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Surpporting Information

Synthesis of Aromatic Ruthenabenzothiophenes via C–H Activation of Thiophenes

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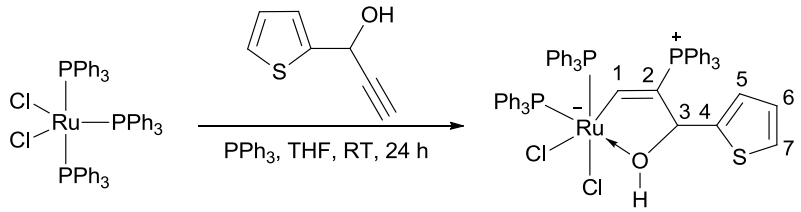
Contents

1. Experimental Procedures

General Procedures. All syntheses were performed at room temperature under a nitrogen atmosphere using standard Schlenk techniques, unless otherwise stated. The solvents were distilled from sodium/benzophenone (tetrahydrofuran and diethyl ether) or calcium hydride (dichloromethane) under a nitrogen atmosphere prior to use. Other reagents were used as received from commercial sources without further purification. Column chromatography was performed on alumina gel (200-300 mesh) in air. The nuclear magnetic resonance (NMR) experiments were performed on a Bruker AVIII-400 spectrometer (^{1}H 400.0 MHz, ^{13}C 100.6 MHz, ^{31}P 161.9 MHz) for compound **1** at 239 K, a Bruker AVIII-500 spectrometer (^{1}H 500.2 MHz, ^{13}C 125.8 MHz, ^{31}P 202.5 MHz) for complex **2** and **4**, a Bruker AVIII-300 spectrometer (^{1}H 300.1 MHz, ^{13}C 75.5 MHz, ^{31}P 121.5 MHz) for complex **5** at room temperature, and a Bruker AVIII-600 spectrometer (^{1}H 600.1 MHz, ^{13}C 150.9 MHz, ^{31}P 242.9 MHz) for complex **3** at 278 K. ^{1}H and ^{13}C NMR chemical shifts (δ) are relative to tetramethylsilane, while ^{31}P NMR chemical shifts(δ) are relative to 85% H_3PO_4. The absolute values of the coupling constants are given in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). Elemental analyses data were performed on a Vario EL III elemental analyzer. High-resolution mass spectrometry (HRMS) experiments were performed on a Bruker En Apex Ultra 7.0T FT-MS.

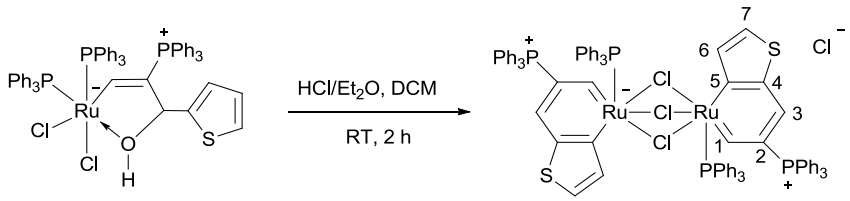
Preparation and characterization of complex 1:



1: 65%

1-(2-thienyl)-2-propyn-1-ol (0.36 mL, 3.23 mmol) was added to a solution of $RuCl_2(PPh_3)_3$ (2.06 g, 2.15 mmol) and PPh_3 (2.82 g, 10.75 mmol) in tetrahydrofuran (20 mL). The reaction mixture was stirred at room temperature for 24 h to give a yellow suspension. The yellow solid was collected by filtration, washed with Et_2O (3 × 40 mL) and dried in vacuo. Yield: 1.53 g, 65%; ^{1}H NMR (400.0 MHz, CD_2Cl_2, 239 K): δ = 11.06 (d, *J*(P,H) = 22.91 Hz, 1H, C^{1}*H*), 6.72-7.57 (m, 45H, Ph), 6.46 (br, 1H, C^{3}*H*), 5.93-6.28 (m, 3H, Th), 2.02 (br, 1H, O*H*); ^{31}P {^{1}H} NMR (161.9 MHz, CD_2Cl_2, 239 K): δ = 60.25 (d, *J*(P,P) = 40.43 Hz, Ru*P*Ph_3), 55.84 (d, *J*(P,P) = 40.43 Hz, Ru*P*Ph_3), −3.69 (s, C*P*Ph_3); Unfortunately, the poor solubility of **1** prevented ^{13}C {^{1}H} NMR characterization; Elemental analysis calcd (%) for $C_{61}H_{51}Cl_2OP_3RuS$: C 66.79, H 4.69; Found: C 66.42, H 5.03; HRMS (ESI): *m/z* calcd for $[C_{61}H_{51}ClOP_3RuS]^+$: 1061.1613 $[M\text{-}Cl]^+$, found: 1061.1641.

