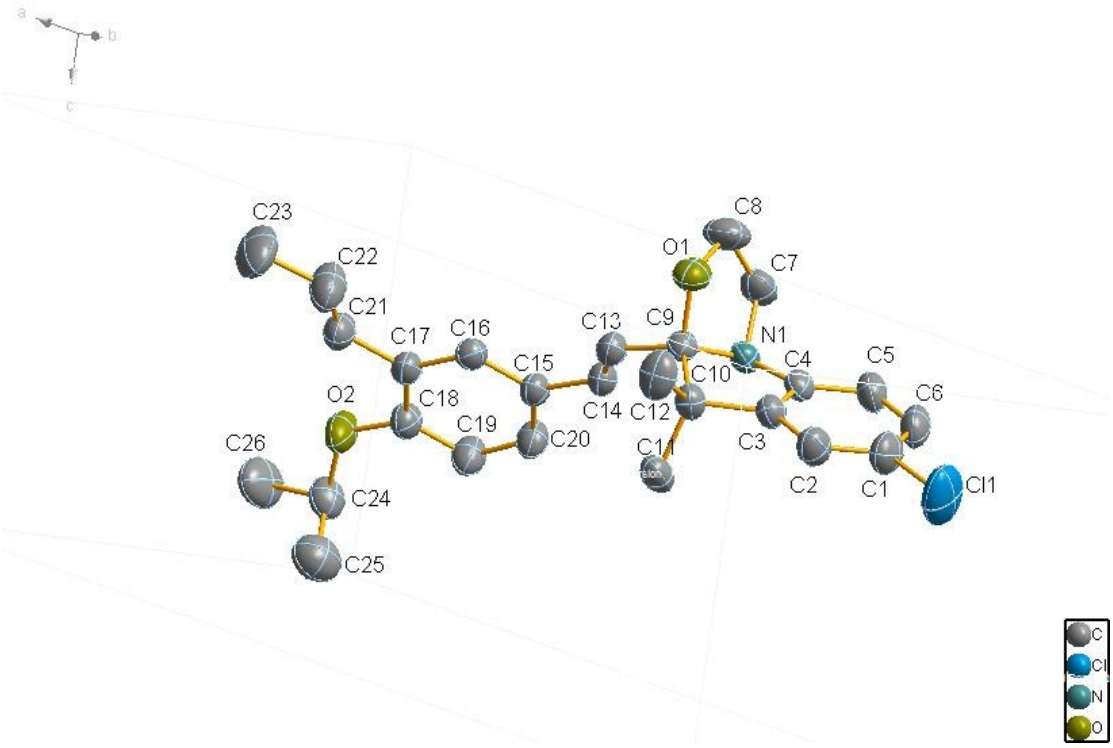


Table 1. Crystal data and structure refinement for **9**

Identification code	160330a
Empirical formula	C26 H30 Cl N O2
Formula weight	423.96
Temperature	294(2) K
Wavelength	0.71073 A
Crystal system, space group	MONOCLINIC, P2(1)/c
Unit cell dimensions	a = 17.3687(19) A alpha = 90 deg.
b = 17.0036(16) A beta = 100.326(6) deg.	
c = 8.0980(9) A gamma = 90 deg.	
Volume	2352.9(4) A^3
Z, Calculated density	4, 1.197 Mg/m^3
Absorption coefficient	0.184 mm^-1
F(000)	904
Crystal size	0.40 x 0.23 x 0.16 mm
Theta range for data collection	3.24 to 27.46 deg.
Limiting indices	-22<=h<=22, -21<=k<=22, -10<=l<=10
Reflections collected / unique	24316 / 5367 [R(int) = 0.0503]

Completeness to theta = 27.46	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9712 and 0.9302
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5367 / 0 / 276
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0565, wR2 = 0.1462
R indices (all data)	R1 = 0.0674, wR2 = 0.1536
Largest diff. peak and hole	0.220 and -0.339 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**.

	x	y	z	U(eq)
C(1)	1517(1)	6193(2)	2157(3)	61(1)
C(2)	2130(1)	5658(1)	2468(3)	54(1)
C(3)	2845(1)	5881(1)	2089(2)	40(1)
C(4)	2945(1)	6627(1)	1449(2)	39(1)
C(5)	2326(1)	7158(1)	1136(3)	50(1)
C(6)	1605(1)	6929(1)	1497(3)	59(1)
C(7)	3874(1)	7097(1)	-292(2)	53(1)
C(8)	3971(2)	6389(2)	-1379(3)	71(1)
C(9)	4103(1)	5971(1)	1369(2)	37(1)
C(10)	3624(1)	5454(1)	2417(2)	41(1)
C(11)	3953(1)	5529(1)	4310(2)	54(1)
C(12)	3594(1)	4589(1)	1893(3)	64(1)
C(13)	4976(1)	5985(1)	2007(2)	41(1)
C(14)	5358(1)	6571(1)	2863(2)	41(1)
C(15)	6194(1)	6601(1)	3653(2)	39(1)
C(16)	6753(1)	6075(1)	3259(2)	40(1)
C(17)	7530(1)	6082(1)	4093(2)	41(1)
C(18)	7748(1)	6636(1)	5387(2)	45(1)
C(19)	7206(1)	7168(1)	5779(3)	53(1)
C(20)	6441(1)	7153(1)	4909(2)	48(1)
C(21)	8118(1)	5523(1)	3688(3)	53(1)
C(22)	8022(2)	4945(2)	2673(4)	81(1)
C(23)	8659(2)	4392(2)	2334(4)	103(1)
C(24)	8769(1)	6949(1)	7807(3)	57(1)
C(25)	8517(2)	6447(2)	9109(4)	83(1)
C(26)	9650(1)	7017(2)	8012(4)	92(1)
Cl(1)	601(1)	5912(1)	2573(1)	105(1)
N(1)	3737(1)	6754(1)	1294(2)	37(1)
O(1)	3959(1)	5706(1)	-362(2)	51(1)
O(2)	8522(1)	6620(1)	6148(2)	65(1)

Table 3. Bond lengths [A] and angles [deg] for **9**.

