

Supporting Information for

**Substituent Effect on the Catalytic Activity of Ru(II) Complexes Bearing a
Pyridyl-Supported Pyrazolyl-Imidazolyl Ligand for Transfer Hydrogenation of
Ketones**

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1. Copies of NMR spectra

CHN-117 ^1H NMR in DMSO- d_6

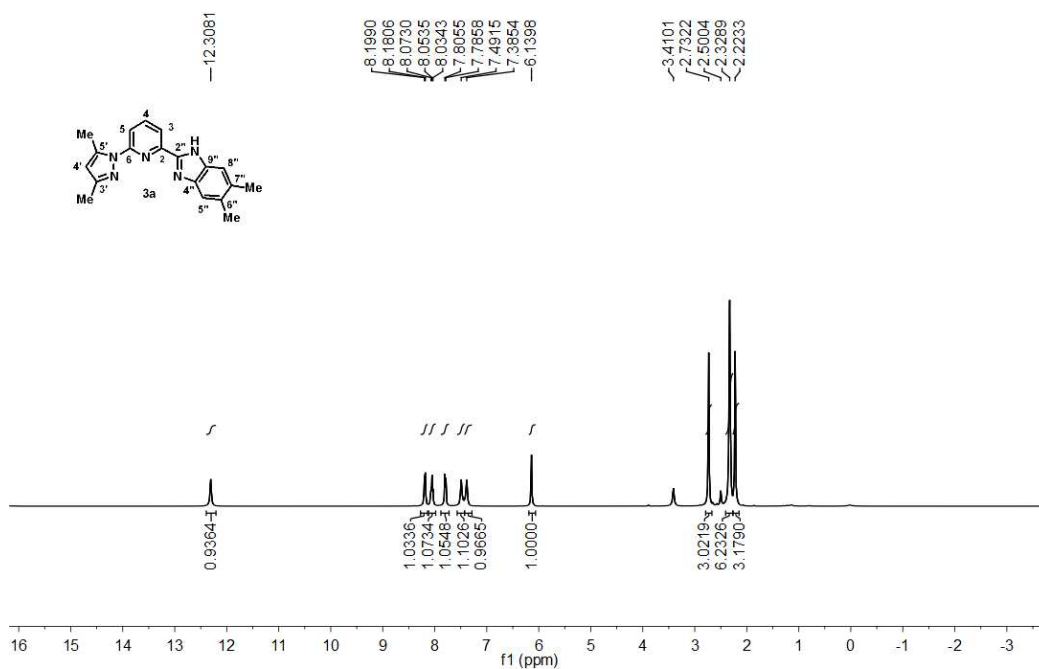


Figure S1. ^1H NMR spectrum of **3a** in DMSO- d_6 .

CHN-117 ^{13}C NMR in DMSO- d_6

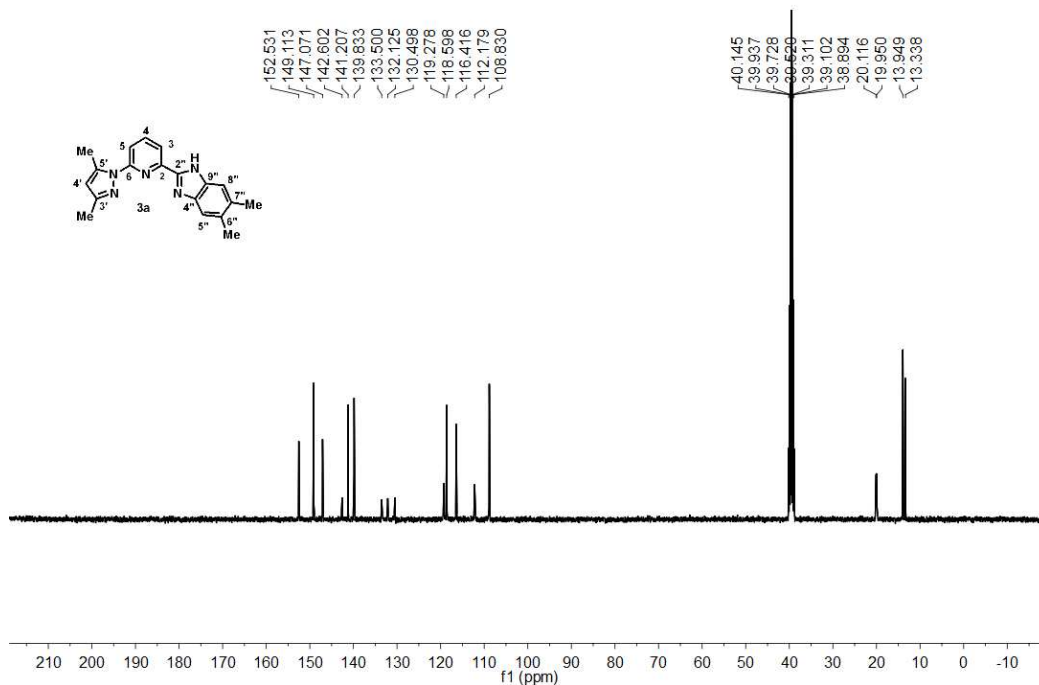


Figure S2. ^{13}C NMR spectrum of **3a** in DMSO- d_6 .

CHN-124 ^1H NMR in DMSO- d_6

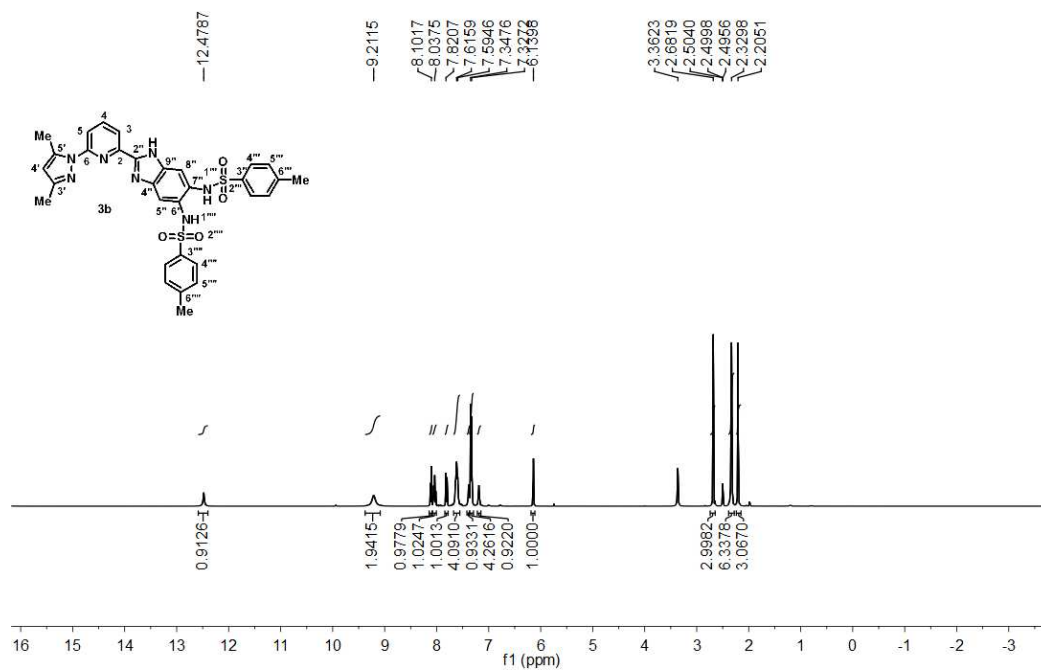


Figure S3. ^1H NMR spectrum of **3b** in DMSO- d_6 .

CHN-124 ^{13}C NMR in DMSO- d_6

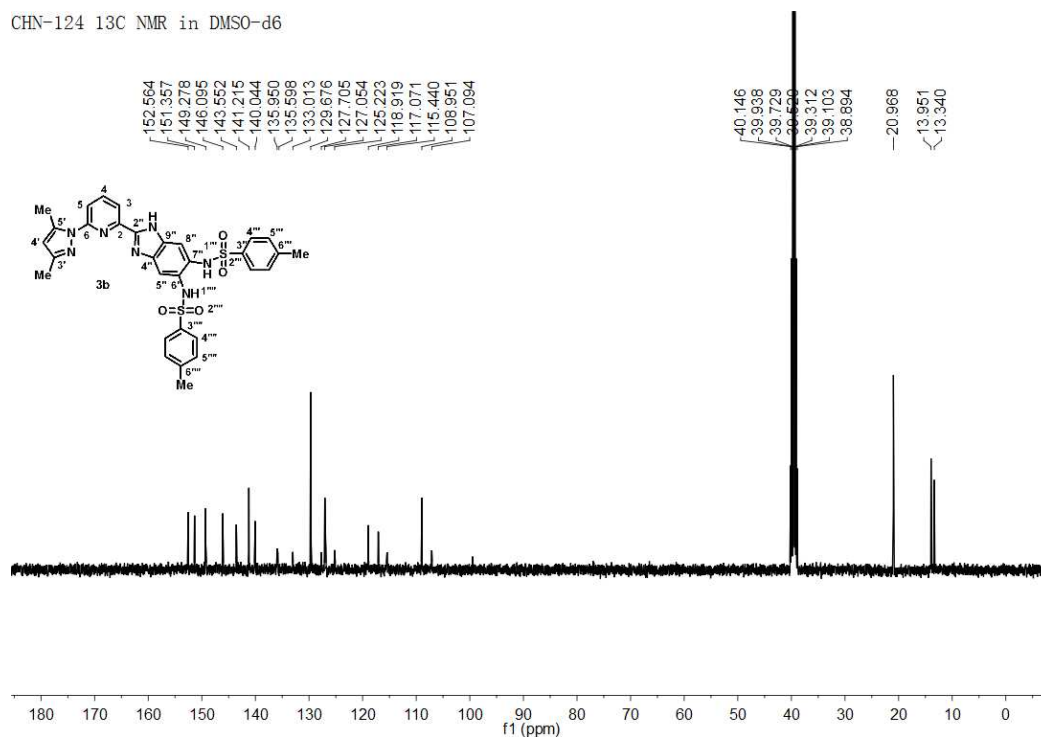


Figure S4. ^{13}C NMR spectrum of **3b** in DMSO- d_6 .

CHN-097 ^1H NMR in DMSO- d_6

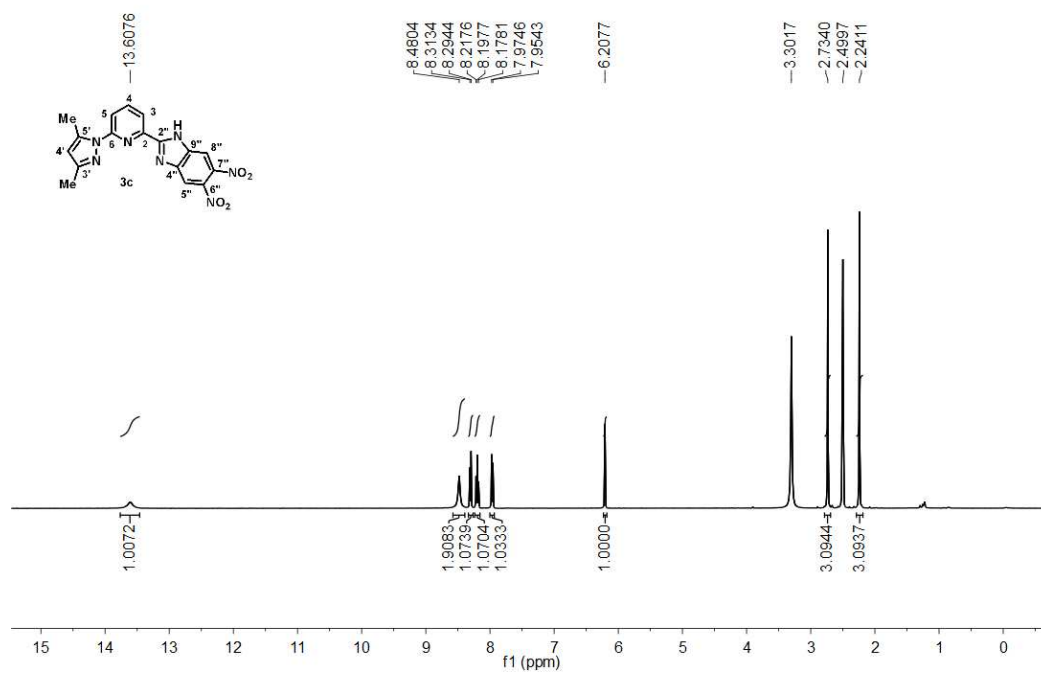


Figure S5. ^1H NMR spectrum of **3c** in DMSO- d_6 .