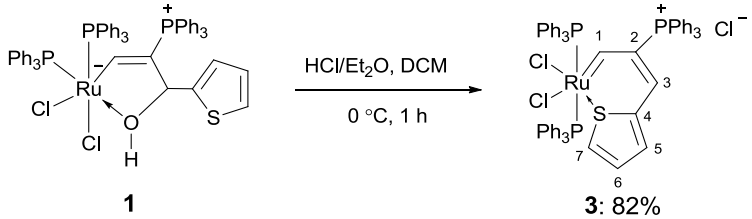
Preparation and characterization of complex 2:



1 **2**: 74%

Method a: To a suspension of compound **1** (450 mg, 0.41 mmol) in DCM (15 mL) was added HCl/Et_2O (0.20 mL, 0.49 mmol). The reaction mixture was stirred at room temperature for 2 h to give a red solution. The solvent was reduced to about 3 mL under vacuum and washed with Et_2O (3 × 30 mL) to give a red solid. Yield: 247 mg, 74%; **Method b**: The solution of compound **3** (200 mg, 0.18 mmol) in DCM (10 mL) was stirred at room temperature for 2 h to give a red solution. The solvent was reduced to about 2 mL under vacuum and washed with Et_2O (3 × 15 mL) to give a red solid. Yield: 114 mg, 78%; ^{1}H NMR (500.2 MHz, CD_2Cl_2): δ = 16.26 (dd, *J*(P,H) = 15.18 Hz, *J*(P,H) = 7.10 Hz, 2H, C^1*H*), 7.97 (d, *J*(H,H) = 3.60 Hz, 2H, C^6*H*), 7.73 (d, *J*(P,H) = 14.25 Hz, 2H, C^3*H*), 6.89 (d, *J*(H,H) = 3.60 Hz, 2H, C^7*H*), 6.68-7.55 ppm (62H, Ph and above-mentioned C^7*H*); ^{31}P {^{1}H} NMR (202.5 MHz, CD_2Cl_2): δ = 47.05 (s, Ru*P*Ph_3), 18.69 ppm (s, C*P*Ph_3); ^{13}C {^{1}H} NMR (125.8 MHz, CD_2Cl_2, plus ^{13}C-dept 135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC): δ = 282.10 (dd, *J*(P,C) = 35.90 Hz, *J*(P,C) = 15.91 Hz, C^1), 244.79 (d, *J*(P,C) = 13.86 Hz, C^5), 143.20 (s, C^7), 137.96 (s, C^6), 135.20 (d, *J*(P,C) = 22.08 Hz, C^3), 133.14-133.53 (Ph), 132.47 (d, *J*(P,C) = 47.58 Hz, C^4), 126.49-129.12 (Ph), 120.04 (d, *J*(P,C) = 86.94 Hz, Ph), 113.53 ppm (d, *J*(P,C) = 75.87 Hz, C^2). Elemental analysis calcd (%) for $C_{86}H_{68}Cl_4P_4Ru_2S_2$: C 63.24, H 4.20. Found: C 63.21, H 4.44; HRMS (ESI): *m/z* calcd for $[C_{86}H_{68}Cl_3P_4Ru_2S_2]^+$: 1599.0874 $[M\text{-}Cl]^+$, found: 1599.0867.

Preparation and characterization of complex 3:

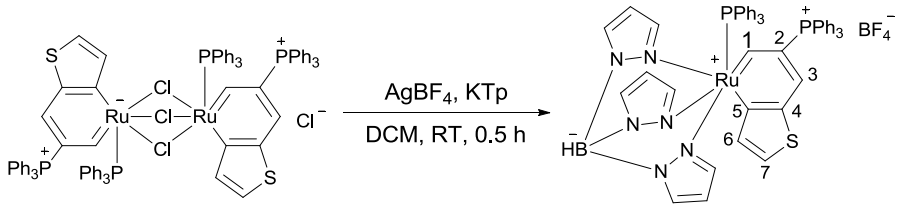


1 **3**: 82%

To a suspension of compound **1** (606 mg, 0.55 mmol) in DCM (20 mL) was added HCl/Et_2O (1.10 mL, 2.75 mmol). The reaction mixture was stirred at 0 ℃ for 1 h to give a red solution. The solvent was reduced to about 5 mL under vacuum and washed with Et_2O (3 × 15 mL) to give a red solid. Yield: 505 mg, 82%; ^{1}H NMR (600.1 MHz, CD_2Cl_2, 278K): δ = 17.87 (d, *J*(P,H) = 20.95 Hz, 1H, C^1*H*), 9.19 (d, *J*(P,H) = 16.81 Hz, 1H, C^3*H*), 8.59 (s, 1H, C^5*H*), 7.91 (dd, *J*(H,H) = 10.58 Hz, *J*(H,H) = 4.60 Hz, 1H, C^6*H*), 6.85-7.80 (Ph, 45H), 6.71 (d, *J*(H,H) = 4.60 Hz, 1H, C^7*H*); ^{31}P {^{1}H} NMR (242.9 MHz, CD_2Cl_2, 278K): δ = 24.18 (s, Ru*P*Ph_3), 11.79 (s, C*P*Ph_3); Elemental analysis calcd (%) for $C_{61}H_{50}Cl_3P_3RuS$: C 65.68, H 4.52; found: C 65.69, H 4.91; HRMS (ESI): *m/z* calcd for $[C_{61}H_{50}Cl_2P_3RuS]^+$: 1079.1261 $[M\text{-}Cl]^+$, found:

1079.1293.

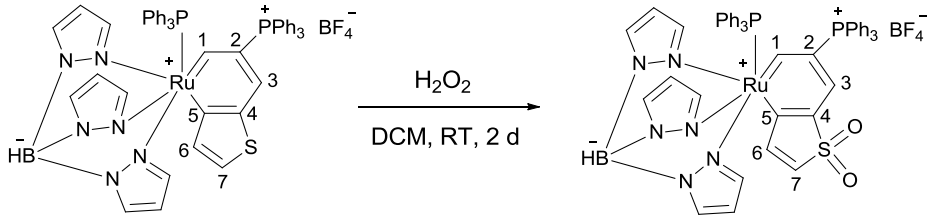
Preparation and characterization of complex 4:



2 **4:** 82%

A mixture of **2** (310 mg, 0.19 mmol), $AgBF_4$ (184.93 mg, 0.95 mmol) and KTp (105.40 mg, 0.42 mmol) in DCM (20 mL) was stirred at room temperature for about 0.5 h to give a red solution, the solid suspension was removed through a filter. The filtrate was reduced to about 3 mL under vacuum and washed with Et_2O (3 × 30 mL) to give a red solid. The residue was purified by column chromatography (neutral alumina, eluent: acetone/dichloromethane, 1:3) to give complex **4** as a red solid (325 mg, 82%); ^{1}H NMR (500.2 MHz, CD_2Cl_2): δ = 17.11 (d, *J*(P,H) = 19.91 Hz, 1H, C^1*H*), 8.23 (d, *J*(H,H) = 4.95 Hz, 1H, C^6*H*), 8.11 (d, *J*(P,H) = 12.47 Hz, 1H, C^3*H*), 7.85 (s, 1H, Tp), 7.55-7.77 (10H, Ph), 7.39 (d, *J*(H,H) = 4.95 Hz, 1H, C^7*H*), 7.31 (s, 3H, Tp), 7.16-7.30 (8H, Ph), 6.98 (s, 1H, Tp), 6.11-6.88 (12H, Ph), 6.06 (s, 2H, Tp), 5.56 (s, 1H, Tp), 5.05 ppm (s, 1H, Tp); ^{31}P {^{1}H} NMR (202.5 MHz, CD_2Cl_2): δ = 39.35 (s, Ru*P*Ph$_3$), 16.05 ppm (s, C*P*Ph$_3$); ^{13}C {^{1}H} NMR (125.8 MHz, CD_2Cl_2, plus ^{13}C-dept 135 , ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC): δ = 283.63 (dd, apparent t, *J*(P,C) = 21.44 Hz, C^1), 246.33 (d, *J*(P,C) = 13.55 Hz, C^5), 145.35 (s, C^6), 145.26 (s, Tp), 143.51 (s, C^7), 142.79 (s, Tp), 141.71 (s, Tp), 138.30 (d, *J*(P,C) = 22.15 Hz, C^3), 135.75 (s, Tp), 135.08 (s, Tp), 134.14 (s, Ph), 133.92 (s, Tp), 133.57 (d, *J*(P,C) = 10.10 Hz, Ph), 133.11 (d, *J*(P,C) = 13.43 Hz, C^4), 127.08-132.72 (Ph), 120.07 (d, *J*(P,C) = 87.18 Hz, Ph), 108.98 (d, *J*(P,C) = 75.41 Hz, C^2), 105.80 (s, Tp), 105.48 (s, Tp), 103.97 ppm (s, Tp); Elemental analysis calcd (%) for $C_{52}H_{44}B_2F_4N_6P_2RuS$: N 8.04, C 59.73; H 4.24; Found: N 8.29, C 59.78, H 4.39; HRMS (ESI): *m/z* calcd for $[C_{52}H_{44}BN_6P_2RuS]^+$: 959.1974 $[M\text{-}BF_4]^+$, found: 959.1974.