C(1)-C(6)	1.380(3)	C(13)-H(13)	0.9300
C(1)-C(2)	1.388(3)	C(14)-C(15)	1.478(2)
C(1)-Cl(1)	1.751(2)	C(14)-H(14)	0.9300
C(2)-C(3)	1.384(3)	C(15)-C(20)	1.394(2)
C(2)-H(2)	0.9300	C(15)-C(16)	1.399(2)
C(3)-C(4)	1.393(2)	C(16)-C(17)	1.397(2)
C(3)-C(10)	1.517(2)	C(16)-H(16)	0.9300
C(4)-C(5)	1.393(2)	C(17)-C(18)	1.409(3)
C(4)-N(1)	1.420(2)	C(17)-C(21)	1.474(3)
C(5)-C(6)	1.391(3)	C(18)-O(2)	1.376(2)
C(5)-H(5)	0.9300	C(18)-C(19)	1.383(3)
C(6)-H(6)	0.9300	C(19)-C(20)	1.388(3)
C(7)-N(1)	1.468(2)	C(19)-H(19)	0.9300
C(7)-C(8)	1.519(3)	C(20)-H(20)	0.9300
C(7)-H(7A)	0.9700	C(21)-C(22)	1.273(3)
C(7)-H(7B)	0.9700	C(21)-H(21)	0.9300
C(8)-O(1)	1.426(3)	C(22)-C(23)	1.514(3)
C(8)-H(8A)	0.9700	C(22)-H(22)	0.9300
C(8)-H(8B)	0.9700	C(23)-H(23A)	0.9600
C(9)-O(1)	1.451(2)	C(23)-H(23B)	0.9600
C(9)-N(1)	1.472(2)	C(23)-H(23C)	0.9600
C(9)-C(13)	1.512(2)	C(24)-O(2)	1.447(2)
C(9)-C(10)	1.561(2)	C(24)-C(25)	1.482(4)
C(10)-C(12)	1.529(3)	C(24)-C(26)	1.513(3)
C(10)-C(11)	1.543(3)	C(24)-H(24)	0.9800
C(11)-H(11A)	0.9600	C(25)-H(25A)	0.9600
C(11)-H(11B)	0.9600	C(25)-H(25B)	0.9600
C(11)-H(11C)	0.9600	C(25)-H(25C)	0.9600
C(12)-H(12A)	0.9600	C(26)-H(26A)	0.9600
C(12)-H(12B)	0.9600	C(26)-H(26B)	0.9600
C(12)-H(12C)	0.9600	C(26)-H(26C)	0.9600
C(13)-C(14)	1.323(2)		
C(6)-C(1)-C(2)	121.96(19)	C(4)-C(3)-C(10)	109.43(15)
C(6)-C(1)-Cl(1)	119.36(17)	C(5)-C(4)-C(3)	120.93(17)
C(2)-C(1)-Cl(1)	118.67(19)	C(5)-C(4)-N(1)	127.84(17)
C(3)-C(2)-C(1)	118.0(2)	C(3)-C(4)-N(1)	111.12(14)
C(3)-C(2)-H(2)	121.0	C(6)-C(5)-C(4)	118.35(19)
C(1)-C(2)-H(2)	121.0	C(6)-C(5)-H(5)	120.8
C(2)-C(3)-C(4)	120.61(17)	C(4)-C(5)-H(5)	120.8
C(2)-C(3)-C(10)	129.68(17)	C(1)-C(6)-C(5)	120.13(19)

C(1)-C(6)-H(6)	119.9	C(20)-C(15)-C(16)	117.51(15)
C(5)-C(6)-H(6)	119.9	C(20)-C(15)-C(14)	119.21(15)
N(1)-C(7)-C(8)	104.12(16)	C(16)-C(15)-C(14)	123.21(16)
N(1)-C(7)-H(7A)	110.9	C(17)-C(16)-C(15)	122.30(16)
C(8)-C(7)-H(7A)	110.9	C(17)-C(16)-H(16)	118.8
N(1)-C(7)-H(7B)	110.9	C(15)-C(16)-H(16)	118.8
C(8)-C(7)-H(7B)	110.9	C(16)-C(17)-C(18)	118.22(16)
H(7A)-C(7)-H(7B)	109.0	C(16)-C(17)-C(21)	122.32(17)
O(1)-C(8)-C(7)	107.23(16)	C(18)-C(17)-C(21)	119.45(16)
O(1)-C(8)-H(8A)	110.3	O(2)-C(18)-C(19)	124.17(17)
C(7)-C(8)-H(8A)	110.3	O(2)-C(18)-C(17)	115.51(16)
O(1)-C(8)-H(8B)	110.3	C(19)-C(18)-C(17)	120.28(16)
C(7)-C(8)-H(8B)	110.3	C(18)-C(19)-C(20)	120.09(17)
H(8A)-C(8)-H(8B)	108.5	C(18)-C(19)-H(19)	120.0
O(1)-C(9)-N(1)	104.04(13)	C(20)-C(19)-H(19)	120.0
O(1)-C(9)-C(13)	108.84(14)	C(19)-C(20)-C(15)	121.56(17)
N(1)-C(9)-C(13)	113.50(14)	C(19)-C(20)-H(20)	119.2
O(1)-C(9)-C(10)	109.52(13)	C(15)-C(20)-H(20)	119.2
N(1)-C(9)-C(10)	105.33(13)	C(22)-C(21)-C(17)	128.7(2)
C(13)-C(9)-C(10)	115.00(14)	C(22)-C(21)-H(21)	115.6
C(3)-C(10)-C(12)	115.23(16)	C(17)-C(21)-H(21)	115.6
C(3)-C(10)-C(11)	107.08(15)	C(21)-C(22)-C(23)	125.5(2)
C(12)-C(10)-C(11)	110.09(17)	C(21)-C(22)-H(22)	117.2
C(3)-C(10)-C(9)	100.46(13)	C(23)-C(22)-H(22)	117.2
C(12)-C(10)-C(9)	112.73(16)	C(22)-C(23)-H(23A)	109.5
C(11)-C(10)-C(9)	110.81(14)	C(22)-C(23)-H(23B)	109.5
C(10)-C(11)-H(11A)	109.5	H(23A)-C(23)-H(23B)	109.5
C(10)-C(11)-H(11B)	109.5	C(22)-C(23)-H(23C)	109.5
H(11A)-C(11)-H(11B)	109.5	H(23A)-C(23)-H(23C)	109.5
C(10)-C(11)-H(11C)	109.5	H(23B)-C(23)-H(23C)	109.5
H(11A)-C(11)-H(11C)	109.5	O(2)-C(24)-C(25)	111.17(19)
H(11B)-C(11)-H(11C)	109.5	O(2)-C(24)-C(26)	104.89(19)
C(10)-C(12)-H(12A)	109.5	C(25)-C(24)-C(26)	112.9(2)
C(10)-C(12)-H(12B)	109.5	O(2)-C(24)-H(24)	109.3
H(12A)-C(12)-H(12B)	109.5	C(25)-C(24)-H(24)	109.3
C(10)-C(12)-H(12C)	109.5	C(26)-C(24)-H(24)	109.3
H(12A)-C(12)-H(12C)	109.5	C(24)-C(25)-H(25A)	109.5
H(12B)-C(12)-H(12C)	109.5	C(24)-C(25)-H(25B)	109.5
C(14)-C(13)-C(9)	124.70(16)	H(25A)-C(25)-H(25B)	109.5
C(14)-C(13)-H(13)	117.7	C(24)-C(25)-H(25C)	109.5
C(9)-C(13)-H(13)	117.7	H(25A)-C(25)-H(25C)	109.5
C(13)-C(14)-C(15)	127.87(16)	H(25B)-C(25)-H(25C)	109.5
C(13)-C(14)-H(14)	116.1	C(24)-C(26)-H(26A)	109.5
C(15)-C(14)-H(14)	116.1	C(24)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5	C(4)-N(1)-C(9)	106.01(13)
C(24)-C(26)-H(26C)	109.5	C(7)-N(1)-C(9)	105.04(14)
H(26A)-C(26)-H(26C)	109.5	C(8)-O(1)-C(9)	106.75(15)
H(26B)-C(26)-H(26C)	109.5	C(18)-O(2)-C(24)	120.77(15)
C(4)-N(1)-C(7)	116.71(14)		