CHN-097 ^{13}C NMR in DMSO- d_6

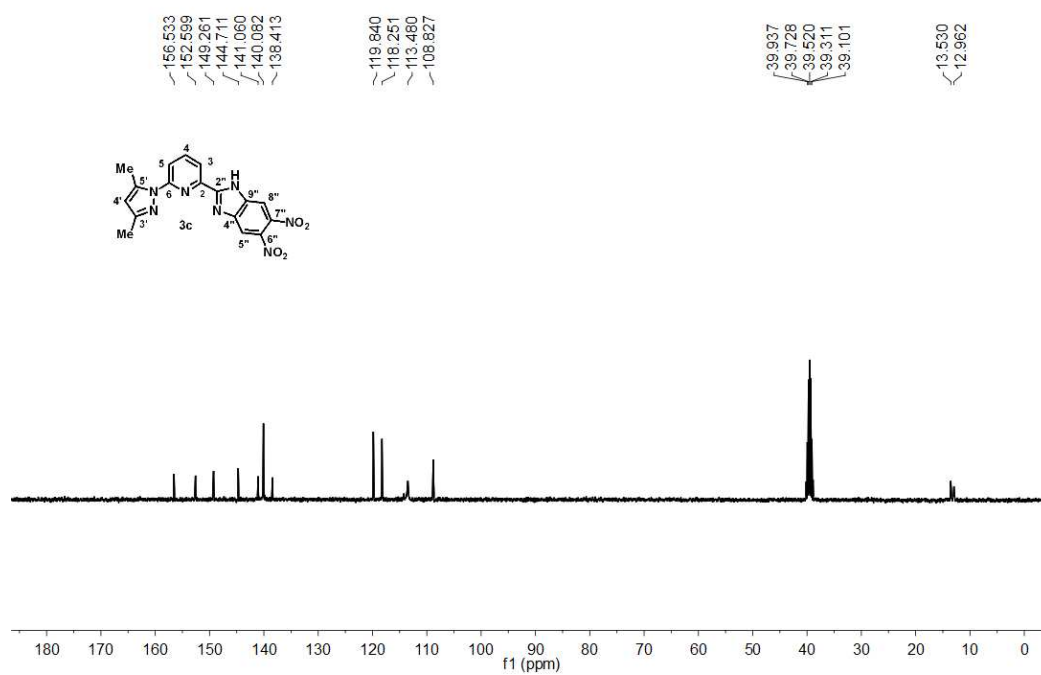


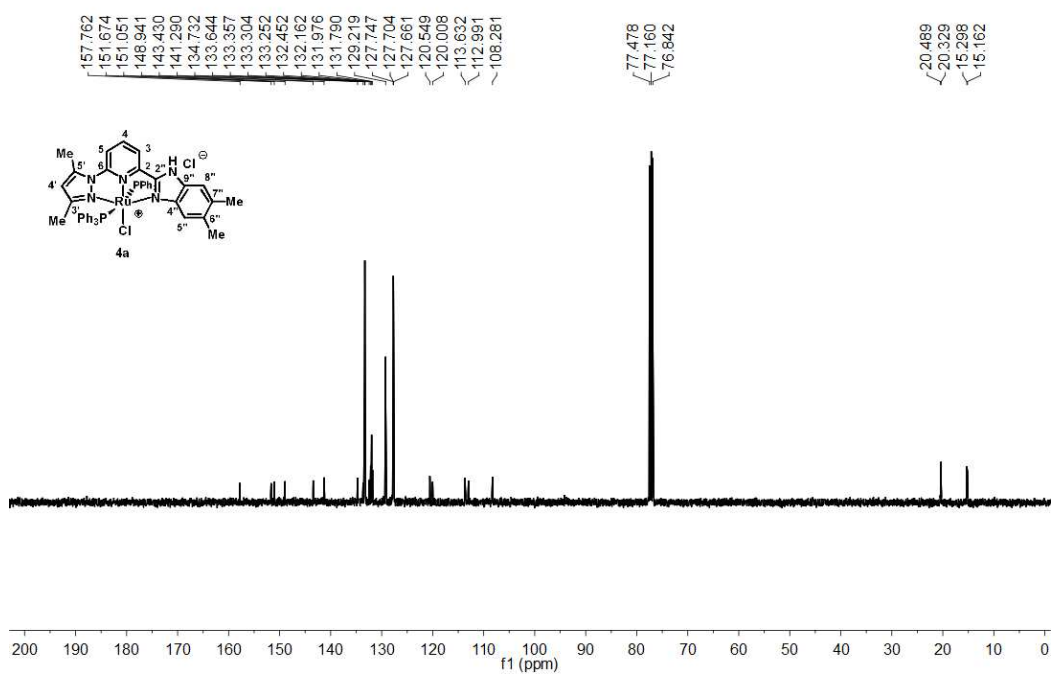
Figure S6. ^{13}C NMR spectrum of **3c** in DMSO- d_6 .

Chemical structure of **4a** is shown above the spectrum. The structure is a macrocyclic complex with a central Ru(II) atom coordinated by two phosphorus atoms (PPh₃ and PPh₂), two nitrogen atoms (NMe₂ and NMe), and a chloride ligand. The macrocycle contains two methyl groups and a chloride ligand.

¹H NMR spectrum (CDCl₃) of **4a** is shown below. The x-axis represents the chemical shift in ppm (δ), ranging from 0 to 16. The y-axis represents the intensity of the signal.

Peak list (ppm): 0.8741, 1.0001, 1.0224, 1.1689, 1.0912, 12.4502, 6.3801, 12.4824, 1.0155, 1.0000, 6.0895, 3.0428, 3.0158.

Integration values are provided below the baseline: 1.0001, 1.0224, 1.1689, 1.0912, 12.4502, 6.3801, 12.4824, 1.0155, 1.0000, 6.0895, 3.0428, 3.0158.

CHN-120 ¹³C NMR in CDCl₃

S5

CHN-120 ^{31}P NMR in CDCl_3

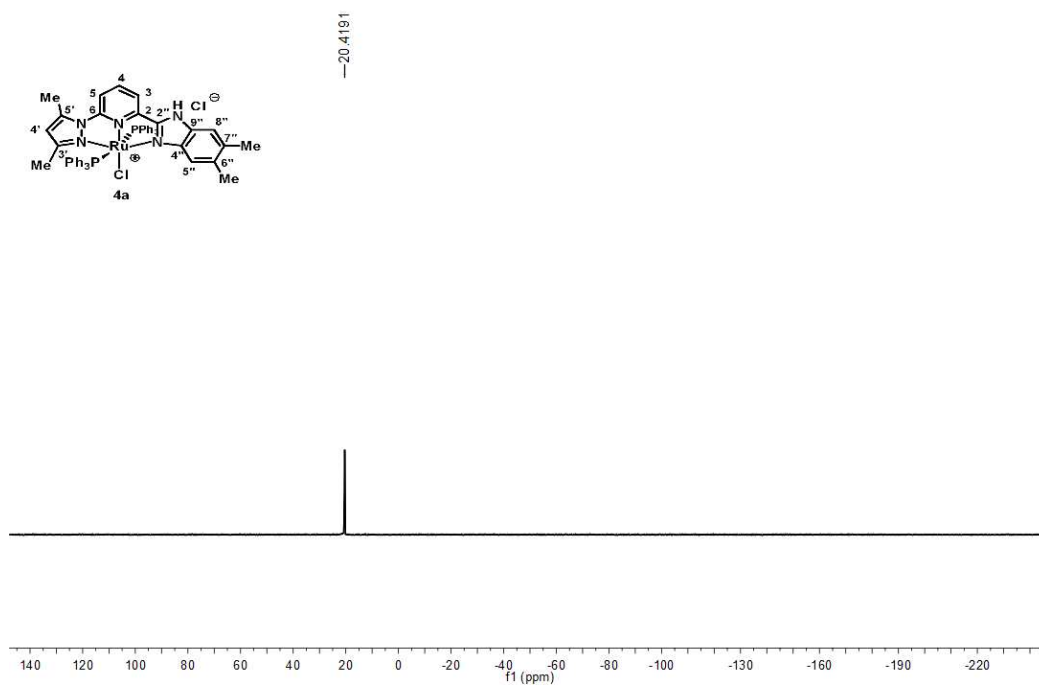


Figure S9. ^{31}P NMR spectrum of **4a** in CDCl_3 .

CHN-084 ^1H NMR in $\text{CDCl}_3/\text{CD}_3\text{OD}$

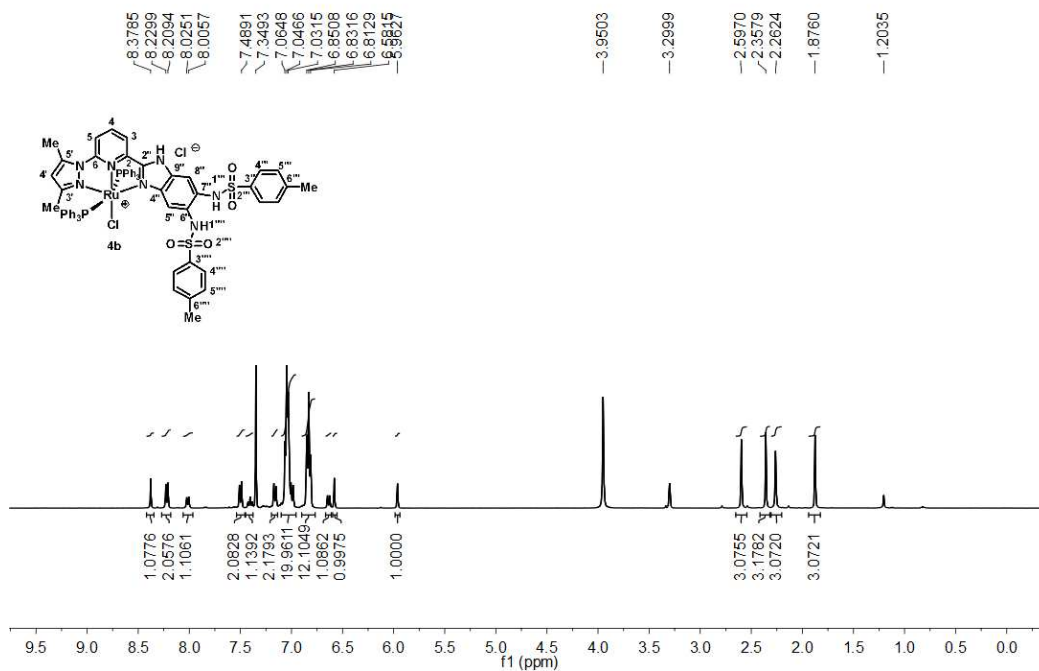


Figure S10. ^1H NMR spectrum of **4b** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

CHN-084 ^{13}C NMR in $\text{CDCl}_3/\text{CD}_3\text{OD}$

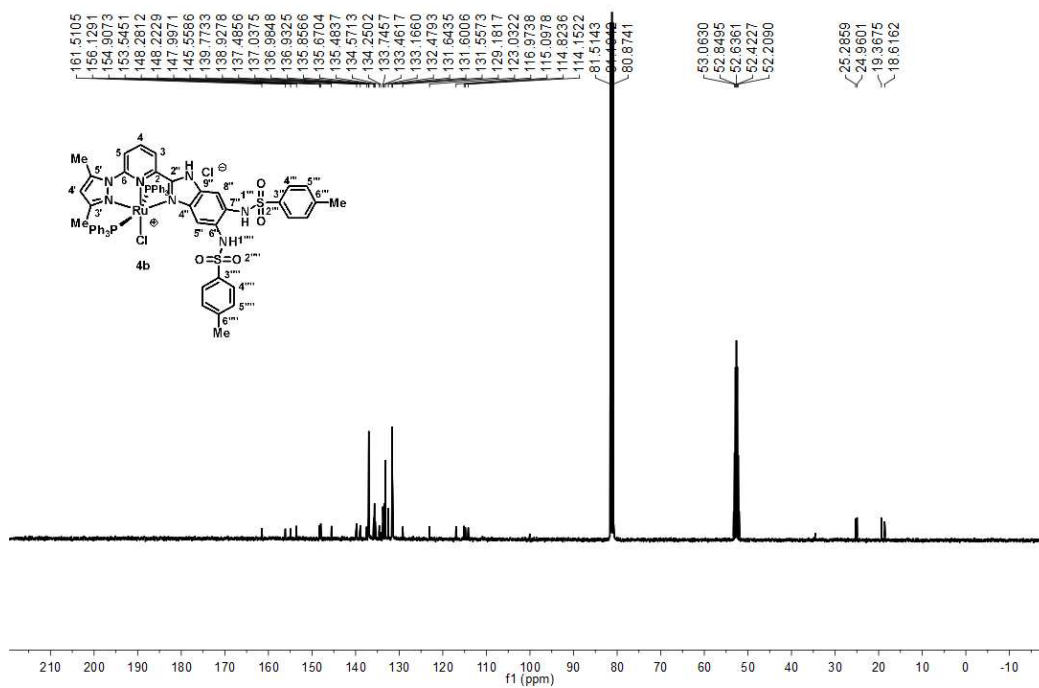


Figure S11. ^{13}C NMR spectrum of **4b** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

CHN-084 ^{31}P NMR in CDCl_3

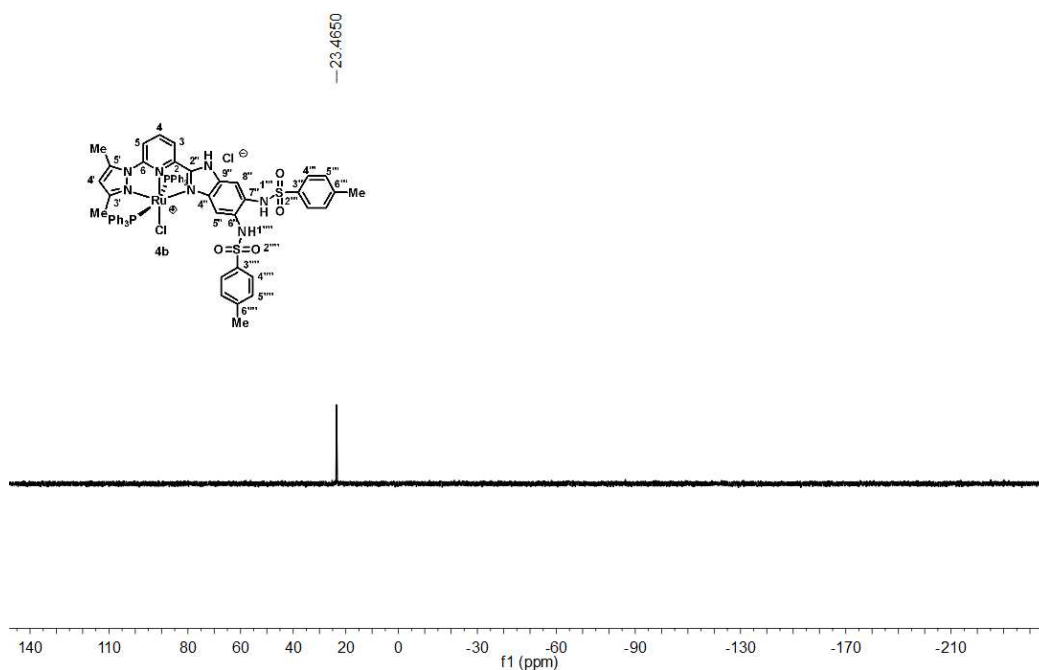


Figure S12. ^{31}P NMR spectrum of **4b** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

CHN-125 ^1H NMR in CDCl_3

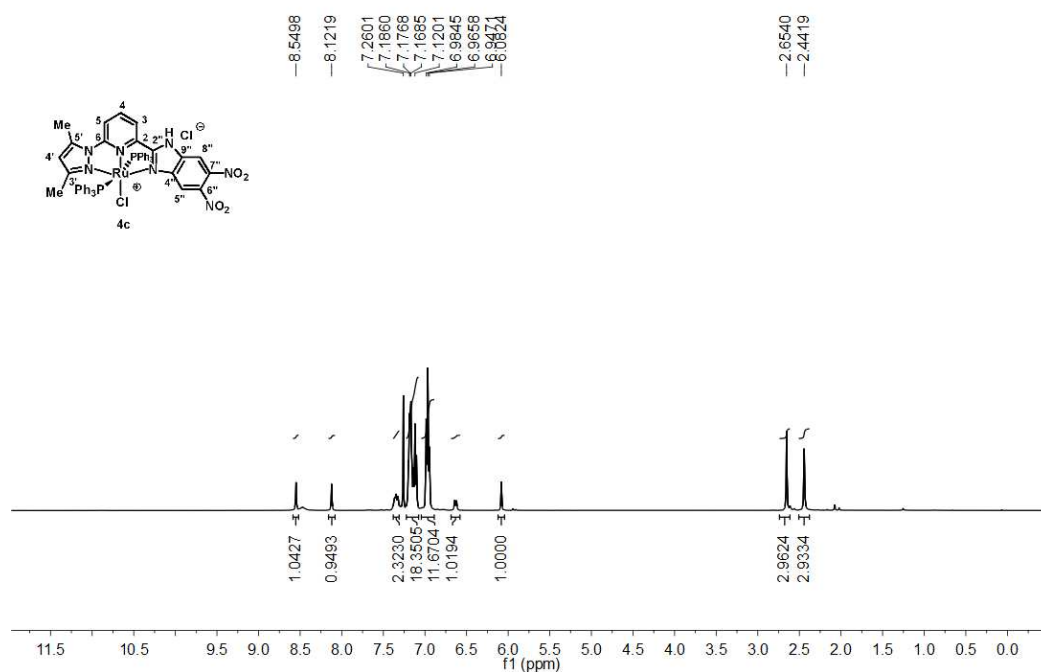


Figure S13. ^1H NMR spectrum of **4c** in CDCl_3 .