Preparation and characterization of complex 5:



4 **5:** 90%

A mixture of **4** (200 mg, 0.19 mmol) and H_2O_2 (30% in H_2O, 116 μL, 3.8 mmol) in DCM (10 mL) was stirred at room temperature for about 2 d to give a dark yellow solution. The solvent was reduced to about 3 mL under vacuum and washed with Et_2O (3 × 30 mL) to give a yellow solid (184 mg, 90%). ^{1}H NMR (300.1 MHz, CD_2Cl_2): δ = 15.84 (dd, *J*(P,H) = 21.30 Hz, *J*(P,H) = 1.92 Hz, 1H, C^1*H*), 8.21 (d, *J*(P,H) = 10.45 Hz, 1H, C^3*H*), 7.88 (d, *J*(H,H) = 1.87 Hz, 1H, Tp), 7.57 (d, *J*(H,H) = 6.82 Hz, 1H,

C^6H, determined by HSQC), 7.41 (d, *J*(H,H) = 1.83 Hz, 1H, Tp), 7.35 (s, 2H, Tp), 7.08 (d, *J*(H,H) = 6.82 Hz, 1H, C^7H), 6.64 (d, *J*(H,H) = 1.82 Hz, 1H, Tp), 6.26-7.80 (36H, Ph and Tp, C^6H, C^7H mentioned above), 6.09 (s, 2H, Tp), 5.63 (s, 1H, Tp), 5.04 ppm (s, 1H, Tp); $^{31}P\{^1H\}$ NMR (121.5 MHz, CD_2Cl_2): δ = 34.01 (s, Ru*P*Ph_3), 17.26 ppm (s, C*P*Ph_3); $^{13}C\{^1H\}$ NMR (75.5 MHz, CD_2Cl_2, plus ^{13}C-dept 135, ^1H-^{13}C HSQC and ^1H-^{13}C HMBC): δ = 275.49 (d, *J*(P,C) = 16.30 Hz, C^5), 273.99 (dd, *J*(P,C) = 14.87 Hz, *J*(P,C) = 3.42 Hz, C^1), 145.42 (s, Tp), 142.74 (s, Tp), 142.55 (s, C^6), 140.61 (s, Tp), 136.48 (s, Tp), 136.00 (d, *J*(P,C) = 4.65 Hz, C^4), 135.76 (s, Ph), 134.89 (s, Ph), 134.48 (s, Tp), 134.44 (s, Tp), 132.61-133.54 (Ph), 131.84 (d, *J*(P,C) = 21.91 Hz, C^3), 128.90-130.07 (Ph), 128.45 (s, C^7), 118.48-127.79 (Ph), 108.74 (dd, *J*(P,C) = 78.35 Hz, *J*(P,C) = 2.75 Hz, C^2), 106.55 (s, Tp), 106.18 (s, Tp), 104.90 ppm (d, *J*(P,C) = 1.72 Hz, Tp); Elemental analysis calcd (%) for $C_{52}H_{44}O_2B_2F_4N_6P_2RuS$: N 7.80, C 57.96, H 4.12. Found: N 7.63, C 57.63, H 4.36; HRMS (ESI): *m/z* calcd for $[C_{52}H_{44}BN_6O_2P_2RuS]^+$: 991.1872 $[M\text{-}BF_4]^+$, found: 991.1860.