Figure S11. Crystal structure of 10

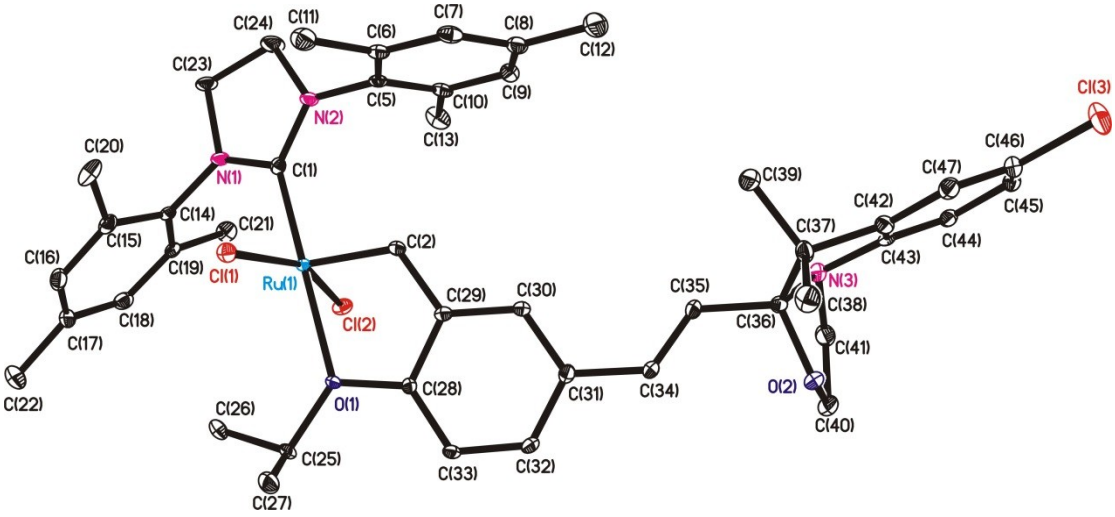


Table 4. Crystal data and structure refinement for **10**

Identification code	n151221a
Empirical formula	C96 H116 C118 N6 O4 Ru2
Formula weight	2258.18
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 15.4470(4) A alpha = 93.4050(10) deg.
	b = 16.2633(4) A beta = 90 deg.
	c = 20.7349(6) A gamma = 90 deg.
Volume	5199.8(2) A^3
Z, Calculated density	2, 1.442 Mg/m^3
Absorption coefficient	0.804 mm^-1
F(000)	2320
Crystal size	0.220 x 0.210 x 0.180 mm
Theta range for data collection	0.984 to 26.499 deg.
Limiting indices	-19<=h<=19, -20<=k<=10, -24<=l<=26
Reflections collected / unique	34278 / 21536 [R(int) = 0.0217]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	21536 / 12 / 1155
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.0990
R indices (all data)	R1 = 0.0529, wR2 = 0.1058
Extinction coefficient	n/a
Largest diff. peak and hole	1.643 and -0.867 e.A^-3

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10**.

	x	y	z	U(eq)
Ru(1)	4988(1)	5823(1)	8247(1)	11(1)
Ru(2)	0(1)	11062(1)	1754(1)	11(1)
C(91)	2792(17)	3809(7)	8531(7)	45(1)
Cl(6)	1840(20)	4301(17)	8839(9)	49(1)
Cl(7)	2539(1)	3095(1)	7884(1)	54(1)
C(91')	2781(17)	3776(6)	8531(8)	45(1)
Cl(6')	1810(30)	4269(17)	8786(9)	49(1)
Cl(7')	2848(1)	2783(2)	8828(1)	54(1)
O(1)	5699(1)	5026(1)	8926(1)	15(1)
C(92)	1627(4)	1517(4)	6708(3)	59(2)
Cl(8)	851(1)	961(1)	6263(1)	69(1)
Cl(9)	2044(1)	2337(1)	6285(1)	70(1)
C(92')	1780(20)	1360(9)	6553(15)	59(2)
Cl(8')	1036(4)	1324(5)	5908(4)	69(1)
Cl(9')	2124(5)	2380(4)	6767(4)	70(1)
O(2)	4549(2)	101(1)	7763(1)	23(1)
O(3)	-714(1)	10164(1)	1101(1)	16(1)
O(4)	392(2)	5396(1)	2268(1)	23(1)
N(1)	4132(2)	7311(2)	7868(1)	18(1)
N(2)	4021(2)	6390(2)	7069(1)	17(1)
N(3)	3349(2)	485(2)	7214(1)	18(1)
N(4)	789(2)	12637(2)	2100(1)	20(1)
N(5)	978(2)	11857(2)	2898(1)	19(1)
N(6)	1626(2)	5832(2)	2786(1)	19(1)
Cl(1)	6356(1)	6206(1)	7873(1)	18(1)
Cl(2)	3807(1)	5687(1)	8951(1)	19(1)
Cl(3)	3750(1)	-1978(1)	5024(1)	37(1)
Cl(4)	1163(1)	10818(1)	1029(1)	19(1)
Cl(5)	-1353(1)	11500(1)	2172(1)	19(1)
Cl(10)	1378(1)	3575(1)	4900(1)	34(1)
Cl(11)	6551(1)	8049(1)	5937(1)	49(1)
Cl(12)	6875(1)	9301(1)	5014(1)	52(1)
Cl(13)	3177(1)	5779(1)	5141(1)	38(1)
Cl(14)	1502(1)	6468(1)	5520(1)	82(1)
Cl(15)	3808(1)	6654(1)	3514(1)	46(1)
Cl(16)	2564(1)	7963(1)	3261(1)	67(1)
Cl(17)	7874(1)	2111(1)	8790(1)	66(1)
Cl(18)	6841(1)	617(1)	8795(1)	45(1)

C(1)	4336(2)	6525(2)	7669(1)	14(1)
C(2)	4896(2)	4811(2)	7821(1)	16(1)
C(3)	638(2)	11879(2)	2302(1)	14(1)
C(4)	128(2)	10126(2)	2190(1)	16(1)
C(5)	4017(2)	5622(2)	6693(1)	16(1)
C(6)	4684(2)	5449(2)	6244(1)	19(1)
C(7)	4671(2)	4694(2)	5891(1)	22(1)
C(8)	4014(2)	4127(2)	5969(2)	23(1)
C(9)	3355(2)	4335(2)	6411(2)	23(1)
C(10)	3339(2)	5078(2)	6778(1)	19(1)
C(11)	5397(2)	6052(2)	6146(2)	30(1)
C(12)	4011(3)	3317(2)	5574(2)	37(1)
C(13)	2626(2)	5286(2)	7259(2)	29(1)
C(14)	4443(2)	7734(2)	8445(1)	16(1)
C(15)	5265(2)	8091(2)	8439(2)	21(1)
C(16)	5558(2)	8481(2)	9008(2)	27(1)
C(17)	5048(2)	8555(2)	9564(2)	27(1)
C(18)	4209(2)	8253(2)	9538(2)	22(1)
C(19)	3892(2)	7845(2)	8986(1)	17(1)
C(20)	5796(2)	8134(2)	7830(2)	31(1)
C(21)	2961(2)	7571(2)	8964(2)	24(1)
C(22)	5395(3)	8966(3)	10182(2)	42(1)
C(23)	3698(2)	7772(2)	7368(2)	23(1)
C(24)	3536(3)	7099(2)	6842(2)	32(1)
C(25)	6146(2)	5269(2)	9527(1)	18(1)
C(26)	5950(2)	6175(2)	9664(2)	23(1)
C(27)	7107(2)	5090(2)	9439(2)	25(1)
C(28)	5545(2)	4214(2)	8762(1)	13(1)
C(29)	5127(2)	4096(2)	8167(1)	14(1)
C(30)	4922(2)	3298(2)	7940(1)	15(1)
C(31)	5124(2)	2620(2)	8290(1)	16(1)
C(32)	5553(2)	2764(2)	8878(2)	18(1)
C(33)	5763(2)	3551(2)	9119(1)	16(1)
C(34)	4927(2)	1771(2)	8054(1)	18(1)
C(35)	4387(2)	1559(2)	7583(2)	20(1)
C(36)	4271(2)	689(2)	7311(2)	18(1)
C(37)	4722(2)	493(2)	6648(2)	21(1)
C(38)	5666(2)	226(2)	6723(2)	29(1)
C(39)	4674(2)	1227(2)	6230(2)	27(1)
C(40)	3830(2)	-29(2)	8191(2)	27(1)
C(41)	3026(2)	281(2)	7850(2)	26(1)
C(42)	4134(2)	-174(2)	6370(2)	19(1)
C(43)	3357(2)	-151(2)	6709(1)	16(1)
C(44)	2686(2)	-678(2)	6539(2)	19(1)