CHN-125 ^{13}C NMR in CDCl_3

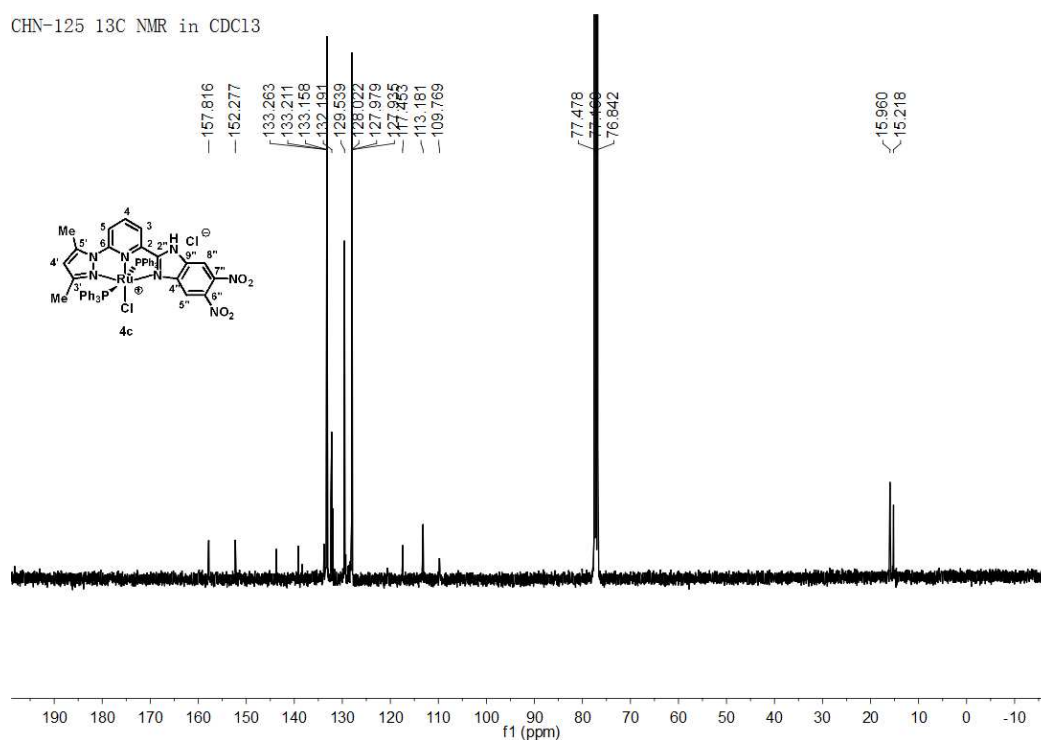


Figure S14. ^{13}C NMR spectrum of **4c** in CDCl_3 .

CHN-125 ^{31}P NMR in CDCl_3

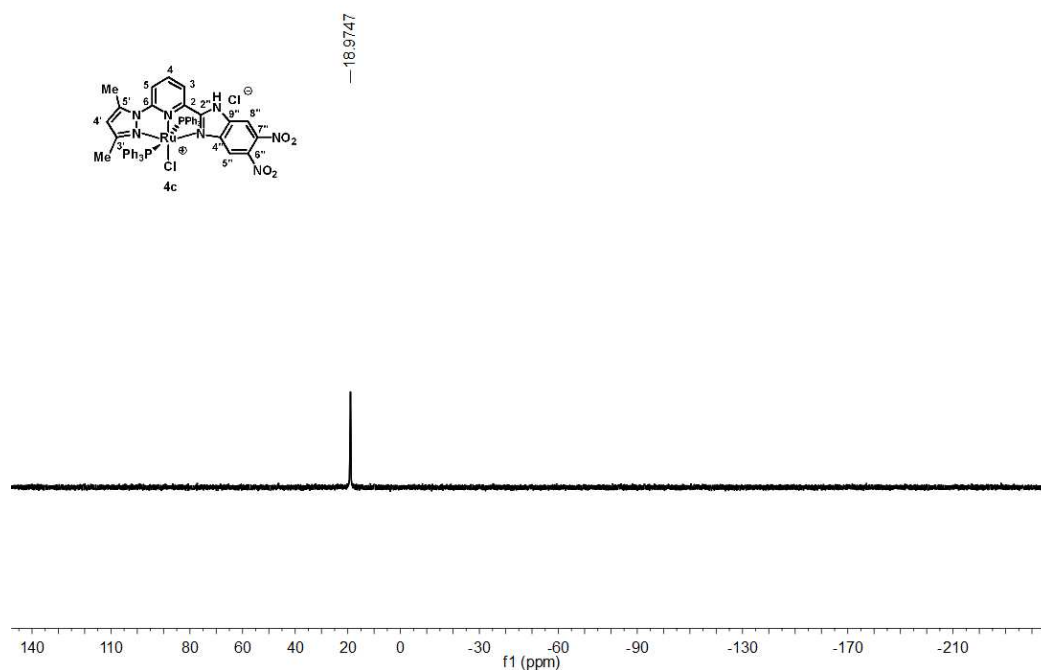


Figure S15. ^{31}P NMR spectrum of **4c** in CDCl_3 .

CHN-472 ^1H NMR in CDCl_3

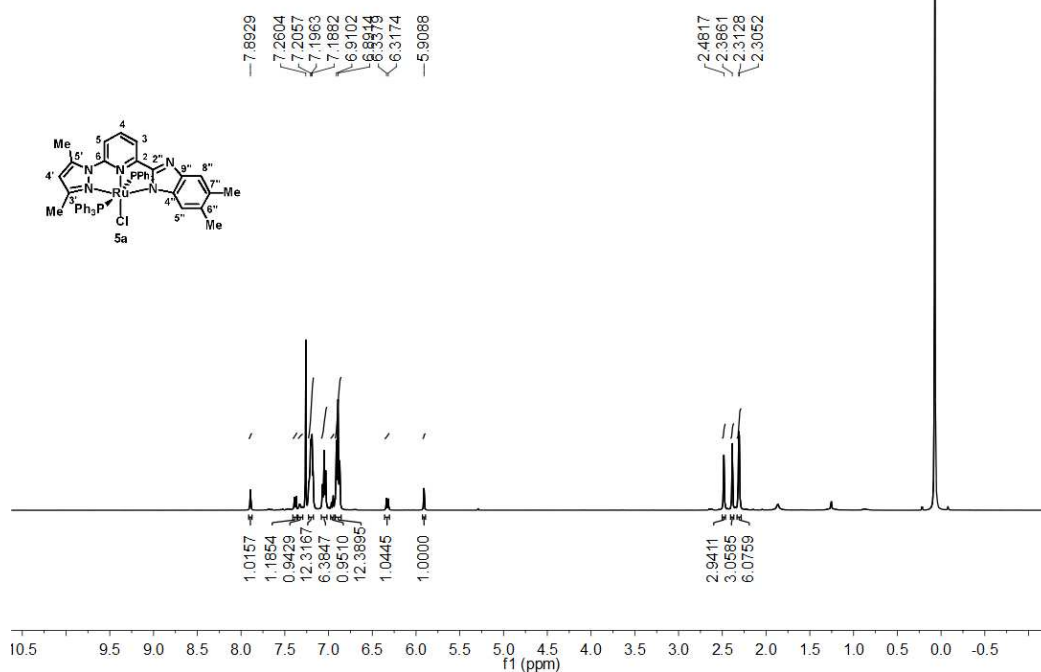


Figure S16. ^1H NMR spectrum of **5a** in CDCl_3 .

CHN-472 ^{13}C NMR in CDCl_3

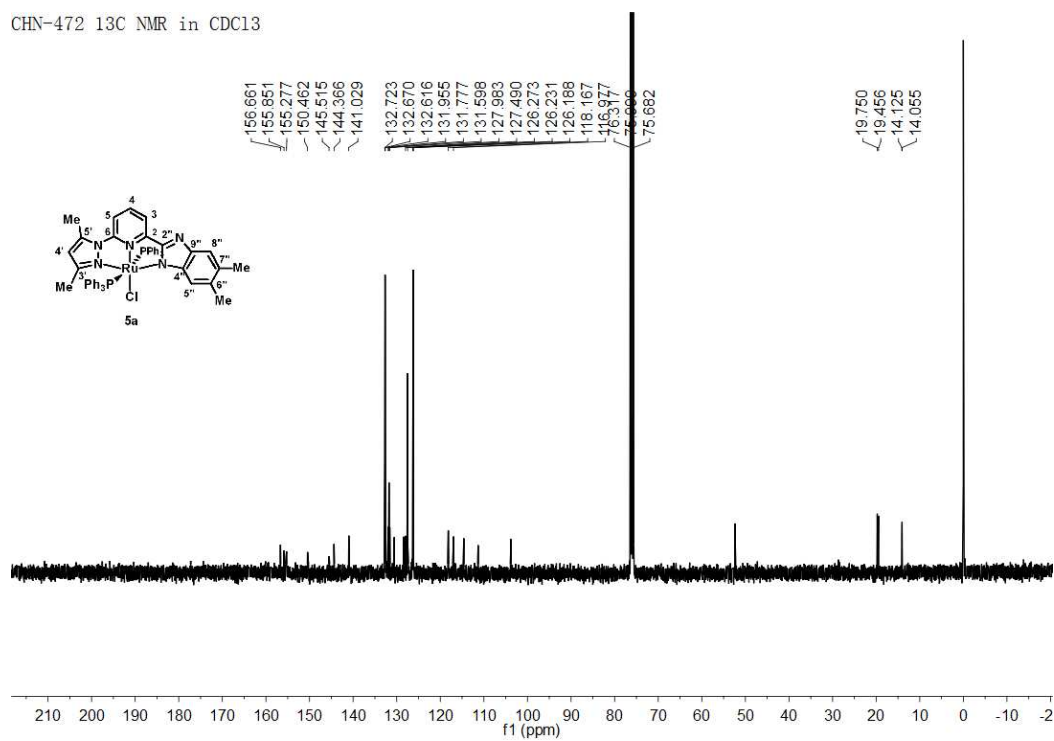


Figure S17. ^{13}C NMR spectrum of **5a** in CDCl_3 .

CHN-472 ^{31}P NMR in CDCl_3

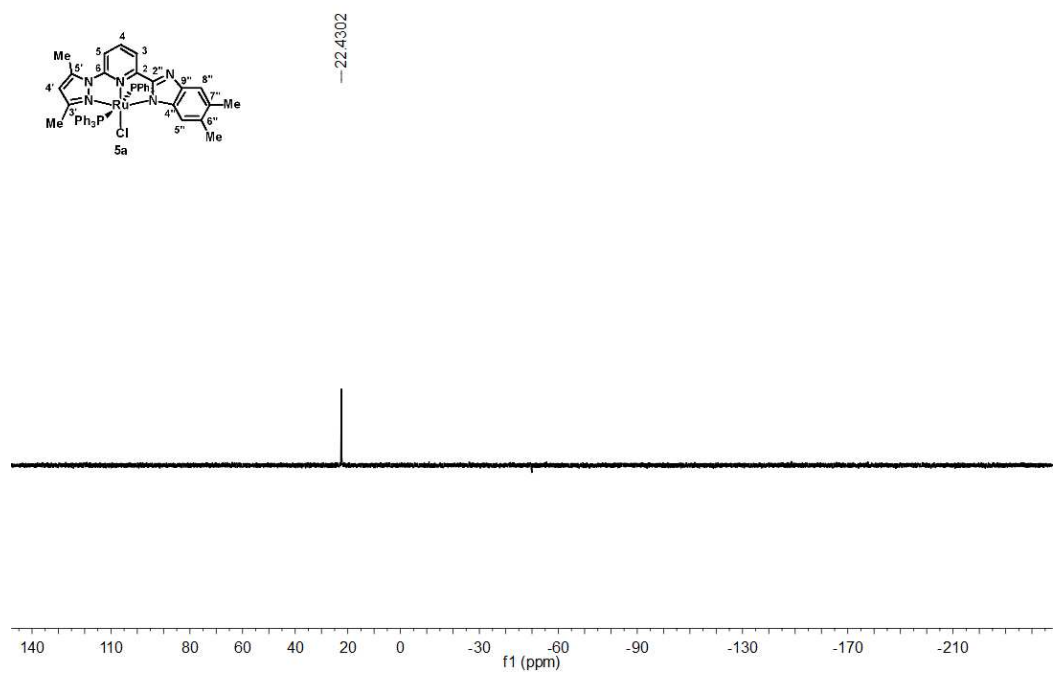


Figure S18. ^{31}P NMR spectrum of **5a** in CDCl_3 .