2. NMR spectra and HRMS

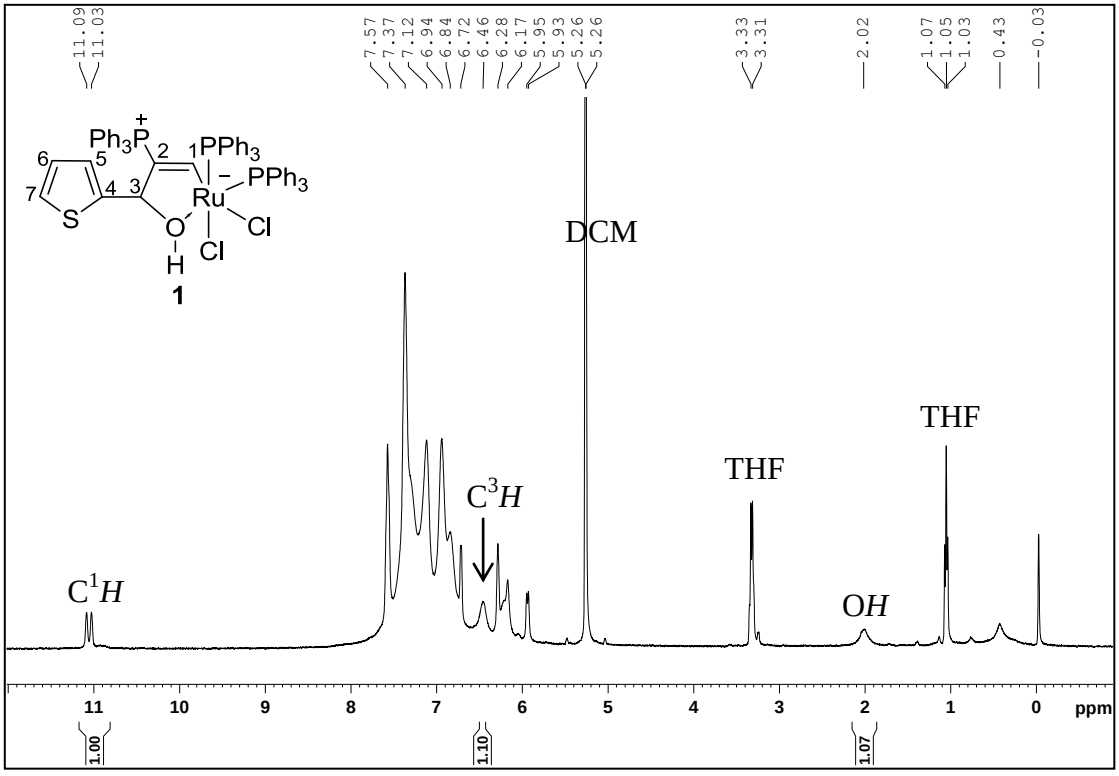


Figure S1 The ^1H-NMR (400.0 MHz, CD_2Cl_2) spectrum for compound **1** at 239 K.