C(45)	2823(2)	-1240(2)	6009(2)	21(1)
C(46)	3594(2)	-1260(2)	5680(2)	23(1)
C(47)	4271(2)	-737(2)	5852(2)	22(1)
C(48)	480(2)	12953(2)	1511(1)	17(1)
C(49)	1048(2)	12971(2)	978(1)	18(1)
C(50)	742(2)	13294(2)	419(2)	23(1)
C(51)	-96(2)	13597(2)	379(2)	26(1)
C(52)	-625(2)	13613(2)	923(2)	25(1)
C(53)	-342(2)	13312(2)	1504(2)	20(1)
C(54)	1982(2)	12701(2)	1018(2)	26(1)
C(55)	-893(2)	13467(2)	2102(2)	29(1)
C(56)	-426(3)	13914(3)	-245(2)	39(1)
C(57)	1057(2)	11167(2)	3293(1)	17(1)
C(58)	1745(2)	10624(2)	3182(1)	18(1)
C(59)	1840(2)	9985(2)	3595(2)	22(1)
C(60)	1271(2)	9892(2)	4105(2)	31(1)
C(61)	592(2)	10448(2)	4198(2)	34(1)
C(62)	464(2)	11093(2)	3796(2)	24(1)
C(63)	2368(2)	10718(3)	2628(2)	32(1)
C(64)	-279(3)	11691(3)	3903(2)	40(1)
C(65)	1406(3)	9207(3)	4559(2)	46(1)
C(66)	1422(3)	12621(2)	3108(2)	42(1)
C(67)	1228(2)	13193(2)	2578(2)	24(1)
C(68)	-1158(2)	10307(2)	493(1)	16(1)
C(69)	-2118(2)	10179(2)	580(2)	24(1)
C(70)	-941(2)	11182(2)	334(2)	21(1)
C(71)	-572(2)	9375(2)	1280(1)	14(1)
C(72)	-816(2)	8663(2)	943(1)	18(1)
C(73)	-629(2)	7910(2)	1201(2)	22(1)
C(74)	-192(2)	7854(2)	1784(2)	19(1)
C(75)	45(2)	8585(2)	2114(1)	17(1)
C(76)	-137(2)	9353(2)	1872(1)	14(1)
C(77)	0(2)	7036(2)	2020(2)	22(1)
C(78)	569(2)	6873(2)	2468(2)	21(1)
C(79)	699(2)	6032(2)	2719(2)	20(1)
C(80)	1078(2)	5214(2)	1808(2)	28(1)
C(81)	1914(2)	5534(2)	2130(2)	26(1)
C(82)	284(2)	5914(2)	3392(2)	19(1)
C(83)	-661(2)	5653(2)	3351(2)	28(1)
C(84)	367(2)	6705(2)	3834(2)	24(1)
C(85)	889(2)	5267(2)	3631(2)	18(1)
C(86)	790(2)	4753(2)	4140(2)	21(1)
C(87)	1484(2)	4249(2)	4276(1)	21(1)
C(88)	2253(2)	4243(2)	3928(2)	21(1)

C(89)	2352(2)	4754(2)	3419(2)	19(1)
C(90)	1660(2)	5259(2)	3275(1)	17(1)
C(93)	7287(3)	8430(2)	5375(2)	42(1)
C(94)	2258(2)	6284(2)	4882(2)	33(1)
C(95)	3220(3)	7161(3)	2930(2)	45(1)
C(96)	7810(3)	1065(3)	8530(2)	44(1)

Table 6. Bond lengths [A] and angles [deg] for **10**

Ru(1)-C(2)	1.825(3)	N(3)-C(43)	1.427(4)
Ru(1)-C(1)	1.979(3)	N(3)-C(41)	1.466(4)
Ru(1)-O(1)	2.2552(19)	N(3)-C(36)	1.473(4)
Ru(1)-Cl(1)	2.3470(7)	N(4)-C(3)	1.347(4)
Ru(1)-Cl(2	2.3566(7)	N(4)-C(48)	1.434(4)
Ru(2)-C(4)	1.828(3)	N(4)-C(67)	1.466(4)
Ru(2)-C(3)	1.962(3)	N(5)-C(3)	1.344(4)
Ru(2)-O(3)	2.2240(19)	N(5)-C(57)	1.433(4)
Ru(2)-Cl(5)	2.3563(8)	N(5)-C(66)	1.464(4)
Ru(2)-Cl(4)	2.3616(8)	N(6)-C(90)	1.419(4)
C(91)-Cl(7)	1.764(10)	N(6)-C(79)	1.478(4)
C(91)-Cl(6)	1.773(8)	N(6)-C(81)	1.484(4)
C(91)-H(91A)	0.9900	Cl(3)-C(46)	1.757(3)
C(91)-H(91B)	0.9900	Cl(10)-C(87)	1.753(3)
C(91')-Cl(7')	1.767(10)	Cl(11)-C(93)	1.766(5)
C(91')-Cl(6')	1.771(8)	Cl(12)-C(93)	1.761(4)
C(91')-H(91C)	0.9900	Cl(13)-C(94)	1.740(4)
C(91')-H(91D)	0.9900	Cl(14)-C(94)	1.776(4)
O(1)-C(28)	1.365(3)	Cl(15)-C(95)	1.759(4)
O(1)-C(25)	1.458(3)	Cl(16)-C(95)	1.758(4)
C(92)-Cl(8)	1.734(6)	Cl(17)-C(96)	1.757(5)
C(92)-Cl(9)	1.762(6)	Cl(18)-C(96)	1.766(4)
C(92)-H(92A)	0.9900	C(2)-C(29)	1.446(4)
C(92)-H(92B)	0.9900	C(2)-H(2)	0.9500
C(92')-Cl(8')	1.761(10)	C(4)-C(76)	1.444(4)
C(92')-Cl(9')	1.774(10)	C(4)-H(4)	0.9500
C(92')-H(92C)	0.9900	C(5)-C(10)	1.389(4)
C(92')-H(92D)	0.9900	C(5)-C(6)	1.405(4)
O(2)-C(36)	1.443(3)	C(6)-C(7)	1.391(4)
O(2)-C(40)	1.446(4)	C(6)-C(11)	1.498(5)
O(3)-C(71)	1.374(3)	C(7)-C(8)	1.387(5)
O(3)-C(68)	1.466(3)	C(7)-H(7)	0.9500
O(4)-C(79)	1.433(4)	C(8)-C(9)	1.398(5)
O(4)-C(80)	1.445(4)	C(8)-C(12)	1.510(5)
N(1)-C(1)	1.357(4)	C(9)-C(10)	1.390(5)
N(1)-C(14)	1.427(4)	C(9)-H(9)	0.9500
N(1)-C(23)	1.475(4)	C(10)-C(13)	1.511(4)
N(2)-C(1)	1.342(4)	C(11)-H(11A)	0.9800
N(2)-C(5)	1.432(4)	C(11)-H(11B)	0.9800
N(2)-C(24)	1.476(4)	C(11)-H(11C)	0.9801