CHN-129 ^1H NMR in CDCl_3

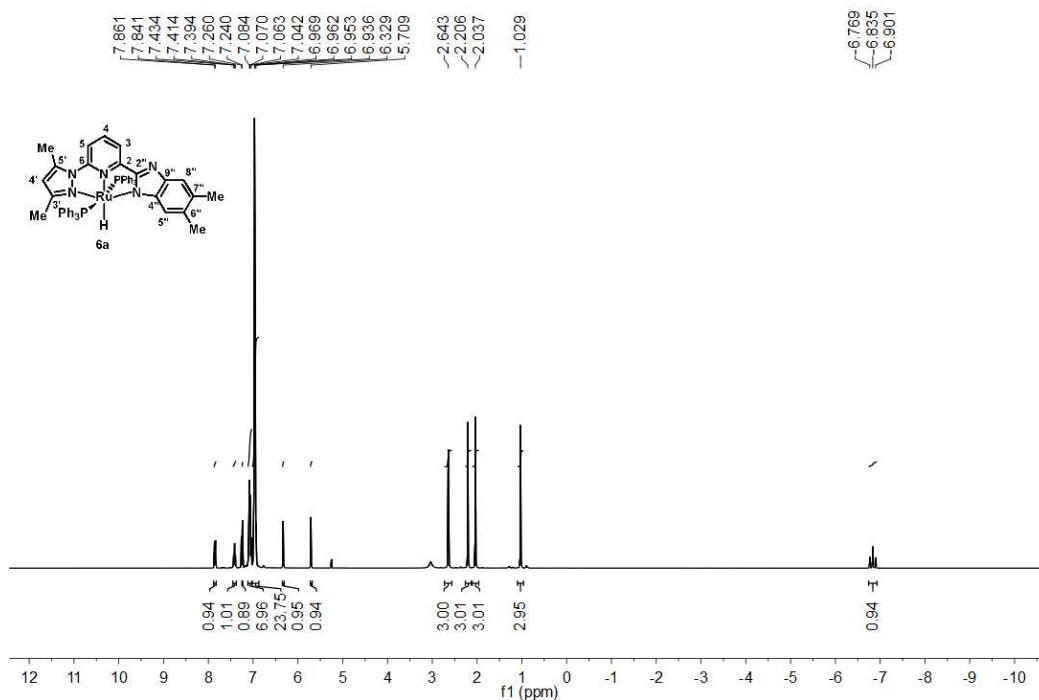


Figure S19. ^1H NMR spectrum of **6a** in CDCl_3 .

CHN-129 ^{13}C NMR in CDCl_3

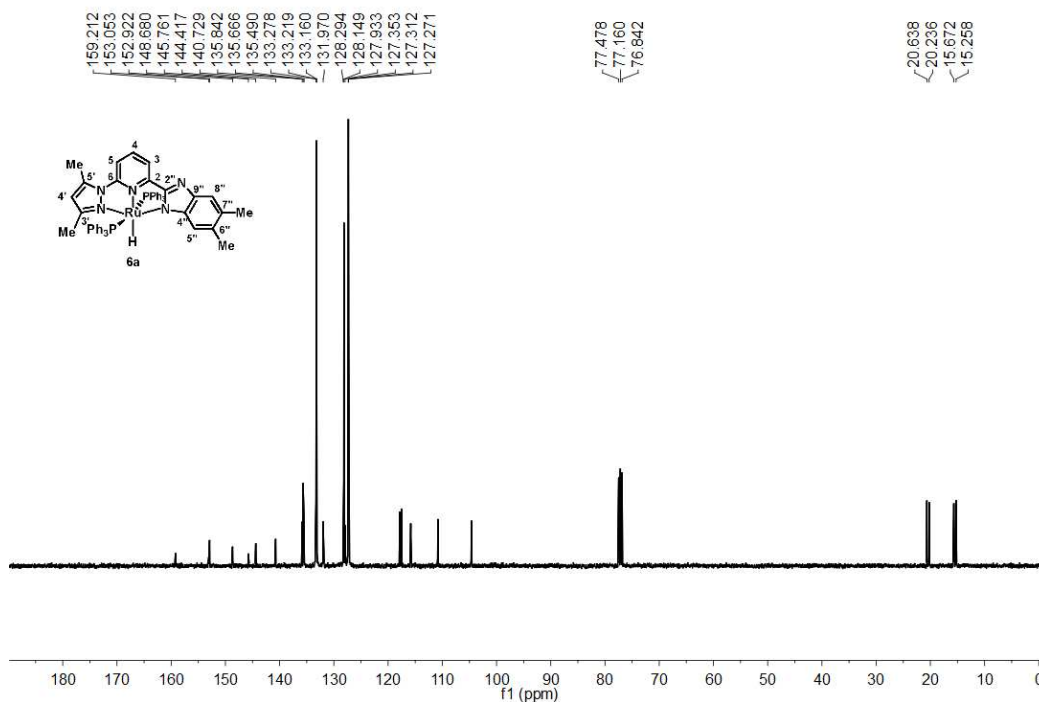


Figure S20. ^{13}C NMR spectrum of **6a** in CDCl_3 .

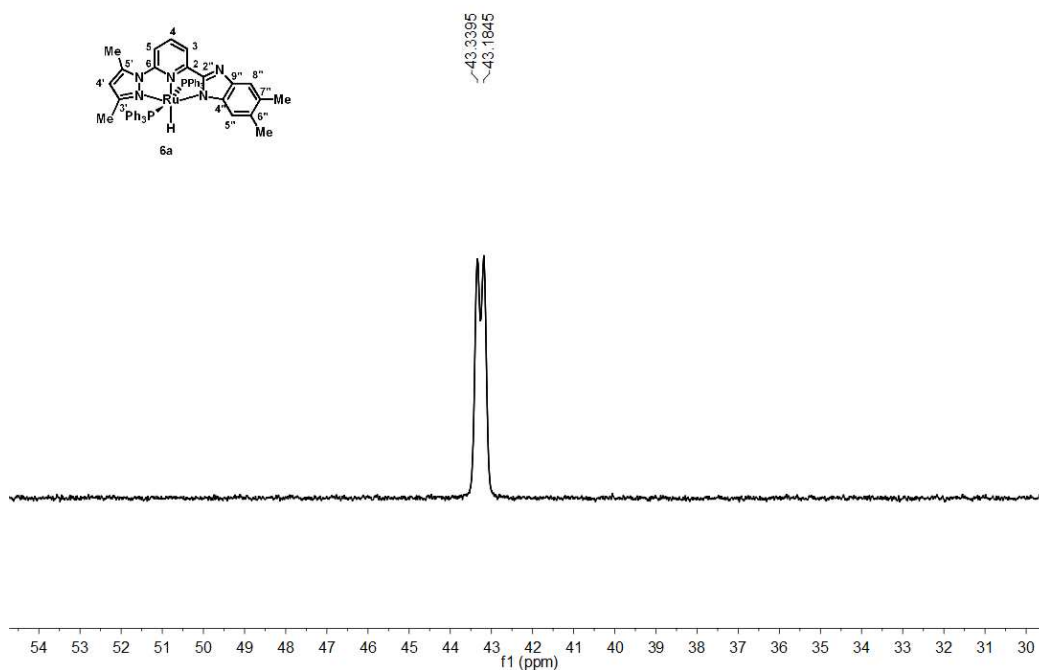


Figure S21. ^{31}P NMR spectrum of **6a** in CDCl_3 .

2. X-Ray crystallographic data

The supplemental file (4b_6a.xyz) contains the computed Cartesian coordinates of all of the molecules reported in this study. The file may be opened as a text file to read the coordinates, or opened directly by a molecular modeling program such as Mercury (version 3.3 or later, <http://www.ccdc.cam.ac.uk/pages/Home.aspx>) for visualization and analysis.

2.1 X-Ray crystallographic data for 4b

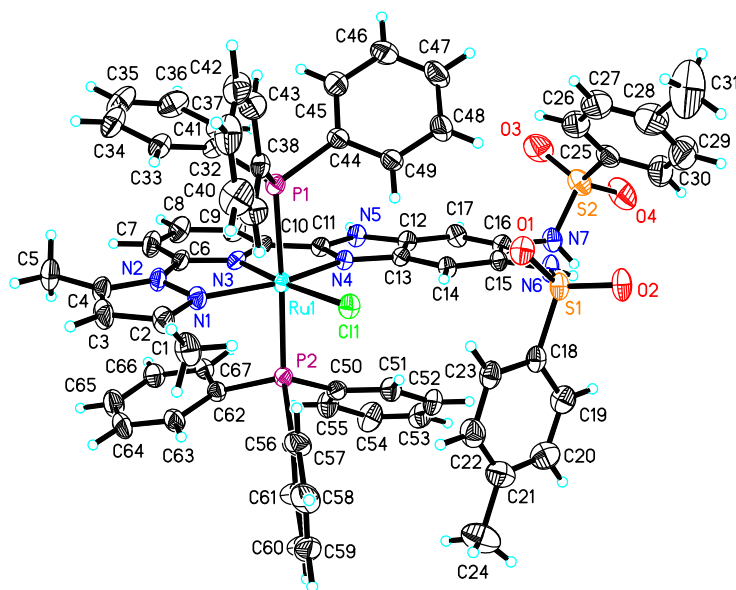


Figure S22. Molecular structure of complex **4b**. Two CHCl₃ molecules are omitted for clarity.

Table S1. Crystal data and structure refinement for **4b**.

Identification code	cd214121	
Empirical formula	C ₁₃₈ H ₁₂₂ Cl ₁₆ N ₁₄ O ₈ P ₄ Ru ₂ S ₄	
Formula weight	3125.95	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /c	
Unit cell dimensions	a = 17.2774(7) Å	α = 90°.
	b = 18.1856(7) Å	β = 100.0810(10)°.
	c = 24.7095(11) Å	γ = 90°.
Volume	7643.9(5) Å ³	
Z	2	
Density (calculated)	1.358 Mg/m ³	
Absorption coefficient	0.630 mm ⁻¹	
F(000)	3192	
Crystal size	0.143 x 0.121 x 0.105 mm ³	
Theta range for data collection	1.639 to 25.500°.	
Index ranges	−? ≤ h ≤ ?, −? ≤ k ≤ ?, −? ≤ l ≤ ?	
Reflections collected	?	

Independent reflections	14208 [R(int) = ?]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6669
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	14208 / 7 / 864
Goodness-of-fit on F ²	0.993
Final R indices [I>2sigma(I)]	R1 = 0.0552, wR2 = 0.1339
R indices (all data)	R1 = 0.0837, wR2 = 0.1463
Extinction coefficient	n/a
Largest diff. peak and hole	0.757 and -0.828 e.Å ⁻³

Table S2. Bond lengths [Å] and angles [°] for **4b**.

Ru(1)-N(3)	1.978(3)
Ru(1)-N(1)	2.097(3)
Ru(1)-N(4)	2.116(3)
Ru(1)-P(1)	2.3947(11)
Ru(1)-P(2)	2.4033(11)
Ru(1)-Cl(1)	2.4467(9)
S(1)-O(1)	1.417(3)
S(1)-O(2)	1.429(3)
S(1)-N(6)	1.623(3)
S(1)-C(18)	1.751(5)
S(2)-O(4)	1.418(4)
S(2)-O(3)	1.422(4)
S(2)-N(7)	1.625(4)
S(2)-C(25)	1.757(5)
P(1)-C(32)	1.831(4)
P(1)-C(44)	1.832(4)
P(1)-C(38)	1.834(4)
P(2)-C(50)	1.829(4)
P(2)-C(62)	1.836(4)
P(2)-C(56)	1.839(4)
Cl(3)-C(68)	1.744(7)
Cl(4)-C(68)	1.709(7)
Cl(5)-C(68)	1.742(7)
Cl(6)-C(69)	1.745(6)

Cl(7)-C(69)	1.748(5)
Cl(8)-C(69)	1.733(5)
N(1)-C(2)	1.324(5)
N(1)-N(2)	1.418(4)
N(2)-C(4)	1.382(5)
N(2)-C(6)	1.387(5)
N(3)-C(6)	1.346(5)
N(3)-C(10)	1.354(4)
N(4)-C(11)	1.344(4)
N(4)-C(13)	1.395(4)
N(5)-C(11)	1.345(5)
N(5)-C(12)	1.374(5)
N(5)-H(5)	0.85(5)
N(6)-C(15)	1.410(5)
N(6)-H(6)	0.69(3)
N(7)-C(16)	1.427(5)
N(7)-H(7A)	0.83(4)
C(1)-C(2)	1.492(6)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.397(6)
C(3)-C(4)	1.326(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.501(7)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-C(7)	1.391(6)
C(7)-C(8)	1.356(6)
C(7)-H(7)	0.9300
C(8)-C(9)	1.379(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.379(5)
C(9)-H(9)	0.9300
C(10)-C(11)	1.442(5)
C(12)-C(17)	1.377(5)
C(12)-C(13)	1.395(5)

C(13)-C(14)	1.387(5)
C(14)-C(15)	1.376(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.420(5)
C(16)-C(17)	1.373(5)
C(17)-H(17)	0.9300
C(18)-C(23)	1.370(5)
C(18)-C(19)	1.379(6)
C(19)-C(20)	1.365(7)
C(19)-H(19)	0.9300
C(20)-C(21)	1.387(7)
C(20)-H(20)	0.9300
C(21)-C(22)	1.369(7)
C(21)-C(24)	1.514(8)
C(22)-C(23)	1.365(7)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(30)	1.354(7)
C(25)-C(26)	1.367(7)
C(26)-C(27)	1.357(8)
C(26)-H(26)	0.9300
C(27)-C(28)	1.359(9)
C(27)-H(27)	0.9300
C(28)-C(29)	1.354(9)
C(28)-C(31)	1.37(2)
C(28)-C(31')	1.485(17)
C(29)-C(30)	1.381(8)
C(29)-H(29)	0.9300
C(30)-H(30)	0.9300
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(31')-H(31D)	0.9600
C(31')-H(31E)	0.9600
C(31')-H(31F)	0.9600

C(32)-C(37)	1.390(6)
C(32)-C(33)	1.395(6)
C(33)-C(34)	1.385(6)
C(33)-H(33)	0.9300
C(34)-C(35)	1.367(7)
C(34)-H(34)	0.9300
C(35)-C(36)	1.379(7)
C(35)-H(35)	0.9300
C(36)-C(37)	1.392(6)
C(36)-H(36)	0.9300
C(37)-H(37)	0.9300
C(38)-C(39)	1.377(6)
C(38)-C(43)	1.380(7)
C(39)-C(40)	1.389(7)
C(39)-H(39)	0.9300
C(40)-C(41)	1.365(8)
C(40)-H(40)	0.930
0	
C(41)-C(42)	1.372(8)
C(41)-H(41)	0.9300
C(42)-C(43)	1.378(7)
C(42)-H(42)	0.9300
C(43)-H(43)	0.9300
C(44)-C(45)	1.382(6)
C(44)-C(49)	1.382(6)
C(45)-C(46)	1.365(7)
C(45)-H(45)	0.9300
C(46)-C(47)	1.366(7)
C(46)-H(46)	0.9300
C(47)-C(48)	1.383(7)
C(47)-H(47)	0.9300
C(48)-C(49)	1.373(6)
C(48)-H(48)	0.9300
C(49)-H(49)	0.9300
C(50)-C(55)	1.380(6)
C(50)-C(51)	1.390(6)
C(51)-C(52)	1.397(6)
C(51)-H(51)	0.9300

C(52)-C(53)	1.358(7)
C(52)-H(52)	0.9300
C(53)-C(54)	1.354(7)
C(53)-H(53)	0.9300
C(54)-C(55)	1.393(6)
C(54)-H(54)	0.9300
C(55)-H(55)	0.9300
C(56)-C(61)	1.363(7)
C(56)-C(57)	1.378(6)
C(57)-C(58)	1.385(7)
C(57)-H(57)	0.9300
C(58)-C(59)	1.340(8)
C(58)-H(58)	0.9300
C(59)-C(60)	1.346(8)
C(59)-H(59)	0.9300
C(60)-C(61)	1.372(7)
C(60)-H(60)	0.9300
C(61)-H(61)	0.9300
C(62)-C(67)	1.390(5)
C(62)-C(63)	1.393(5)
C(63)-C(64)	1.385(6)
C(63)-H(63)	0.9300
C(64)-C(65)	1.369(7)
C(64)-H(64)	0.9300
C(65)-C(66)	1.373(6)
C(65)-H(65)	0.9300
C(66)-C(67)	1.386(5)
C(66)-H(66)	0.9300
C(67)-H(67)	0.9300
C(68)-H(68)	0.9800
C(69)-H(69)	0.9800
N(3)-Ru(1)-N(1)	78.41(13)
N(3)-Ru(1)-N(4)	78.95(12)
N(1)-Ru(1)-N(4)	157.33(12)
N(3)-Ru(1)-P(1)	88.78(10)
N(1)-Ru(1)-P(1)	89.38(10)
N(4)-Ru(1)-P(1)	91.40(9)

N(3)-Ru(1)-P(2)	89.18(10)
N(1)-Ru(1)-P(2)	88.53(10)
N(4)-Ru(1)-P(2)	89.90(9)
P(1)-Ru(1)-P(2)	177.33(4)
N(3)-Ru(1)-Cl(1)	174.52(10)
N(1)-Ru(1)-Cl(1)	106.68(9)
N(4)-Ru(1)-Cl(1)	95.99(8)
P(1)-Ru(1)-Cl(1)	89.25(4)
P(2)-Ru(1)-Cl(1)	92.94(4)
O(1)-S(1)-O(2)	119.14(19)
O(1)-S(1)-N(6)	108.34(19)
O(2)-S(1)-N(6)	105.25(18)
O(1)-S(1)-C(18)	108.6(2)
O(2)-S(1)-C(18)	108.4(2)
N(6)-S(1)-C(18)	106.48(19)
O(4)-S(2)-O(3)	120.2(2)
O(4)-S(2)-N(7)	105.6(2)
O(3)-S(2)-N(7)	107.1(2)
O(4)-S(2)-C(25)	107.7(2)
O(3)-S(2)-C(25)	108.1(3)
N(7)-S(2)-C(25)	107.5(2)
C(32)-P(1)-C(44)	105.6(2)
C(32)-P(1)-C(38)	99.77(17)
C(44)-P(1)-C(38)	100.09(18)
C(32)-P(1)-Ru(1)	111.35(14)
C(44)-P(1)-Ru(1)	117.19(13)
C(38)-P(1)-Ru(1)	120.53(15)
C(50)-P(2)-C(62)	106.97(18)
C(50)-P(2)-C(56)	97.71(18)
C(62)-P(2)-C(56)	100.84(19)
C(50)-P(2)-Ru(1)	116.22(14)
C(62)-P(2)-Ru(1)	109.31(14)
C(56)-P(2)-Ru(1)	123.74(15)
C(2)-N(1)-N(2)	104.8(3)
C(2)-N(1)-Ru(1)	144.9(3)
N(2)-N(1)-Ru(1)	110.3(2)
C(4)-N(2)-C(6)	132.6(4)
C(4)-N(2)-N(1)	109.2(3)

C(6)-N(2)-N(1)	118.0(3)
C(6)-N(3)-C(10)	120.3(3)
C(6)-N(3)-Ru(1)	120.1(3)
C(10)-N(3)-Ru(1)	119.7(2)
C(11)-N(4)-C(13)	105.0(3)
C(11)-N(4)-Ru(1)	110.1(2)
C(13)-N(4)-Ru(1)	144.8(2)
C(11)-N(5)-C(12)	107.6(3)
C(11)-N(5)-H(5)	127(3)
C(12)-N(5)-H(5)	125(3)
C(15)-N(6)-S(1)	126.4(3)
C(15)-N(6)-H(6)	117(3)
S(1)-N(6)-H(6)	112(3)
C(16)-N(7)-S(2)	122.1(3)
C(16)-N(7)-H(7A)	112(3)
S(2)-N(7)-H(7A)	114(3)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	110.4(4)
N(1)-C(2)-C(1)	123.1(4)
C(3)-C(2)-C(1)	126.4(4)
C(4)-C(3)-C(2)	108.7(4)
C(4)-C(3)-H(3)	125.7
C(2)-C(3)-H(3)	125.7
C(3)-C(4)-N(2)	106.8(4)
C(3)-C(4)-C(5)	128.3(4)
N(2)-C(4)-C(5)	124.9(5)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(3)-C(6)-N(2)	112.9(3)

N(3)-C(6)-C(7)	119.7(4)
N(2)-C(6)-C(7)	127.4(4)
C(8)-C(7)-C(6)	119.7(4)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(7)-C(8)-C(9)	121.2(4)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(8)-C(9)-C(10)	117.4(4)
C(8)-C(9)-H(9)	121.3
C(10)-C(9)-H(9)	121.3
N(3)-C(10)-C(9)	121.8(3)
N(3)-C(10)-C(11)	110.9(3)
C(9)-C(10)-C(11)	127.3(4)
N(4)-C(11)-N(5)	112.2(3)
N(4)-C(11)-C(10)	120.3(3)
N(5)-C(11)-C(10)	127.5(3)
N(5)-C(12)-C(17)	131.8(3)
N(5)-C(12)-C(13)	106.4(3)
C(17)-C(12)-C(13)	121.8(3)
C(14)-C(13)-C(12)	120.8(3)
C(14)-C(13)-N(4)	130.4(3)
C(12)-C(13)-N(4)	108.8(3)
C(15)-C(14)-C(13)	117.9(3)
C(15)-C(14)-H(14)	121.1
C(13)-C(14)-H(14)	121.1
C(14)-C(15)-N(6)	122.3(3)
C(14)-C(15)-C(16)	120.8(3)
N(6)-C(15)-C(16)	116.8(3)
C(17)-C(16)-C(15)	120.9(3)
C(17)-C(16)-N(7)	117.7(3)
C(15)-C(16)-N(7)	121.4(3)
C(16)-C(17)-C(12)	117.8(3)
C(16)-C(17)-H(17)	121.1
C(12)-C(17)-H(17)	121.1
C(23)-C(18)-C(19)	120.7(5)
C(23)-C(18)-S(1)	120.2(4)
C(19)-C(18)-S(1)	119.1(3)

C(20)-C(19)-C(18)	118.7(5)
C(20)-C(19)-H(19)	120.6
C(18)-C(19)-H(19)	120.6
C(19)-C(20)-C(21)	121.7(5)
C(19)-C(20)-H(20)	119.2
C(21)-C(20)-H(20)	119.2
C(22)-C(21)-C(20)	117.8(5)
C(22)-C(21)-C(24)	120.8(6)
C(20)-C(21)-C(24)	121.3(6)
C(23)-C(22)-C(21)	121.7(5)
C(23)-C(22)-H(22)	119.1
C(21)-C(22)-H(22)	119.1
C(22)-C(23)-C(18)	119.3(5)
C(22)-C(23)-H(23)	120.3
C(18)-C(23)-H(23)	120.3
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(30)-C(25)-C(26)	120.5(5)
C(30)-C(25)-S(2)	119.7(4)
C(26)-C(25)-S(2)	119.5(4)
C(27)-C(26)-C(25)	120.2(6)
C(27)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(26)-C(27)-C(28)	119.5(6)
C(26)-C(27)-H(27)	120.2
C(28)-C(27)-H(27)	120.2
C(29)-C(28)-C(27)	120.8(6)
C(29)-C(28)-C(31)	110.4(13)
C(27)-C(28)-C(31)	125.8(16)
C(29)-C(28)-C(31')	122.3(12)
C(27)-C(28)-C(31')	116.3(11)
C(28)-C(29)-C(30)	119.7(6)
C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1

C(25)-C(30)-C(29)	119.2(6)
C(25)-C(30)-H(30)	120.4
C(29)-C(30)-H(30)	120.4
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(31')-H(31D)	109.5
C(28)-C(31')-H(31E)	109.5
H(31D)-C(31')-H(31E)	109.5
C(28)-C(31')-H(31F)	109.5
H(31D)-C(31')-H(31F)	109.5
H(31E)-C(31')-H(31F)	109.5
C(37)-C(32)-C(33)	117.6(4)
C(37)-C(32)-P(1)	122.5(3)
C(33)-C(32)-P(1)	119.5(3)
C(34)-C(33)-C(32)	121.3(4)
C(34)-C(33)-H(33)	119.4
C(32)-C(33)-H(33)	119.4
C(35)-C(34)-C(33)	120.0(5)
C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	120.3(5)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(35)-C(36)-C(37)	119.7(5)
C(35)-C(36)-H(36)	120.1
C(37)-C(36)-H(36)	120.1
C(32)-C(37)-C(36)	121.0(5)
C(32)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(39)-C(38)-C(43)	118.8(4)
C(39)-C(38)-P(1)	120.8(4)
C(43)-C(38)-P(1)	120.3(3)
C(38)-C(39)-C(40)	120.8(5)
C(38)-C(39)-H(39)	119.6

C(40)-C(39)-H(39)	119.6
C(41)-C(40)-C(39)	119.9(6)
C(41)-C(40)-H(40)	120.1
C(39)-C(40)-H(40)	120.1
C(40)-C(41)-C(42)	119.6(5)
C(40)-C(41)-H(41)	120.2
C(42)-C(41)-H(41)	120.2
C(41)-C(42)-C(43)	120.9(6)
C(41)-C(42)-H(42)	119.6
C(43)-C(42)-H(42)	119.6
C(42)-C(43)-C(38)	120.1(5)
C(42)-C(43)-H(43)	119.9
C(38)-C(43)-H(43)	119.9
C(45)-C(44)-C(49)	118.1(4)
C(45)-C(44)-P(1)	125.7(3)
C(49)-C(44)-P(1)	116.2(3)
C(46)-C(45)-C(44)	121.4(5)
C(46)-C(45)-H(45)	119.3
C(44)-C(45)-H(45)	119.3
C(45)-C(46)-C(47)	119.9(5)
C(45)-C(46)-H(46)	120.0
C(47)-C(46)-H(46)	120.0
C(46)-C(47)-C(48)	120.1(5)
C(46)-C(47)-H(47)	119.9
C(48)-C(47)-H(47)	119.9
C(49)-C(48)-C(47)	119.4(5)
C(49)-C(48)-H(48)	120.3
C(47)-C(48)-H(48)	120.3
C(48)-C(49)-C(44)	121.1(5)
C(48)-C(49)-H(49)	119.5
C(44)-C(49)-H(49)	119.5
C(55)-C(50)-C(51)	118.3(4)
C(55)-C(50)-P(2)	126.8(3)
C(51)-C(50)-P(2)	114.7(3)
C(50)-C(51)-C(52)	120.4(4)
C(50)-C(51)-H(51)	119.8
C(52)-C(51)-H(51)	119.8
C(53)-C(52)-C(51)	119.9(5)

C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0
C(54)-C(53)-C(52)	120.5(4)
C(54)-C(53)-H(53)	119.8
C(52)-C(53)-H(53)	119.8
C(53)-C(54)-C(55)	120.6(5)
C(53)-C(54)-H(54)	119.7
C(55)-C(54)-H(54)	119.7
C(50)-C(55)-C(54)	120.3(4)
C(50)-C(55)-H(55)	119.9
C(54)-C(55)-H(55)	119.9
C(61)-C(56)-C(57)	118.1(4)
C(61)-C(56)-P(2)	120.0(3)
C(57)-C(56)-P(2)	121.9(4)
C(56)-C(57)-C(58)	119.1(5)
C(56)-C(57)-H(57)	120.4
C(58)-C(57)-H(57)	120.4
C(59)-C(58)-C(57)	121.8(5)
C(59)-C(58)-H(58)	119.1
C(57)-C(58)-H(58)	119.1
C(58)-C(59)-C(60)	119.2(5)
C(58)-C(59)-H(59)	120.4
C(60)-C(59)-H(59)	120.4
C(59)-C(60)-C(61)	120.4(6)
C(59)-C(60)-H(60)	119.8
C(61)-C(60)-H(60)	119.8
C(56)-C(61)-C(60)	121.3(5)
C(56)-C(61)-H(61)	119.3
C(60)-C(61)-H(61)	119.3
C(67)-C(62)-C(63)	118.5(4)
C(67)-C(62)-P(2)	122.3(3)
C(63)-C(62)-P(2)	118.7(3)
C(64)-C(63)-C(62)	119.9(4)
C(64)-C(63)-H(63)	120.1
C(62)-C(63)-H(63)	120.1
C(65)-C(64)-C(63)	120.7(4)
C(65)-C(64)-H(64)	119.7
C(63)-C(64)-H(64)	119.7

C(64)-C(65)-C(66)	120.6(4)
C(64)-C(65)-H(65)	119.7
C(66)-C(65)-H(65)	119.7
C(65)-C(66)-C(67)	119.1(4)
C(65)-C(66)-H(66)	120.4
C(67)-C(66)-H(66)	120.4
C(66)-C(67)-C(62)	121.3(4)
C(66)-C(67)-H(67)	119.4
C(62)-C(67)-H(67)	119.4
Cl(4)-C(68)-Cl(5)	112.2(4)
Cl(4)-C(68)-Cl(3)	110.9(4)
Cl(5)-C(68)-Cl(3)	109.9(4)
Cl(4)-C(68)-H(68)	107.9
Cl(5)-C(68)-H(68)	107.9
Cl(3)-C(68)-H(68)	107.9
Cl(8)-C(69)-Cl(6)	111.1(3)
Cl(8)-C(69)-Cl(7)	111.0(3)
Cl(6)-C(69)-Cl(7)	109.8(3)
Cl(8)-C(69)-H(69)	108.3
Cl(6)-C(69)-H(69)	108.3
Cl(7)-C(69)-H(69)	108.3

Table S3. Torsion angles [°] for **4b**.