C(12)-H(12A)	0.9800	C(30)-H(30)	0.9500
C(12)-H(12B)	0.9800	C(31)-C(32)	1.393(4)
C(12)-H(12C)	0.9800	C(31)-C(34)	1.470(4)
C(13)-H(13A)	0.9800	C(32)-C(33)	1.385(4)
C(13)-H(13B)	0.9800	C(32)-H(32)	0.9500
C(13)-H(13C)	0.9800	C(33)-H(33)	0.9500
C(14)-C(15)	1.397(4)	C(34)-C(35)	1.315(4)
C(14)-C(19)	1.411(4)	C(34)-H(34)	0.9500
C(15)-C(16)	1.382(5)	C(35)-C(36)	1.502(4)
C(15)-C(20)	1.510(5)	C(35)-H(35)	0.9500
C(16)-C(17)	1.394(5)	C(36)-C(37)	1.558(5)
C(16)-H(16)	0.9500	C(37)-C(42)	1.503(4)
C(17)-C(18)	1.386(5)	C(37)-C(39)	1.518(4)
C(17)-C(22)	1.509(5)	C(37)-C(38)	1.534(4)
C(18)-C(19)	1.379(4)	C(38)-H(38A)	0.9800
C(18)-H(18)	0.9500	C(38)-H(38B)	0.9800
C(19)-C(21)	1.505(4)	C(38)-H(38C)	0.9800
C(20)-H(20A)	0.9800	C(39)-H(39A)	0.9800
C(20)-H(20B)	0.9800	C(39)-H(39B)	0.9800
C(20)-H(20C)	0.9800	C(39)-H(39C)	0.9800
C(21)-H(21A)	0.9800	C(40)-C(41)	1.530(5)
C(21)-H(21B)	0.9800	C(40)-H(40A)	0.9900
C(21)-H(21C)	0.9800	C(40)-H(40B)	0.9900
C(22)-H(22A)	0.9800	C(41)-H(41A)	0.9900
C(22)-H(22B)	0.9800	C(41)-H(41B)	0.9900
C(22)-H(22C)	0.9800	C(42)-C(47)	1.386(5)
C(23)-C(24)	1.520(5)	C(42)-C(43)	1.390(4)
C(23)-H(23A)	0.9900	C(43)-C(44)	1.378(4)
C(23)-H(23B)	0.9900	C(44)-C(45)	1.402(4)
C(24)-H(24A)	0.9900	C(44)-H(44)	0.9500
C(24)-H(24B)	0.9900	C(45)-C(46)	1.371(5)
C(25)-C(26)	1.515(4)	C(45)-H(45)	0.9500
C(25)-C(27)	1.521(4)	C(46)-C(47)	1.383(5)
C(25)-H(25)	1.0000	C(47)-H(47)	0.9500
C(26)-H(26A)	0.9800	C(48)-C(53)	1.400(4)
C(26)-H(26B)	0.9800	C(48)-C(49)	1.412(4)
C(26)-H(26C)	0.9800	C(49)-C(50)	1.384(4)
C(27)-H(27A)	0.9800	C(49)-C(54)	1.511(4)
C(27)-H(27B)	0.9800	C(50)-C(51)	1.390(5)
C(27)-H(27C)	0.9800	C(50)-H(50)	0.9500
C(28)-C(33)	1.385(4)	C(51)-C(52)	1.393(5)
C(28)-C(29)	1.397(4)	C(51)-C(56)	1.509(4)
C(29)-C(30)	1.391(4)	C(52)-C(53)	1.397(4)
C(30)-C(31)	1.391(4)	C(52)-H(52)	0.9500

C(53)-C(55)	1.512(5)	C(71)-C(72)	1.370(4)
C(54)-H(54A)	0.9800	C(71)-C(76)	1.402(4)
C(54)-H(54B)	0.9800	C(72)-C(73)	1.394(4)
C(54)-H(54C)	0.9800	C(72)-H(72)	0.9500
C(55)-H(55A)	0.9800	C(73)-C(74)	1.393(4)
C(55)-H(55B)	0.9800	C(73)-H(73)	0.9500
C(55)-H(55C)	0.9800	C(74)-C(75)	1.385(4)
C(56)-H(56A)	0.9800	C(74)-C(77)	1.475(4)
C(56)-H(56B)	0.9800	C(75)-C(76)	1.403(4)
C(56)-H(56C)	0.9800	C(75)-H(75)	0.9500
C(57)-C(58)	1.392(4)	C(77)-C(78)	1.318(4)
C(57)-C(62)	1.399(4)	C(77)-H(77)	0.9500
C(58)-C(59)	1.392(4)	C(78)-C(79)	1.505(4)
C(58)-C(63)	1.513(4)	C(78)-H(78)	0.9500
C(59)-C(60)	1.392(5)	C(79)-C(82)	1.558(4)
C(59)-H(59)	0.9500	C(80)-C(81)	1.531(5)
C(60)-C(61)	1.391(5)	C(80)-H(80A)	0.9900
C(60)-C(65)	1.516(5)	C(80)-H(80B)	0.9900
C(61)-C(62)	1.392(5)	C(81)-H(81A)	0.9900
C(61)-H(61)	0.9500	C(81)-H(81B)	0.9900
C(62)-C(64)	1.511(5)	C(82)-C(85)	1.512(4)
C(63)-H(63A)	0.9800	C(82)-C(83)	1.521(4)
C(63)-H(63B)	0.9800	C(82)-C(84)	1.540(4)
C(63)-H(63C)	0.9800	C(83)-H(83A)	0.9800
C(64)-H(64A)	0.9800	C(83)-H(83B)	0.9800
C(64)-H(64B)	0.9800	C(83)-H(83C)	0.9800
C(64)-H(64C)	0.9800	C(84)-H(84A)	0.9800
C(65)-H(65A)	0.9800	C(84)-H(84B)	0.9800
C(65)-H(65B)	0.9800	C(84)-H(84C)	0.9800
C(65)-H(65C)	0.9800	C(85)-C(86)	1.393(4)
C(66)-C(67)	1.512(4)	C(85)-C(90)	1.400(4)
C(66)-H(66A)	0.9900	C(86)-C(87)	1.390(5)
C(66)-H(66B)	0.9900	C(86)-H(86)	0.9500
C(67)-H(67A)	0.9900	C(87)-C(88)	1.390(5)
C(67)-H(67B)	0.9900	C(88)-C(89)	1.391(4)
C(68)-C(69)	1.510(4)	C(88)-H(88)	0.9500
C(68)-C(70)	1.518(4)	C(89)-C(90)	1.391(4)
C(68)-H(68)	1.0000	C(89)-H(89)	0.9500
C(69)-H(69A)	0.9800	C(93)-H(93A)	0.9900
C(69)-H(69B)	0.9800	C(93)-H(93B)	0.9900
C(69)-H(69C)	0.9800	C(94)-H(94A)	0.9900
C(70)-H(70A)	0.9800	C(94)-H(94B)	0.9900
C(70)-H(70B)	0.9800	C(95)-H(95A)	0.9900
C(70)-H(70C)	0.9800	C(95)-H(95B)	0.9900