C(2)-N(1)-N(2)-C(4)	1.2(4)
Ru(1)-N(1)-N(2)-C(4)	-179.3(3)
C(2)-N(1)-N(2)-C(6)	-175.0(4)
Ru(1)-N(1)-N(2)-C(6)	4.6(4)
O(1)-S(1)-N(6)-C(15)	-46.9(4)
O(2)-S(1)-N(6)-C(15)	-175.3(4)
C(18)-S(1)-N(6)-C(15)	69.7(4)
O(4)-S(2)-N(7)-C(16)	-171.3(3)
O(3)-S(2)-N(7)-C(16)	-42.0(4)
C(25)-S(2)-N(7)-C(16)	74.0(4)
N(2)-N(1)-C(2)-C(3)	-1.1(5)
Ru(1)-N(1)-C(2)-C(3)	179.5(4)
N(2)-N(1)-C(2)-C(1)	177.1(4)
Ru(1)-N(1)-C(2)-C(1)	-2.2(8)

N(1)-C(2)-C(3)-C(4)	0.7(6)
C(1)-C(2)-C(3)-C(4)	-177.4(5)
C(2)-C(3)-C(4)-N(2)	0.1(6)
C(2)-C(3)-C(4)-C(5)	-179.3(5)
C(6)-N(2)-C(4)-C(3)	174.7(4)
N(1)-N(2)-C(4)-C(3)	-0.7(5)
C(6)-N(2)-C(4)-C(5)	-5.9(8)
N(1)-N(2)-C(4)-C(5)	178.7(4)
C(10)-N(3)-C(6)-N(2)	178.3(3)
Ru(1)-N(3)-C(6)-N(2)	-2.7(5)
C(10)-N(3)-C(6)-C(7)	-0.6(6)
Ru(1)-N(3)-C(6)-C(7)	178.4(3)
C(4)-N(2)-C(6)-N(3)	-176.6(4)
N(1)-N(2)-C(6)-N(3)	-1.5(5)
C(4)-N(2)-C(6)-C(7)	2.1(8)
N(1)-N(2)-C(6)-C(7)	177.2(4)
N(3)-C(6)-C(7)-C(8)	0.9(7)
N(2)-C(6)-C(7)-C(8)	-177.8(4)
C(6)-C(7)-C(8)-C(9)	0.0(8)
C(7)-C(8)-C(9)-C(10)	-1.1(7)
C(6)-N(3)-C(10)-C(9)	-0.6(6)
Ru(1)-N(3)-C(10)-C(9)	-179.6(3)
C(6)-N(3)-C(10)-C(11)	179.1(4)
Ru(1)-N(3)-C(10)-C(11)	0.1(4)
C(8)-C(9)-C(10)-N(3)	1.4(7)
C(8)-C(9)-C(10)-C(11)	-178.2(4)
C(13)-N(4)-C(11)-N(5)	-0.3(4)
Ru(1)-N(4)-C(11)-N(5)	-177.2(3)
C(13)-N(4)-C(11)-C(10)	-178.5(4)
Ru(1)-N(4)-C(11)-C(10)	4.6(4)
C(12)-N(5)-C(11)-N(4)	0.0(5)
C(12)-N(5)-C(11)-C(10)	178.0(4)
N(3)-C(10)-C(11)-N(4)	-3.4(5)
C(9)-C(10)-C(11)-N(4)	176.3(4)
N(3)-C(10)-C(11)-N(5)	178.8(4)
C(9)-C(10)-C(11)-N(5)	-1.5(7)
C(11)-N(5)-C(12)-C(17)	178.4(4)
C(11)-N(5)-C(12)-C(13)	0.3(4)

N(5)-C(12)-C(13)-C(14)	178.6(4)
C(17)-C(12)-C(13)-C(14)	0.3(6)
N(5)-C(12)-C(13)-N(4)	-0.5(4)
C(17)-C(12)-C(13)-N(4)	-178.8(4)
C(11)-N(4)-C(13)-C(14)	-178.5(4)
Ru(1)-N(4)-C(13)-C(14)	-3.6(7)
C(11)-N(4)-C(13)-C(12)	0.5(4)
Ru(1)-N(4)-C(13)-C(12)	175.4(3)
C(12)-C(13)-C(14)-C(15)	0.8(6)
N(4)-C(13)-C(14)-C(15)	179.7(4)
C(13)-C(14)-C(15)-N(6)	177.6(4)
C(13)-C(14)-C(15)-C(16)	-1.2(6)
S(1)-N(6)-C(15)-C(14)	-0.3(6)
S(1)-N(6)-C(15)-C(16)	178.6(3)
C(14)-C(15)-C(16)-C(17)	0.5(6)
N(6)-C(15)-C(16)-C(17)	-178.4(4)
C(14)-C(15)-C(16)-N(7)	-178.0(4)
N(6)-C(15)-C(16)-N(7)	3.1(6)
S(2)-N(7)-C(16)-C(17)	79.7(5)
S(2)-N(7)-C(16)-C(15)	-101.8(4)
C(15)-C(16)-C(17)-C(12)	0.6(6)
N(7)-C(16)-C(17)-C(12)	179.2(4)
N(5)-C(12)-C(17)-C(16)	-178.9(4)
C(13)-C(12)-C(17)-C(16)	-1.0(6)
O(1)-S(1)-C(18)-C(23)	-3.5(4)
O(2)-S(1)-C(18)-C(23)	127.2(3)
N(6)-S(1)-C(18)-C(23)	-120.0(3)
O(1)-S(1)-C(18)-C(19)	176.1(3)
O(2)-S(1)-C(18)-C(19)	-53.2(4)
N(6)-S(1)-C(18)-C(19)	59.6(4)
C(23)-C(18)-C(19)-C(20)	-0.5(7)
S(1)-C(18)-C(19)-C(20)	179.9(4)
C(18)-C(19)-C(20)-C(21)	-1.0(8)
C(19)-C(20)-C(21)-C(22)	1.9(8)
C(19)-C(20)-C(21)-C(24)	-178.8(5)
C(20)-C(21)-C(22)-C(23)	-1.5(8)
C(24)-C(21)-C(22)-C(23)	179.2(5)
C(21)-C(22)-C(23)-C(18)	0.1(7)

C(19)-C(18)-C(23)-C(22)	0.9(6)
S(1)-C(18)-C(23)-C(22)	-179.5(3)
O(4)-S(2)-C(25)-C(30)	-27.4(5)
O(3)-S(2)-C(25)-C(30)	-158.7(5)
N(7)-S(2)-C(25)-C(30)	85.9(5)
O(4)-S(2)-C(25)-C(26)	158.8(5)
O(3)-S(2)-C(25)-C(26)	27.5(5)
N(7)-S(2)-C(25)-C(26)	-87.9(5)
C(30)-C(25)-C(26)-C(27)	1.7(10)
S(2)-C(25)-C(26)-C(27)	175.4(5)
C(25)-C(26)-C(27)-C(28)	-1.3(11)
C(26)-C(27)-C(28)-C(29)	0.1(13)
C(26)-C(27)-C(28)-C(31)	158.9(17)
C(26)-C(27)-C(28)-C(31')	-171.3(16)
C(27)-C(28)-C(29)-C(30)	0.9(14)
C(31)-C(28)-C(29)-C(30)	-160.9(18)
C(31')-C(28)-C(29)-C(30)	171.7(17)
C(26)-C(25)-C(30)-C(29)	-0.7(10)
S(2)-C(25)-C(30)-C(29)	-174.5(6)
C(28)-C(29)-C(30)-C(25)	-0.6(12)
C(44)-P(1)-C(32)-C(37)	46.8(4)
C(38)-P(1)-C(32)-C(37)	150.3(4)
Ru(1)-P(1)-C(32)-C(37)	-81.4(4)
C(44)-P(1)-C(32)-C(33)	-139.9(4)
C(38)-P(1)-C(32)-C(33)	-36.5(4)
Ru(1)-P(1)-C(32)-C(33)	91.9(4)
C(37)-C(32)-C(33)-C(34)	-2.2(7)
P(1)-C(32)-C(33)-C(34)	-175.8(4)
C(32)-C(33)-C(34)-C(35)	0.9(8)
C(33)-C(34)-C(35)-C(36)	0.3(9)
C(34)-C(35)-C(36)-C(37)	0.0(9)
C(33)-C(32)-C(37)-C(36)	2.5(7)
P(1)-C(32)-C(37)-C(36)	175.9(4)
C(35)-C(36)-C(37)-C(32)	-1.4(8)
C(32)-P(1)-C(38)-C(39)	123.0(4)
C(44)-P(1)-C(38)-C(39)	-129.1(4)
Ru(1)-P(1)-C(38)-C(39)	1.0(4)
C(32)-P(1)-C(38)-C(43)	-53.8(4)

C(44)-P(1)-C(38)-C(43)	54.1(4)
Ru(1)-P(1)-C(38)-C(43)	-175.8(3)
C(43)-C(38)-C(39)-C(40)	1.0(7)
P(1)-C(38)-C(39)-C(40)	-175.8(4)
C(38)-C(39)-C(40)-C(41)	-1.3(8)
C(39)-C(40)-C(41)-C(42)	0.4(9)
C(40)-C(41)-C(42)-C(43)	0.8(8)
C(41)-C(42)-C(43)-C(38)	-1.0(7)
C(39)-C(38)-C(43)-C(42)	0.1(7)
P(1)-C(38)-C(43)-C(42)	177.0(4)
C(32)-P(1)-C(44)-C(45)	9.4(5)
C(38)-P(1)-C(44)-C(45)	-93.8(4)
Ru(1)-P(1)-C(44)-C(45)	134.0(4)
C(32)-P(1)-C(44)-C(49)	-174.2(3)
C(38)-P(1)-C(44)-C(49)	82.6(3)
Ru(1)-P(1)-C(44)-C(49)	-49.6(4)
C(49)-C(44)-C(45)-C(46)	0.5(8)
P(1)-C(44)-C(45)-C(46)	176.9(4)
C(44)-C(45)-C(46)-C(47)	0.3(9)
C(45)-C(46)-C(47)-C(48)	-1.5(9)
C(46)-C(47)-C(48)-C(49)	1.7(9)
C(47)-C(48)-C(49)-C(44)	-0.8(8)
C(45)-C(44)-C(49)-C(48)	-0.3(7)
P(1)-C(44)-C(49)-C(48)	-176.9(4)
C(62)-P(2)-C(50)-C(55)	3.3(5)
C(56)-P(2)-C(50)-C(55)	107.1(4)
Ru(1)-P(2)-C(50)-C(55)	-119.1(4)
C(62)-P(2)-C(50)-C(51)	-171.2(3)
C(56)-P(2)-C(50)-C(51)	-67.3(4)
Ru(1)-P(2)-C(50)-C(51)	66.5(3)
C(55)-C(50)-C(51)-C(52)	0.7(7)
P(2)-C(50)-C(51)-C(52)	175.6(4)
C(50)-C(51)-C(52)-C(53)	-0.5(8)
C(51)-C(52)-C(53)-C(54)	-0.5(9)
C(52)-C(53)-C(54)-C(55)	1.4(9)
C(51)-C(50)-C(55)-C(54)	0.1(7)
P(2)-C(50)-C(55)-C(54)	-174.1(4)
C(53)-C(54)-C(55)-C(50)	-1.2(8)

C(50)-P(2)-C(56)-C(61)	-48.3(4)
C(62)-P(2)-C(56)-C(61)	60.8(4)
Ru(1)-P(2)-C(56)-C(61)	-177.1(3)
C(50)-P(2)-C(56)-C(57)	131.1(4)
C(62)-P(2)-C(56)-C(57)	-119.9(4)
Ru(1)-P(2)-C(56)-C(57)	2.3(4)
C(61)-C(56)-C(57)-C(58)	-0.8(7)
P(2)-C(56)-C(57)-C(58)	179.9(4)
C(56)-C(57)-C(58)-C(59)	0.4(8)
C(57)-C(58)-C(59)-C(60)	1.0(9)
C(58)-C(59)-C(60)-C(61)	-2.0(9)
C(57)-C(56)-C(61)-C(60)	-0.2(7)
P(2)-C(56)-C(61)-C(60)	179.1(4)
C(59)-C(60)-C(61)-C(56)	1.6(9)
C(50)-P(2)-C(62)-C(67)	-50.6(4)
C(56)-P(2)-C(62)-C(67)	-152.2(3)
Ru(1)-P(2)-C(62)-C(67)	76.0(4)
C(50)-P(2)-C(62)-C(63)	138.2(4)
C(56)-P(2)-C(62)-C(63)	36.6(4)
Ru(1)-P(2)-C(62)-C(63)	-95.2(4)
C(67)-C(62)-C(63)-C(64)	0.8(7)
P(2)-C(62)-C(63)-C(64)	172.4(4)
C(62)-C(63)-C(64)-C(65)	1.0(8)
C(63)-C(64)-C(65)-C(66)	-1.5(9)
C(64)-C(65)-C(66)-C(67)	0.2(8)
C(65)-C(66)-C(67)-C(62)	1.6(7)
C(63)-C(62)-C(67)-C(66)	-2.1(6)
P(2)-C(62)-C(67)-C(66)	-173.4(3)

Table S4. Hydrogen bonds for **4b** [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
C(68)-H(68)...Cl(2)#1	0.98	2.51	3.422(8)	154.8

C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9
C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
C(68)-H(68)...Cl(2)#1	0.98	2.51	3.422(8)	154.8
C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9
C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9

C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9
C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9
C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
C(1)-H(1A)...Cl(1)	0.96	2.94	3.846(5)	157.9
C(3)-H(3)...O(1)#4	0.93	2.52	3.168(5)	127.1
C(9)-H(9)...Cl(2)#2	0.93	2.89	3.763(4)	156.2
C(14)-H(14)...Cl(1)	0.93	2.90	3.646(3)	137.8

C(14)-H(14)...O(1)	0.93	2.45	3.000(4)	117.9
C(19)-H(19)...Cl(2)#1	0.93	2.91	3.782(5)	156.4
C(23)-H(23)...Cl(1)	0.93	2.89	3.539(4)	127.9
C(39)-H(39)...Cl(1)	0.93	2.70	3.400(5)	132.2
C(49)-H(49)...Cl(1)	0.93	2.76	3.612(5)	153.6
C(57)-H(57)...Cl(1)	0.93	2.58	3.328(5)	138.1
C(67)-H(67)...O(4)#3	0.93	2.56	3.190(5)	125.6
C(69)-H(69)...O(2)	0.98	2.24	3.019(6)	136.0
N(5)-H(5)...Cl(2)#2	0.85(5)	2.33(5)	3.160(3)	168(5)
N(6)-H(6)...Cl(2)#1	0.69(3)	2.61(3)	3.277(4)	165(4)
N(7)-H(7A)...Cl(2)#1	0.83(4)	2.38(4)	3.209(4)	175(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+3/2 #2 x-1,y,z #3 -x,y+1/2,-z+3/2

#4 -x+1,y+1/2,-z+3/2

2.2 X-Ray crystallographic data for 6a

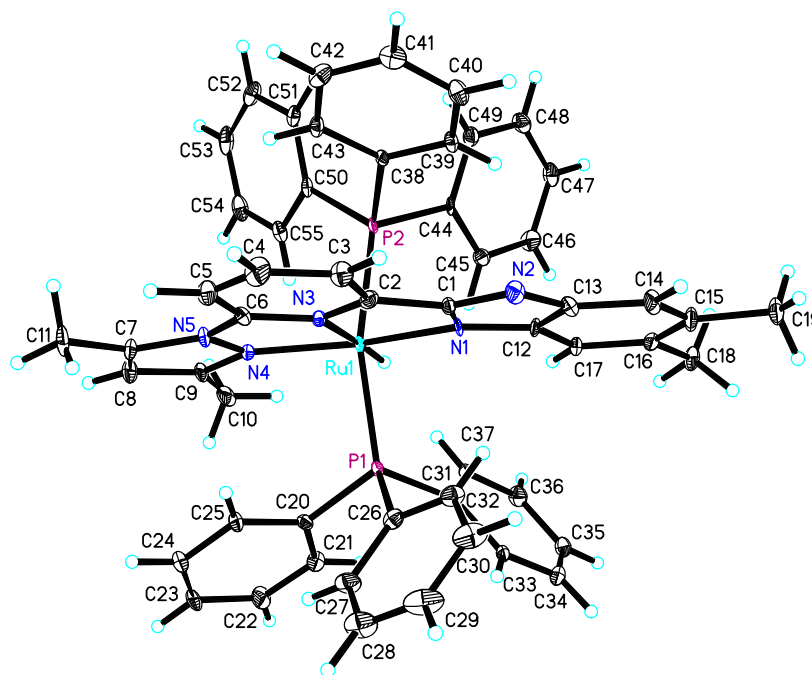


Figure S23. The molecular structure of complex **6a**.