C(96)-H(96A)	0.9900	C(96)-H(96B)	0.9900

C(2)-Ru(1)-C(1)	101.76(12)	Cl(8')-C(92')-H(92C)	109.2
C(2)-Ru(1)-O(1)	78.77(10)	Cl(9')-C(92')-H(92C)	109.2
C(1)-Ru(1)-O(1)	178.28(10)	Cl(8')-C(92')-H(92D)	109.2
C(2)-Ru(1)-Cl(1)	99.24(10)	Cl(9')-C(92')-H(92D)	109.2
C(1)-Ru(1)-Cl(1)	94.84(8)	H(92C)-C(92')-H(92D)	107.9
O(1)-Ru(1)-Cl(1)	86.68(6)	C(36)-O(2)-C(40)	107.2(2)
C(2)-Ru(1)-Cl(2)	97.08(10)	C(71)-O(3)-C(68)	120.3(2)
C(1)-Ru(1)-Cl(2)	93.41(8)	C(71)-O(3)-Ru(2)	110.28(16)
O(1)-Ru(1)-Cl(2)	84.89(6)	C(68)-O(3)-Ru(2)	128.58(16)
Cl(1)-Ru(1)-Cl(2)	159.79(3)	C(79)-O(4)-C(80)	107.5(2)
C(4)-Ru(2)-C(3)	102.33(12)	C(1)-N(1)-C(14)	125.0(2)
C(4)-Ru(2)-O(3)	79.56(10)	C(1)-N(1)-C(23)	113.6(2)
C(3)-Ru(2)-O(3)	177.91(10)	C(14)-N(1)-C(23)	120.2(2)
C(4)-Ru(2)-Cl(5)	99.03(10)	C(1)-N(2)-C(5)	126.7(2)
C(3)-Ru(2)-Cl(5)	93.05(9)	C(1)-N(2)-C(24)	113.1(3)
O(3)-Ru(2)-Cl(5)	87.53(6)	C(5)-N(2)-C(24)	119.7(2)
C(4)-Ru(2)-Cl(4)	96.82(10)	C(43)-N(3)-C(41)	118.0(2)
C(3)-Ru(2)-Cl(4)	93.95(9)	C(43)-N(3)-C(36)	103.8(2)
O(3)-Ru(2)-Cl(4)	84.88(6)	C(41)-N(3)-C(36)	105.5(2)
Cl(5)-Ru(2)-Cl(4)	160.88(3)	C(3)-N(4)-C(48)	126.0(2)
Cl(7)-C(91)-Cl(6)	110.6(8)	C(3)-N(4)-C(67)	114.2(2)
Cl(7)-C(91)-H(91A)	109.5	C(48)-N(4)-C(67)	119.4(2)
Cl(6)-C(91)-H(91A)	109.5	C(3)-N(5)-C(57)	128.5(2)
Cl(7)-C(91)-H(91B)	109.5	C(3)-N(5)-C(66)	112.9(2)
Cl(6)-C(91)-H(91B)	109.5	C(57)-N(5)-C(66)	117.9(2)
H(91A)-C(91)-H(91B)	108.1	C(90)-N(6)-C(79)	105.0(2)
Cl(7')-C(91')-Cl(6')	110.7(8)	C(90)-N(6)-C(81)	116.8(2)
Cl(7')-C(91')-H(91C)	109.5	C(79)-N(6)-C(81)	105.5(2)
Cl(6')-C(91')-H(91C)	109.5	N(2)-C(1)-N(1)	107.3(2)
Cl(7')-C(91')-H(91D)	109.5	N(2)-C(1)-Ru(1)	132.6(2)
Cl(6')-C(91')-H(91D)	109.5	N(1)-C(1)-Ru(1)	120.2(2)
H(91C)-C(91')-H(91D)	108.1	C(29)-C(2)-Ru(1)	118.0(2)
C(28)-O(1)-C(25)	120.3(2)	C(29)-C(2)-H(2)	121.0
C(28)-O(1)-Ru(1)	110.08(16)	Ru(1)-C(2)-H(2)	121.0
C(25)-O(1)-Ru(1)	128.87(17)	N(5)-C(3)-N(4)	107.0(2)
Cl(8)-C(92)-Cl(9)	111.9(4)	N(5)-C(3)-Ru(2)	132.4(2)
Cl(8)-C(92)-H(92A)	109.2	N(4)-C(3)-Ru(2)	120.5(2)
Cl(9)-C(92)-H(92A)	109.2	C(76)-C(4)-Ru(2)	118.1(2)
Cl(8)-C(92)-H(92B)	109.2	C(76)-C(4)-H(4)	121.0
Cl(9)-C(92)-H(92B)	109.2	Ru(2)-C(4)-H(4)	121.0
H(92A)-C(92)-H(92B)	107.9	C(10)-C(5)-C(6)	122.1(3)
Cl(8')-C(92')-Cl(9')	112.0(8)	C(10)-C(5)-N(2)	118.4(3)

C(6)-C(5)-N(2)	119.5(3)	C(18)-C(17)-C(22)	120.2(3)
C(7)-C(6)-C(5)	118.3(3)	C(16)-C(17)-C(22)	120.9(3)
C(7)-C(6)-C(11)	120.3(3)	C(19)-C(18)-C(17)	121.0(3)
C(5)-C(6)-C(11)	121.4(3)	C(19)-C(18)-H(18)	119.5
C(8)-C(7)-C(6)	121.3(3)	C(17)-C(18)-H(18)	119.5
C(8)-C(7)-H(7)	119.3	C(18)-C(19)-C(14)	118.6(3)
C(6)-C(7)-H(7)	119.3	C(18)-C(19)-C(21)	119.4(3)
C(7)-C(8)-C(9)	118.3(3)	C(14)-C(19)-C(21)	121.9(3)
C(7)-C(8)-C(12)	120.2(3)	C(15)-C(20)-H(20A)	109.5
C(9)-C(8)-C(12)	121.5(3)	C(15)-C(20)-H(20B)	109.5
C(10)-C(9)-C(8)	122.7(3)	H(20A)-C(20)-H(20B)	109.5
C(10)-C(9)-H(9)	118.7	C(15)-C(20)-H(20C)	109.4
C(8)-C(9)-H(9)	118.7	H(20A)-C(20)-H(20C)	109.5
C(5)-C(10)-C(9)	117.2(3)	H(20B)-C(20)-H(20C)	109.5
C(5)-C(10)-C(13)	120.9(3)	C(19)-C(21)-H(21A)	109.6
C(9)-C(10)-C(13)	121.8(3)	C(19)-C(21)-H(21B)	109.4
C(6)-C(11)-H(11A)	109.4	H(21A)-C(21)-H(21B)	109.5
C(6)-C(11)-H(11B)	109.6	C(19)-C(21)-H(21C)	109.4
H(11A)-C(11)-H(11B)	109.5	H(21A)-C(21)-H(21C)	109.5
C(6)-C(11)-H(11C)	109.4	H(21B)-C(21)-H(21C)	109.5
H(11A)-C(11)-H(11C)	109.5	C(17)-C(22)-H(22A)	109.5
H(11B)-C(11)-H(11C)	109.5	C(17)-C(22)-H(22B)	109.4
C(8)-C(12)-H(12A)	109.4	H(22A)-C(22)-H(22B)	109.5
C(8)-C(12)-H(12B)	109.6	C(17)-C(22)-H(22C)	109.6
H(12A)-C(12)-H(12B)	109.5	H(22A)-C(22)-H(22C)	109.5
C(8)-C(12)-H(12C)	109.4	H(22B)-C(22)-H(22C)	109.5
H(12A)-C(12)-H(12C)	109.5	N(1)-C(23)-C(24)	101.8(2)
H(12B)-C(12)-H(12C)	109.5	N(1)-C(23)-H(23A)	111.4
C(10)-C(13)-H(13A)	109.4	C(24)-C(23)-H(23A)	111.4
C(10)-C(13)-H(13B)	109.5	N(1)-C(23)-H(23B)	111.4
H(13A)-C(13)-H(13B)	109.5	C(24)-C(23)-H(23B)	111.4
C(10)-C(13)-H(13C)	109.5	H(23A)-C(23)-H(23B)	109.3
H(13A)-C(13)-H(13C)	109.5	N(2)-C(24)-C(23)	103.3(2)
H(13B)-C(13)-H(13C)	109.5	N(2)-C(24)-H(24A)	111.1
C(15)-C(14)-C(19)	121.4(3)	C(23)-C(24)-H(24A)	111.1
C(15)-C(14)-N(1)	118.6(3)	N(2)-C(24)-H(24B)	111.1
C(19)-C(14)-N(1)	119.7(3)	C(23)-C(24)-H(24B)	111.1
C(16)-C(15)-C(14)	117.4(3)	H(24A)-C(24)-H(24B)	109.1
C(16)-C(15)-C(20)	119.7(3)	O(1)-C(25)-C(26)	106.1(2)
C(14)-C(15)-C(20)	122.7(3)	O(1)-C(25)-C(27)	108.7(2)
C(15)-C(16)-C(17)	122.3(3)	C(26)-C(25)-C(27)	113.2(3)
C(15)-C(16)-H(16)	118.9	O(1)-C(25)-H(25)	109.6
C(17)-C(16)-H(16)	118.9	C(26)-C(25)-H(25)	109.6
C(18)-C(17)-C(16)	118.9(3)	C(27)-C(25)-H(25)	109.6