Table S5. Crystal data and structure refinement for **6a**.

Identification code	cu_dm14251_0m	
Empirical formula	C55 H49 N5 P2 Ru	
Formula weight	943.00	
Temperature	140(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 12.0044(2) Å	$\alpha = 90^\circ$.
	b = 20.9968(4) Å	$\beta = 93.8990(10)^\circ$.
	c = 38.3562(7) Å	$\gamma = 90^\circ$.
Volume	9645.5(3) Å ³	
Z	8	
Density (calculated)	1.299 Mg/m ³	
Absorption coefficient	3.575 mm ⁻¹	
F(000)	3904	
Crystal size	0.25 x 0.22 x 0.18 mm ³	
Theta range for data collection	4.37 to 69.66°.	
Index ranges	-14 ≤ h ≤ 13, -25 ≤ k ≤ 25, -44 ≤ l ≤ 46	
Reflections collected	32242	
Independent reflections	8886 [R(int) = 0.0395]	
Completeness to theta = 69.66°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5655 and 0.4685	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8886 / 6 / 572	
Goodness-of-fit on F ²	1.068	
Final R indices [I > 2sigma(I)]	R1 = 0.0729, wR2 = 0.1878	
R indices (all data)	R1 = 0.0738, wR2 = 0.1882	
Largest diff. peak and hole	1.434 and -1.515 e.Å ⁻³	

Table S6. Bond lengths [Å] and angles [°] for **6a**.

Ru(1)-N(3)	2.067(5)
Ru(1)-N(4)	2.080(5)
Ru(1)-N(1)	2.109(4)
Ru(1)-P(2)	2.3160(15)
Ru(1)-P(1)	2.3182(15)
Ru(1)-H(1)	1.2808

P(1)-C(20)	1.833(6)
P(1)-C(32)	1.845(6)
P(1)-C(26)	1.852(6)
P(2)-C(38)	1.828(6)
P(2)-C(50)	1.843(6)
P(2)-C(44)	1.861(6)
N(1)-C(1)	1.371(7)
N(1)-C(12)	1.385(7)
N(2)-C(1)	1.344(8)
N(2)-C(13)	1.373(8)
N(3)-C(2)	1.336(8)
N(3)-C(6)	1.337(8)
N(4)-C(9)	1.334(8)
N(4)-N(5)	1.405(8)
N(5)-C(7)	1.371(8)
N(5)-C(6)	1.412(9)
C(1)-C(2)	1.448(8)
C(2)-C(3)	1.386(9)
C(3)-C(4)	1.391(10)
C(3)-H(3)	0.9500
C(4)-C(5)	1.377(11)
C(4)-H(4)	0.9500
C(5)-C(6)	1.395(9)
C(5)-H(5)	0.9500
C(7)-C(8)	1.355(12)
C(7)-C(11)	1.504(10)
C(8)-C(9)	1.411(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.479(10)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.393(8)
C(12)-C(17)	1.401(8)
C(13)-C(14)	1.429(9)

C(14)-C(15)	1.365(10)
C(14)-H(14)	0.9500
C(15)-C(16)	1.427(10)
C(15)-C(19)	1.508(9)
C(16)-C(17)	1.381(8)
C(16)-C(18)	1.522(9)
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(25)	1.380(9)
C(20)-C(21)	1.389(9)
C(21)-C(22)	1.394(9)
C(21)-H(21)	0.9500
C(22)-C(23)	1.393(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.378(11)
C(23)-H(23)	0.9500
C(24)-C(25)	1.396(9)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-C(31)	1.367(9)
C(26)-C(27)	1.409(9)
C(27)-C(28)	1.381(10)
C(27)-H(27)	0.9500
C(28)-C(29)	1.380(13)
C(28)-H(28)	0.9500
C(29)-C(30)	1.382(12)
C(29)-H(29)	0.9500
C(30)-C(31)	1.391(10)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(33)	1.393(8)
C(32)-C(37)	1.394(8)
C(33)-C(34)	1.393(9)

C(33)-H(33)	0.9500
C(34)-C(35)	1.375(10)
C(34)-H(34)	0.9500
C(35)-C(36)	1.388(10)
C(35)-H(35)	0.9500
C(36)-C(37)	1.390(9)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-C(39)	1.392(8)
C(38)-C(43)	1.406(8)
C(39)-C(40)	1.382(9)
C(39)-H(39)	0.9500
C(40)-C(41)	1.375(10)
C(40)-H(40)	0.9500
C(41)-C(42)	1.390(10)
C(41)-H(41)	0.9500
C(42)-C(43)	1.383(9)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44)-C(45)	1.375(9)
C(44)-C(49)	1.407(9)
C(45)-C(46)	1.390(9)
C(45)-H(45)	0.9500
C(46)-C(47)	1.387(10)
C(46)-H(46)	0.9500
C(47)-C(48)	1.378(10)
C(47)-H(47)	0.9500
C(48)-C(49)	1.382(9)
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(55)	1.375(9)
C(50)-C(51)	1.395(9)
C(51)-C(52)	1.394(9)
C(51)-H(51)	0.9500
C(52)-C(53)	1.381(11)
C(52)-H(52)	0.9500
C(53)-C(54)	1.382(11)
C(53)-H(53)	0.9500

C(54)-C(55)	1.385(9)
C(54)-H(54)	0.9500
C(55)-H(55)	0.9500
N(3)-Ru(1)-N(4)	77.4(2)
N(3)-Ru(1)-N(1)	77.02(19)
N(4)-Ru(1)-N(1)	154.3(2)
N(3)-Ru(1)-P(2)	95.60(14)
N(4)-Ru(1)-P(2)	98.47(14)
N(1)-Ru(1)-P(2)	85.65(14)
N(3)-Ru(1)-P(1)	102.68(14)
N(4)-Ru(1)-P(1)	94.05(14)
N(1)-Ru(1)-P(1)	89.96(14)
P(2)-Ru(1)-P(1)	159.73(5)
N(3)-Ru(1)-H(1)	176.1
N(4)-Ru(1)-H(1)	103.7
N(1)-Ru(1)-H(1)	101.8
P(2)-Ru(1)-H(1)	88.0
P(1)-Ru(1)-H(1)	73.5
C(20)-P(1)-C(32)	102.0(3)
C(20)-P(1)-C(26)	101.7(3)
C(32)-P(1)-C(26)	100.3(3)
C(20)-P(1)-Ru(1)	115.9(2)
C(32)-P(1)-Ru(1)	115.6(2)
C(26)-P(1)-Ru(1)	118.7(2)
C(38)-P(2)-C(50)	104.6(3)
C(38)-P(2)-C(44)	102.6(3)
C(50)-P(2)-C(44)	96.5(3)
C(38)-P(2)-Ru(1)	112.48(18)
C(50)-P(2)-Ru(1)	120.4(2)
C(44)-P(2)-Ru(1)	117.7(2)
C(1)-N(1)-C(12)	103.8(5)
C(1)-N(1)-Ru(1)	113.3(4)
C(12)-N(1)-Ru(1)	142.8(4)
C(1)-N(2)-C(13)	102.4(5)
C(2)-N(3)-C(6)	122.2(5)
C(2)-N(3)-Ru(1)	119.2(4)
C(6)-N(3)-Ru(1)	118.4(4)

C(9)-N(4)-N(5)	105.4(5)
C(9)-N(4)-Ru(1)	141.1(5)
N(5)-N(4)-Ru(1)	113.3(4)
C(7)-N(5)-N(4)	110.1(6)
C(7)-N(5)-C(6)	132.5(6)
N(4)-N(5)-C(6)	117.2(5)
N(2)-C(1)-N(1)	115.5(5)
N(2)-C(1)-C(2)	126.6(6)
N(1)-C(1)-C(2)	118.0(5)
N(3)-C(2)-C(3)	120.3(6)
N(3)-C(2)-C(1)	112.4(5)
C(3)-C(2)-C(1)	127.3(6)
C(2)-C(3)-C(4)	117.8(6)
C(2)-C(3)-H(3)	121.1
C(4)-C(3)-H(3)	121.1
C(5)-C(4)-C(3)	121.6(6)
C(5)-C(4)-H(4)	119.2
C(3)-C(4)-H(4)	119.2
C(4)-C(5)-C(6)	117.5(6)
C(4)-C(5)-H(5)	121.3
C(6)-C(5)-H(5)	121.3
N(3)-C(6)-C(5)	120.5(6)
N(3)-C(6)-N(5)	113.6(5)
C(5)-C(6)-N(5)	125.9(6)
C(8)-C(7)-N(5)	107.0(6)
C(8)-C(7)-C(11)	127.6(7)
N(5)-C(7)-C(11)	125.4(7)
C(7)-C(8)-C(9)	107.5(6)
C(7)-C(8)-H(8)	126.3
C(9)-C(8)-H(8)	126.3
N(4)-C(9)-C(8)	110.1(6)
N(4)-C(9)-C(10)	121.4(6)
C(8)-C(9)-C(10)	128.3(6)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5

H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(1)-C(12)-C(13)	106.9(5)
N(1)-C(12)-C(17)	130.8(5)
C(13)-C(12)-C(17)	122.3(5)
N(2)-C(13)-C(12)	111.3(5)
N(2)-C(13)-C(14)	129.7(6)
C(12)-C(13)-C(14)	119.0(6)
C(15)-C(14)-C(13)	119.3(6)
C(15)-C(14)-H(14)	120.4
C(13)-C(14)-H(14)	120.4
C(14)-C(15)-C(16)	120.5(6)
C(14)-C(15)-C(19)	120.2(7)
C(16)-C(15)-C(19)	119.3(6)
C(17)-C(16)-C(15)	121.2(6)
C(17)-C(16)-C(18)	118.4(6)
C(15)-C(16)-C(18)	120.4(6)
C(16)-C(17)-C(12)	117.7(6)
C(16)-C(17)-H(17)	121.1
C(12)-C(17)-H(17)	121.1
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-H(19A)	109.5
C(15)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(15)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(25)-C(20)-C(21)	118.5(6)

C(25)-C(20)-P(1)	118.6(5)
C(21)-C(20)-P(1)	122.9(5)
C(20)-C(21)-C(22)	120.3(6)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	121.0(6)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(24)-C(23)-C(22)	118.4(6)
C(24)-C(23)-H(23)	120.8
C(22)-C(23)-H(23)	120.8
C(23)-C(24)-C(25)	120.6(6)
C(23)-C(24)-H(24)	119.7
C(25)-C(24)-H(24)	119.7
C(20)-C(25)-C(24)	121.2(6)
C(20)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(31)-C(26)-C(27)	118.6(6)
C(31)-C(26)-P(1)	119.1(5)
C(27)-C(26)-P(1)	122.2(5)
C(28)-C(27)-C(26)	120.8(7)
C(28)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(29)-C(28)-C(27)	119.6(7)
C(29)-C(28)-H(28)	120.2
C(27)-C(28)-H(28)	120.2
C(28)-C(29)-C(30)	120.1(7)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
C(29)-C(30)-C(31)	120.0(7)
C(29)-C(30)-H(30)	120.0
C(31)-C(30)-H(30)	120.0
C(26)-C(31)-C(30)	120.9(7)
C(26)-C(31)-H(31)	119.6
C(30)-C(31)-H(31)	119.6
C(33)-C(32)-C(37)	118.4(5)
C(33)-C(32)-P(1)	121.7(5)
C(37)-C(32)-P(1)	119.9(5)

C(34)-C(33)-C(32)	120.1(6)
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(35)-C(34)-C(33)	120.8(6)
C(35)-C(34)-H(34)	119.6
C(33)-C(34)-H(34)	119.6
C(34)-C(35)-C(36)	120.1(6)
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	119.1(6)
C(35)-C(36)-H(36)	120.5
C(37)-C(36)-H(36)	120.5
C(36)-C(37)-C(32)	121.6(6)
C(36)-C(37)-H(37)	119.2
C(32)-C(37)-H(37)	119.2
C(39)-C(38)-C(43)	118.4(5)
C(39)-C(38)-P(2)	121.8(4)
C(43)-C(38)-P(2)	119.2(4)
C(40)-C(39)-C(38)	120.9(6)
C(40)-C(39)-H(39)	119.5
C(38)-C(39)-H(39)	119.5
C(41)-C(40)-C(39)	120.4(6)
C(41)-C(40)-H(40)	119.8
C(39)-C(40)-H(40)	119.8
C(40)-C(41)-C(42)	119.7(6)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1
C(43)-C(42)-C(41)	120.3(6)
C(43)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(42)-C(43)-C(38)	120.3(6)
C(42)-C(43)-H(43)	119.9
C(38)-C(43)-H(43)	119.9
C(45)-C(44)-C(49)	119.0(6)
C(45)-C(44)-P(2)	121.3(5)
C(49)-C(44)-P(2)	119.4(5)
C(44)-C(45)-C(46)	120.2(6)
C(44)-C(45)-H(45)	119.9

C(46)-C(45)-H(45)	119.9
C(47)-C(46)-C(45)	120.9(6)
C(47)-C(46)-H(46)	119.6
C(45)-C(46)-H(46)	119.6
C(48)-C(47)-C(46)	118.9(6)
C(48)-C(47)-H(47)	120.6
C(46)-C(47)-H(47)	120.6
C(47)-C(48)-C(49)	120.9(6)
C(47)-C(48)-H(48)	119.6
C(49)-C(48)-H(48)	119.6
C(48)-C(49)-C(44)	120.1(6)
C(48)-C(49)-H(49)	120.0
C(44)-C(49)-H(49)	120.0
C(55)-C(50)-C(51)	119.0(6)
C(55)-C(50)-P(2)	116.3(5)
C(51)-C(50)-P(2)	124.1(5)
C(52)-C(51)-C(50)	120.0(6)
C(52)-C(51)-H(51)	120.0
C(50)-C(51)-H(51)	120.0
C(53)-C(52)-C(51)	119.8(7)
C(53)-C(52)-H(52)	120.1
C(51)-C(52)-H(52)	120.1
C(52)-C(53)-C(54)	120.3(6)
C(52)-C(53)-H(53)	119.8
C(54)-C(53)-H(53)	119.8
C(53)-C(54)-C(55)	119.5(6)
C(53)-C(54)-H(54)	120.3
C(55)-C(54)-H(54)	120.3
C(50)-C(55)-C(54)	121.3(7)
C(50)-C(55)-H(55)	119.3
C(54)-C(55)-H(55)	119.3

Table S7. Torsion angles [°] for **6a**.