C(25)-C(26)-H(26A)	109.5	C(39)-C(37)-C(38)	110.0(3)
C(25)-C(26)-H(26B)	109.3	C(42)-C(37)-C(36)	100.0(2)
H(26A)-C(26)-H(26B)	109.5	C(39)-C(37)-C(36)	110.9(3)
C(25)-C(26)-H(26C)	109.6	C(38)-C(37)-C(36)	112.3(3)
H(26A)-C(26)-H(26C)	109.5	C(37)-C(38)-H(38A)	109.5
H(26B)-C(26)-H(26C)	109.5	C(37)-C(38)-H(38B)	109.5
C(25)-C(27)-H(27A)	109.4	H(38A)-C(38)-H(38B)	109.5
C(25)-C(27)-H(27B)	109.4	C(37)-C(38)-H(38C)	109.4
H(27A)-C(27)-H(27B)	109.5	H(38A)-C(38)-H(38C)	109.5
C(25)-C(27)-H(27C)	109.5	H(38B)-C(38)-H(38C)	109.5
H(27A)-C(27)-H(27C)	109.5	C(37)-C(39)-H(39A)	109.5
H(27B)-C(27)-H(27C)	109.5	C(37)-C(39)-H(39B)	109.5
O(1)-C(28)-C(33)	126.7(2)	H(39A)-C(39)-H(39B)	109.5
O(1)-C(28)-C(29)	112.3(2)	C(37)-C(39)-H(39C)	109.5
C(33)-C(28)-C(29)	121.0(3)	H(39A)-C(39)-H(39C)	109.5
C(30)-C(29)-C(28)	118.6(3)	H(39B)-C(39)-H(39C)	109.5
C(30)-C(29)-C(2)	122.6(3)	O(2)-C(40)-C(41)	106.0(2)
C(28)-C(29)-C(2)	118.7(3)	O(2)-C(40)-H(40A)	110.5
C(29)-C(30)-C(31)	121.7(3)	C(41)-C(40)-H(40A)	110.5
C(29)-C(30)-H(30)	119.1	O(2)-C(40)-H(40B)	110.5
C(31)-C(30)-H(30)	119.1	C(41)-C(40)-H(40B)	110.5
C(30)-C(31)-C(32)	117.8(3)	H(40A)-C(40)-H(40B)	108.7
C(30)-C(31)-C(34)	122.5(3)	N(3)-C(41)-C(40)	103.7(3)
C(32)-C(31)-C(34)	119.7(3)	N(3)-C(41)-H(41A)	111.0
C(33)-C(32)-C(31)	122.0(3)	C(40)-C(41)-H(41A)	111.0
C(33)-C(32)-H(32)	119.0	N(3)-C(41)-H(41B)	111.0
C(31)-C(32)-H(32)	119.0	C(40)-C(41)-H(41B)	111.0
C(28)-C(33)-C(32)	118.8(3)	H(41A)-C(41)-H(41B)	109.0
C(28)-C(33)-H(33)	120.6	C(47)-C(42)-C(43)	121.4(3)
C(32)-C(33)-H(33)	120.6	C(47)-C(42)-C(37)	129.3(3)
C(35)-C(34)-C(31)	125.4(3)	C(43)-C(42)-C(37)	109.3(3)
C(35)-C(34)-H(34)	117.3	C(44)-C(43)-C(42)	121.5(3)
C(31)-C(34)-H(34)	117.3	C(44)-C(43)-N(3)	126.4(3)
C(34)-C(35)-C(36)	123.7(3)	C(42)-C(43)-N(3)	112.1(3)
C(34)-C(35)-H(35)	118.2	C(43)-C(44)-C(45)	117.0(3)
C(36)-C(35)-H(35)	118.2	C(43)-C(44)-H(44)	121.5
O(2)-C(36)-N(3)	103.0(2)	C(45)-C(44)-H(44)	121.5
O(2)-C(36)-C(35)	111.5(2)	C(46)-C(45)-C(44)	121.1(3)
N(3)-C(36)-C(35)	111.5(3)	C(46)-C(45)-H(45)	119.5
O(2)-C(36)-C(37)	109.3(2)	C(44)-C(45)-H(45)	119.5
N(3)-C(36)-C(37)	106.2(2)	C(45)-C(46)-C(47)	122.2(3)
C(35)-C(36)-C(37)	114.6(3)	C(45)-C(46)-Cl(3)	120.0(2)
C(42)-C(37)-C(39)	109.0(3)	C(47)-C(46)-Cl(3)	117.8(3)
C(42)-C(37)-C(38)	114.3(3)	C(46)-C(47)-C(42)	116.8(3)

C(46)-C(47)-H(47)	121.6	C(60)-C(59)-C(58)	121.3(3)
C(42)-C(47)-H(47)	121.6	C(60)-C(59)-H(59)	119.3
C(53)-C(48)-C(49)	121.8(3)	C(58)-C(59)-H(59)	119.3
C(53)-C(48)-N(4)	118.8(3)	C(61)-C(60)-C(59)	118.8(3)
C(49)-C(48)-N(4)	119.0(3)	C(61)-C(60)-C(65)	121.0(3)
C(50)-C(49)-C(48)	118.0(3)	C(59)-C(60)-C(65)	120.2(3)
C(50)-C(49)-C(54)	119.8(3)	C(60)-C(61)-C(62)	122.1(3)
C(48)-C(49)-C(54)	122.1(3)	C(60)-C(61)-H(61)	118.9
C(49)-C(50)-C(51)	121.5(3)	C(62)-C(61)-H(61)	118.9
C(49)-C(50)-H(50)	119.3	C(61)-C(62)-C(57)	117.1(3)
C(51)-C(50)-H(50)	119.2	C(61)-C(62)-C(64)	121.4(3)
C(50)-C(51)-C(52)	119.2(3)	C(57)-C(62)-C(64)	121.5(3)
C(50)-C(51)-C(56)	120.4(3)	C(58)-C(63)-H(63A)	109.4
C(52)-C(51)-C(56)	120.4(3)	C(58)-C(63)-H(63B)	109.5
C(51)-C(52)-C(53)	121.6(3)	H(63A)-C(63)-H(63B)	109.5
C(51)-C(52)-H(52)	119.2	C(58)-C(63)-H(63C)	109.5
C(53)-C(52)-H(52)	119.2	H(63A)-C(63)-H(63C)	109.5
C(52)-C(53)-C(48)	117.5(3)	H(63B)-C(63)-H(63C)	109.5
C(52)-C(53)-C(55)	118.7(3)	C(62)-C(64)-H(64A)	109.5
C(48)-C(53)-C(55)	123.5(3)	C(62)-C(64)-H(64B)	109.5
C(49)-C(54)-H(54A)	109.4	H(64A)-C(64)-H(64B)	109.5
C(49)-C(54)-H(54B)	109.5	C(62)-C(64)-H(64C)	109.4
H(54A)-C(54)-H(54B)	109.5	H(64A)-C(64)-H(64C)	109.5
C(49)-C(54)-H(54C)	109.4	H(64B)-C(64)-H(64C)	109.5
H(54A)-C(54)-H(54C)	109.5	C(60)-C(65)-H(65A)	109.5
H(54B)-C(54)-H(54C)	109.5	C(60)-C(65)-H(65B)	109.4
C(53)-C(55)-H(55A)	109.4	H(65A)-C(65)-H(65B)	109.5
C(53)-C(55)-H(55B)	109.5	C(60)-C(65)-H(65C)	109.5
H(55A)-C(55)-H(55B)	109.5	H(65A)-C(65)-H(65C)	109.5
C(53)-C(55)-H(55C)	109.5	H(65B)-C(65)-H(65C)	109.5
H(55A)-C(55)-H(55C)	109.5	N(5)-C(66)-C(67)	103.7(2)
H(55B)-C(55)-H(55C)	109.5	N(5)-C(66)-H(66A)	111.0
C(51)-C(56)-H(56A)	109.5	C(67)-C(66)-H(66A)	111.0
C(51)-C(56)-H(56B)	109.4	N(5)-C(66)-H(66B)	111.0
H(56A)-C(56)-H(56B)	109.5	C(67)-C(66)-H(66B)	111.0
C(51)-C(56)-H(56C)	109.5	H(66A)-C(66)-H(66B)	109.0
H(56A)-C(56)-H(56C)	109.5	N(4)-C(67)-C(66)	101.7(2)
H(56B)-C(56)-H(56C)	109.5	N(4)-C(67)-H(67A)	111.4
C(58)-C(57)-C(62)	122.7(3)	C(66)-C(67)-H(67A)	111.4
C(58)-C(57)-N(5)	118.8(3)	N(4)-C(67)-H(67B)	111.4
C(62)-C(57)-N(5)	118.4(3)	C(66)-C(67)-H(67B)	111.4
C(59)-C(58)-C(57)	118.0(3)	H(67A)-C(67)-H(67B)	109.3
C(59)-C(58)-C(63)	120.8(3)	O(3)-C(68)-C(69)	109.0(2)
C(57)-C(58)-C(63)	121.3(3)	O(3)-C(68)-C(70)	106.4(2)