N(3)-Ru(1)-P(1)-C(20)	97.8(3)
N(4)-Ru(1)-P(1)-C(20)	19.9(3)
N(1)-Ru(1)-P(1)-C(20)	174.5(3)
P(2)-Ru(1)-P(1)-C(20)	-108.3(3)

N(3)-Ru(1)-P(1)-C(32)	-142.9(2)
N(4)-Ru(1)-P(1)-C(32)	139.2(3)
N(1)-Ru(1)-P(1)-C(32)	-66.2(2)
P(2)-Ru(1)-P(1)-C(32)	11.0(3)
N(3)-Ru(1)-P(1)-C(26)	-23.7(3)
N(4)-Ru(1)-P(1)-C(26)	-101.6(3)
N(1)-Ru(1)-P(1)-C(26)	53.0(3)
P(2)-Ru(1)-P(1)-C(26)	130.2(3)
N(3)-Ru(1)-P(2)-C(38)	22.4(2)
N(4)-Ru(1)-P(2)-C(38)	100.4(3)
N(1)-Ru(1)-P(2)-C(38)	-54.1(2)
P(1)-Ru(1)-P(2)-C(38)	-132.1(2)
N(3)-Ru(1)-P(2)-C(50)	-101.5(3)
N(4)-Ru(1)-P(2)-C(50)	-23.5(3)
N(1)-Ru(1)-P(2)-C(50)	-178.0(3)
P(1)-Ru(1)-P(2)-C(50)	104.0(3)
N(3)-Ru(1)-P(2)-C(44)	141.4(2)
N(4)-Ru(1)-P(2)-C(44)	-140.6(3)
N(1)-Ru(1)-P(2)-C(44)	64.9(2)
P(1)-Ru(1)-P(2)-C(44)	-13.1(3)
N(3)-Ru(1)-N(1)-C(1)	-1.9(4)
N(4)-Ru(1)-N(1)-C(1)	-5.7(7)
P(2)-Ru(1)-N(1)-C(1)	94.9(4)
P(1)-Ru(1)-N(1)-C(1)	-104.9(4)
N(3)-Ru(1)-N(1)-C(12)	179.2(7)
N(4)-Ru(1)-N(1)-C(12)	175.4(6)
P(2)-Ru(1)-N(1)-C(12)	-84.1(7)
P(1)-Ru(1)-N(1)-C(12)	76.1(7)
N(4)-Ru(1)-N(3)-C(2)	-178.5(5)
N(1)-Ru(1)-N(3)-C(2)	3.2(4)
P(2)-Ru(1)-N(3)-C(2)	-81.0(4)
P(1)-Ru(1)-N(3)-C(2)	90.2(4)
N(4)-Ru(1)-N(3)-C(6)	-2.7(4)
N(1)-Ru(1)-N(3)-C(6)	179.0(5)
P(2)-Ru(1)-N(3)-C(6)	94.8(4)
P(1)-Ru(1)-N(3)-C(6)	-94.0(4)
N(3)-Ru(1)-N(4)-C(9)	-172.3(7)
N(1)-Ru(1)-N(4)-C(9)	-168.5(6)

P(2)-Ru(1)-N(4)-C(9)	93.9(7)
P(1)-Ru(1)-N(4)-C(9)	-70.1(7)
N(3)-Ru(1)-N(4)-N(5)	0.8(4)
N(1)-Ru(1)-N(4)-N(5)	4.6(7)
P(2)-Ru(1)-N(4)-N(5)	-93.1(4)
P(1)-Ru(1)-N(4)-N(5)	102.9(4)
C(9)-N(4)-N(5)-C(7)	0.3(7)
Ru(1)-N(4)-N(5)-C(7)	-175.2(4)
C(9)-N(4)-N(5)-C(6)	176.4(5)
Ru(1)-N(4)-N(5)-C(6)	0.9(6)
C(13)-N(2)-C(1)-N(1)	0.1(7)
C(13)-N(2)-C(1)-C(2)	-179.7(6)
C(12)-N(1)-C(1)-N(2)	0.2(7)
Ru(1)-N(1)-C(1)-N(2)	-179.2(4)
C(12)-N(1)-C(1)-C(2)	180.0(5)
Ru(1)-N(1)-C(1)-C(2)	0.6(7)
C(6)-N(3)-C(2)-C(3)	-0.5(9)
Ru(1)-N(3)-C(2)-C(3)	175.1(5)
C(6)-N(3)-C(2)-C(1)	-179.3(5)
Ru(1)-N(3)-C(2)-C(1)	-3.7(7)
N(2)-C(1)-C(2)-N(3)	-178.3(6)
N(1)-C(1)-C(2)-N(3)	1.9(8)
N(2)-C(1)-C(2)-C(3)	3.0(11)
N(1)-C(1)-C(2)-C(3)	-176.8(6)
N(3)-C(2)-C(3)-C(4)	1.1(10)
C(1)-C(2)-C(3)-C(4)	179.7(6)
C(2)-C(3)-C(4)-C(5)	-1.0(11)
C(3)-C(4)-C(5)-C(6)	0.4(11)
C(2)-N(3)-C(6)-C(5)	-0.2(9)
Ru(1)-N(3)-C(6)-C(5)	-175.8(5)
C(2)-N(3)-C(6)-N(5)	179.6(5)
Ru(1)-N(3)-C(6)-N(5)	3.9(7)
C(4)-C(5)-C(6)-N(3)	0.2(10)
C(4)-C(5)-C(6)-N(5)	-179.5(7)
C(7)-N(5)-C(6)-N(3)	172.0(6)
N(4)-N(5)-C(6)-N(3)	-3.1(8)
C(7)-N(5)-C(6)-C(5)	-8.3(11)
N(4)-N(5)-C(6)-C(5)	176.6(6)

N(4)-N(5)-C(7)-C(8)	-0.5(8)
C(6)-N(5)-C(7)-C(8)	-175.9(7)
N(4)-N(5)-C(7)-C(11)	178.5(7)
C(6)-N(5)-C(7)-C(11)	3.1(12)
N(5)-C(7)-C(8)-C(9)	0.5(8)
C(11)-C(7)-C(8)-C(9)	-178.4(7)
N(5)-N(4)-C(9)-C(8)	0.1(7)
Ru(1)-N(4)-C(9)-C(8)	173.5(5)
N(5)-N(4)-C(9)-C(10)	-175.1(6)
Ru(1)-N(4)-C(9)-C(10)	-1.7(11)
C(7)-C(8)-C(9)-N(4)	-0.3(8)
C(7)-C(8)-C(9)-C(10)	174.4(7)
C(1)-N(1)-C(12)-C(13)	-0.3(6)
Ru(1)-N(1)-C(12)-C(13)	178.6(5)
C(1)-N(1)-C(12)-C(17)	176.6(6)
Ru(1)-N(1)-C(12)-C(17)	-4.4(11)
C(1)-N(2)-C(13)-C(12)	-0.3(7)
C(1)-N(2)-C(13)-C(14)	-179.9(7)
N(1)-C(12)-C(13)-N(2)	0.4(7)
C(17)-C(12)-C(13)-N(2)	-176.8(6)
N(1)-C(12)-C(13)-C(14)	-179.9(6)
C(17)-C(12)-C(13)-C(14)	2.8(9)
N(2)-C(13)-C(14)-C(15)	179.1(7)
C(12)-C(13)-C(14)-C(15)	-0.5(10)
C(13)-C(14)-C(15)-C(16)	-1.4(10)
C(13)-C(14)-C(15)-C(19)	176.7(6)
C(14)-C(15)-C(16)-C(17)	0.9(10)
C(19)-C(15)-C(16)-C(17)	-177.1(6)
C(14)-C(15)-C(16)-C(18)	179.9(6)
C(19)-C(15)-C(16)-C(18)	1.9(10)
C(15)-C(16)-C(17)-C(12)	1.3(9)
C(18)-C(16)-C(17)-C(12)	-177.7(6)
N(1)-C(12)-C(17)-C(16)	-179.8(6)
C(13)-C(12)-C(17)-C(16)	-3.2(9)
C(32)-P(1)-C(20)-C(25)	170.9(5)
C(26)-P(1)-C(20)-C(25)	67.5(5)
Ru(1)-P(1)-C(20)-C(25)	-62.7(5)
C(32)-P(1)-C(20)-C(21)	-9.3(6)

C(26)-P(1)-C(20)-C(21)	-112.6(6)
Ru(1)-P(1)-C(20)-C(21)	117.2(5)
C(25)-C(20)-C(21)-C(22)	0.7(10)
P(1)-C(20)-C(21)-C(22)	-179.1(5)
C(20)-C(21)-C(22)-C(23)	-2.6(11)
C(21)-C(22)-C(23)-C(24)	2.7(11)
C(22)-C(23)-C(24)-C(25)	-0.8(11)
C(21)-C(20)-C(25)-C(24)	1.1(10)
P(1)-C(20)-C(25)-C(24)	-179.0(5)
C(23)-C(24)-C(25)-C(20)	-1.1(11)
C(20)-P(1)-C(26)-C(31)	176.3(5)
C(32)-P(1)-C(26)-C(31)	71.6(6)
Ru(1)-P(1)-C(26)-C(31)	-55.2(6)
C(20)-P(1)-C(26)-C(27)	-3.1(6)
C(32)-P(1)-C(26)-C(27)	-107.8(6)
Ru(1)-P(1)-C(26)-C(27)	125.4(5)
C(31)-C(26)-C(27)-C(28)	0.6(10)
P(1)-C(26)-C(27)-C(28)	-180.0(6)
C(26)-C(27)-C(28)-C(29)	-1.2(12)
C(27)-C(28)-C(29)-C(30)	1.0(12)
C(28)-C(29)-C(30)-C(31)	-0.2(12)
C(27)-C(26)-C(31)-C(30)	0.3(10)
P(1)-C(26)-C(31)-C(30)	-179.2(6)
C(29)-C(30)-C(31)-C(26)	-0.5(11)
C(20)-P(1)-C(32)-C(33)	-96.6(5)
C(26)-P(1)-C(32)-C(33)	7.8(5)
Ru(1)-P(1)-C(32)-C(33)	136.7(4)
C(20)-P(1)-C(32)-C(37)	80.0(5)
C(26)-P(1)-C(32)-C(37)	-175.5(5)
Ru(1)-P(1)-C(32)-C(37)	-46.7(5)
C(37)-C(32)-C(33)-C(34)	1.0(9)
P(1)-C(32)-C(33)-C(34)	177.7(5)
C(32)-C(33)-C(34)-C(35)	-2.5(10)
C(33)-C(34)-C(35)-C(36)	1.8(10)
C(34)-C(35)-C(36)-C(37)	0.4(10)
C(35)-C(36)-C(37)-C(32)	-1.9(10)
C(33)-C(32)-C(37)-C(36)	1.2(9)
P(1)-C(32)-C(37)-C(36)	-175.6(5)

C(50)-P(2)-C(38)-C(39)	-143.2(5)
C(44)-P(2)-C(38)-C(39)	-42.9(5)
Ru(1)-P(2)-C(38)-C(39)	84.6(5)
C(50)-P(2)-C(38)-C(43)	46.2(5)
C(44)-P(2)-C(38)-C(43)	146.4(5)
Ru(1)-P(2)-C(38)-C(43)	-86.1(5)
C(43)-C(38)-C(39)-C(40)	-1.7(9)
P(2)-C(38)-C(39)-C(40)	-172.5(5)
C(38)-C(39)-C(40)-C(41)	-0.6(10)
C(39)-C(40)-C(41)-C(42)	1.9(10)
C(40)-C(41)-C(42)-C(43)	-0.8(10)
C(41)-C(42)-C(43)-C(38)	-1.5(10)
C(39)-C(38)-C(43)-C(42)	2.8(9)
P(2)-C(38)-C(43)-C(42)	173.8(5)
C(38)-P(2)-C(44)-C(45)	148.0(5)
C(50)-P(2)-C(44)-C(45)	-105.4(5)
Ru(1)-P(2)-C(44)-C(45)	23.9(6)
C(38)-P(2)-C(44)-C(49)	-38.0(5)
C(50)-P(2)-C(44)-C(49)	68.5(5)
Ru(1)-P(2)-C(44)-C(49)	-162.1(4)
C(49)-C(44)-C(45)-C(46)	-0.2(9)
P(2)-C(44)-C(45)-C(46)	173.8(5)
C(44)-C(45)-C(46)-C(47)	1.3(11)
C(45)-C(46)-C(47)-C(48)	-1.3(11)
C(46)-C(47)-C(48)-C(49)	0.2(10)
C(47)-C(48)-C(49)-C(44)	0.9(10)
C(45)-C(44)-C(49)-C(48)	-0.9(9)
P(2)-C(44)-C(49)-C(48)	-175.0(5)
C(38)-P(2)-C(50)-C(55)	-163.9(5)
C(44)-P(2)-C(50)-C(55)	91.2(5)
Ru(1)-P(2)-C(50)-C(55)	-36.3(5)
C(38)-P(2)-C(50)-C(51)	25.4(6)
C(44)-P(2)-C(50)-C(51)	-79.5(5)
Ru(1)-P(2)-C(50)-C(51)	153.0(4)
C(55)-C(50)-C(51)-C(52)	1.4(9)
P(2)-C(50)-C(51)-C(52)	171.8(5)
C(50)-C(51)-C(52)-C(53)	-0.5(10)
C(51)-C(52)-C(53)-C(54)	-0.8(10)

C(52)-C(53)-C(54)-C(55)	1.2(10)
C(51)-C(50)-C(55)-C(54)	-0.9(9)
P(2)-C(50)-C(55)-C(54)	-172.1(5)
C(53)-C(54)-C(55)-C(50)	-0.4(10)