C(69)-C(68)-C(70)	112.4(3)	N(6)-C(79)-C(82)	106.0(2)
O(3)-C(68)-H(68)	109.7	C(78)-C(79)-C(82)	114.8(3)
C(69)-C(68)-H(68)	109.7	O(4)-C(80)-C(81)	106.2(3)
C(70)-C(68)-H(68)	109.7	O(4)-C(80)-H(80A)	110.5
C(68)-C(69)-H(69A)	109.4	C(81)-C(80)-H(80A)	110.5
C(68)-C(69)-H(69B)	109.4	O(4)-C(80)-H(80B)	110.5
H(69A)-C(69)-H(69B)	109.5	C(81)-C(80)-H(80B)	110.5
C(68)-C(69)-H(69C)	109.6	H(80A)-C(80)-H(80B)	108.7
H(69A)-C(69)-H(69C)	109.5	N(6)-C(81)-C(80)	103.4(3)
H(69B)-C(69)-H(69C)	109.5	N(6)-C(81)-H(81A)	111.1
C(68)-C(70)-H(70A)	109.6	C(80)-C(81)-H(81A)	111.1
C(68)-C(70)-H(70B)	109.4	N(6)-C(81)-H(81B)	111.1
H(70A)-C(70)-H(70B)	109.5	C(80)-C(81)-H(81B)	111.1
C(68)-C(70)-H(70C)	109.5	H(81A)-C(81)-H(81B)	109.1
H(70A)-C(70)-H(70C)	109.5	C(85)-C(82)-C(83)	114.5(3)
H(70B)-C(70)-H(70C)	109.5	C(85)-C(82)-C(84)	109.1(2)
C(72)-C(71)-O(3)	126.4(3)	C(83)-C(82)-C(84)	109.5(3)
C(72)-C(71)-C(76)	120.9(3)	C(85)-C(82)-C(79)	99.4(2)
O(3)-C(71)-C(76)	112.7(2)	C(83)-C(82)-C(79)	113.2(3)
C(71)-C(72)-C(73)	118.9(3)	C(84)-C(82)-C(79)	110.7(3)
C(71)-C(72)-H(72)	120.6	C(82)-C(83)-H(83A)	109.5
C(73)-C(72)-H(72)	120.6	C(82)-C(83)-H(83B)	109.5
C(74)-C(73)-C(72)	122.5(3)	H(83A)-C(83)-H(83B)	109.5
C(74)-C(73)-H(73)	118.8	C(82)-C(83)-H(83C)	109.5
C(72)-C(73)-H(73)	118.8	H(83A)-C(83)-H(83C)	109.5
C(75)-C(74)-C(73)	117.3(3)	H(83B)-C(83)-H(83C)	109.5
C(75)-C(74)-C(77)	123.2(3)	C(82)-C(84)-H(84A)	109.4
C(73)-C(74)-C(77)	119.5(3)	C(82)-C(84)-H(84B)	109.5
C(74)-C(75)-C(76)	121.7(3)	H(84A)-C(84)-H(84B)	109.5
C(74)-C(75)-H(75)	119.1	C(82)-C(84)-H(84C)	109.5
C(76)-C(75)-H(75)	119.1	H(84A)-C(84)-H(84C)	109.5
C(71)-C(76)-C(75)	118.7(3)	H(84B)-C(84)-H(84C)	109.5
C(71)-C(76)-C(4)	118.0(3)	C(86)-C(85)-C(90)	120.4(3)
C(75)-C(76)-C(4)	123.2(3)	C(86)-C(85)-C(82)	129.7(3)
C(78)-C(77)-C(74)	126.3(3)	C(90)-C(85)-C(82)	109.8(3)
C(78)-C(77)-H(77)	116.9	C(87)-C(86)-C(85)	117.2(3)
C(74)-C(77)-H(77)	116.9	C(87)-C(86)-H(86)	121.4
C(77)-C(78)-C(79)	124.0(3)	C(85)-C(86)-H(86)	121.4
C(77)-C(78)-H(78)	118.0	C(88)-C(87)-C(86)	122.7(3)
C(79)-C(78)-H(78)	118.0	C(88)-C(87)-Cl(10)	118.6(2)
O(4)-C(79)-N(6)	103.1(2)	C(86)-C(87)-Cl(10)	118.7(3)
O(4)-C(79)-C(78)	111.4(2)	C(87)-C(88)-C(89)	120.2(3)
N(6)-C(79)-C(78)	111.8(3)	C(87)-C(88)-H(88)	119.9
O(4)-C(79)-C(82)	109.0(2)	C(89)-C(88)-H(88)	119.9

C(88)-C(89)-C(90)	117.7(3)	Cl(13)-C(94)-H(94B)	109.3
C(88)-C(89)-H(89)	121.2	Cl(14)-C(94)-H(94B)	109.3
C(90)-C(89)-H(89)	121.2	H(94A)-C(94)-H(94B)	108.0
C(89)-C(90)-C(85)	121.9(3)	Cl(16)-C(95)-Cl(15)	113.3(2)
C(89)-C(90)-N(6)	127.0(3)	Cl(16)-C(95)-H(95A)	108.9
C(85)-C(90)-N(6)	111.1(3)	Cl(15)-C(95)-H(95A)	108.9
Cl(12)-C(93)-Cl(11)	111.7(2)	Cl(16)-C(95)-H(95B)	108.9
Cl(12)-C(93)-H(93A)	109.3	Cl(15)-C(95)-H(95B)	108.9
Cl(11)-C(93)-H(93A)	109.3	H(95A)-C(95)-H(95B)	107.7
Cl(12)-C(93)-H(93B)	109.3	Cl(17)-C(96)-Cl(18)	111.2(2)
Cl(11)-C(93)-H(93B)	109.3	Cl(17)-C(96)-H(96A)	109.4
H(93A)-C(93)-H(93B)	107.9	Cl(18)-C(96)-H(96A)	109.4
Cl(13)-C(94)-Cl(14)	111.6(2)	Cl(17)-C(96)-H(96B)	109.4
Cl(13)-C(94)-H(94A)	109.3	Cl(18)-C(96)-H(96B)	109.4
Cl(14)-C(94)-H(94A)	109.3	H(96A)-C(96)-H(96B)	108.0

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