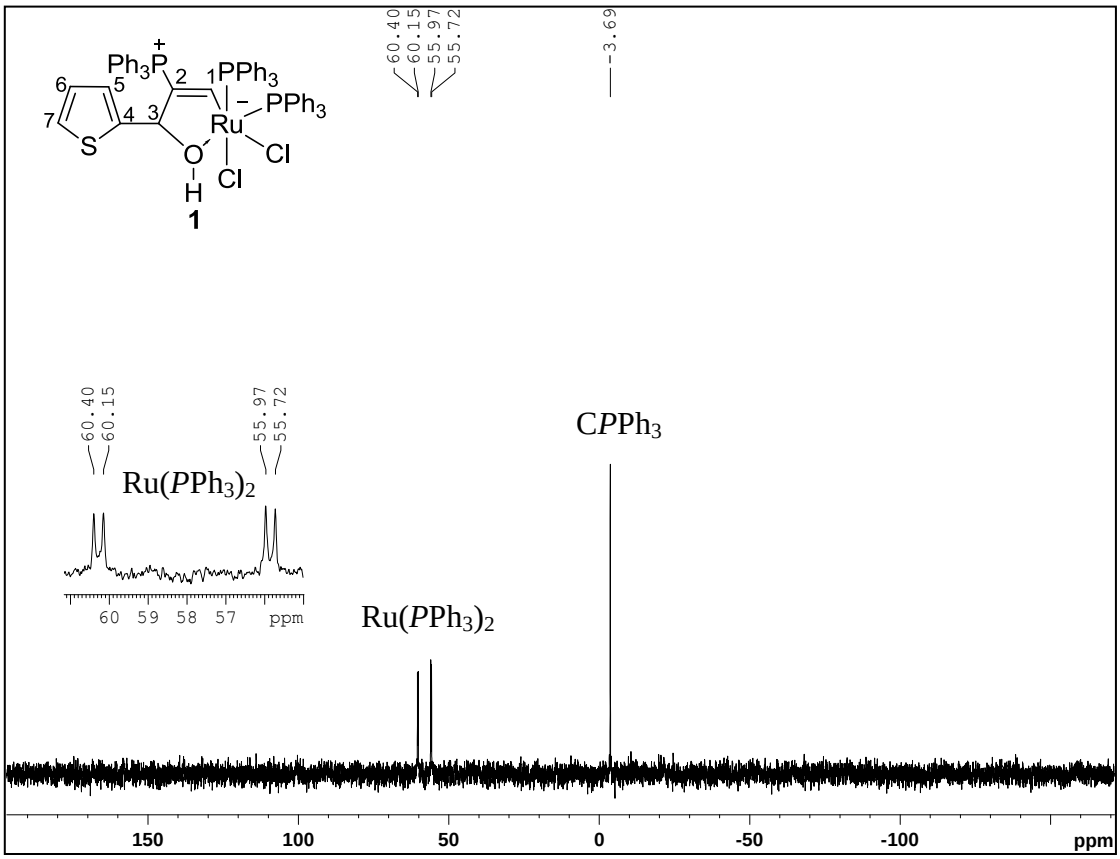


Figure S2 The ^{31}P {^{1}H} NMR (161.9 MHz, CD_2Cl_2) spectrum for compound **1** at 239 K.

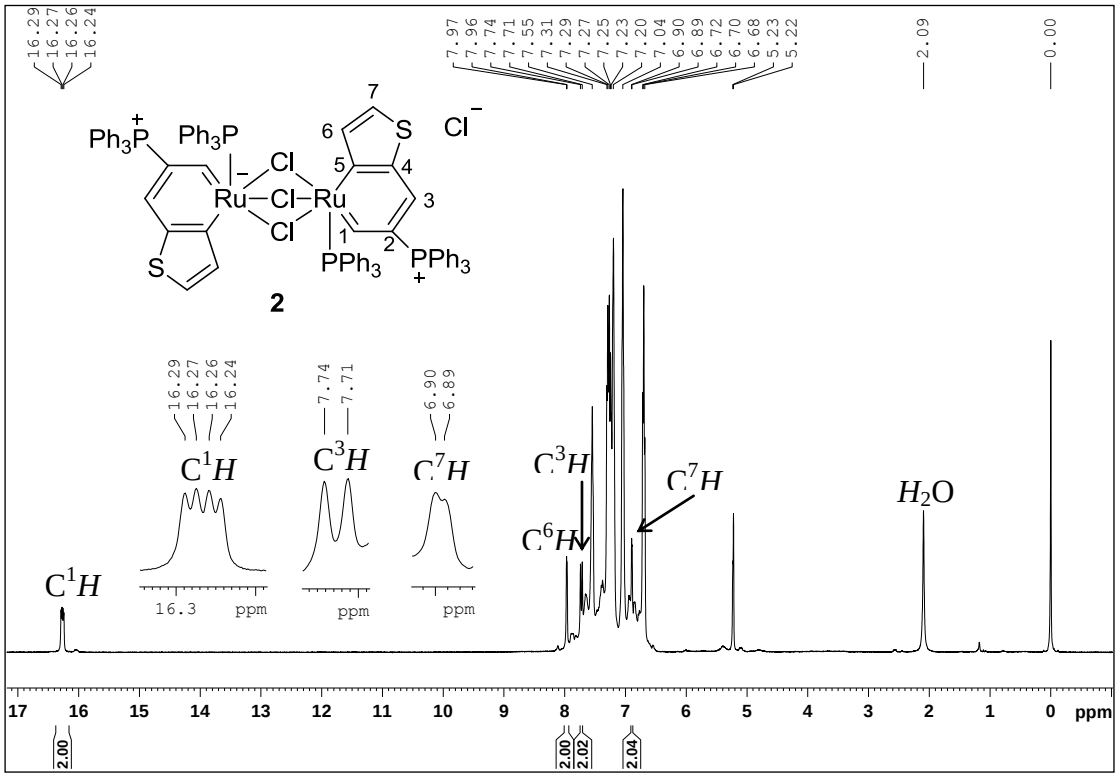


Figure S3 The ^{1}H-NMR (500.2 MHz, CD_2Cl_2) spectrum for complex **2**.

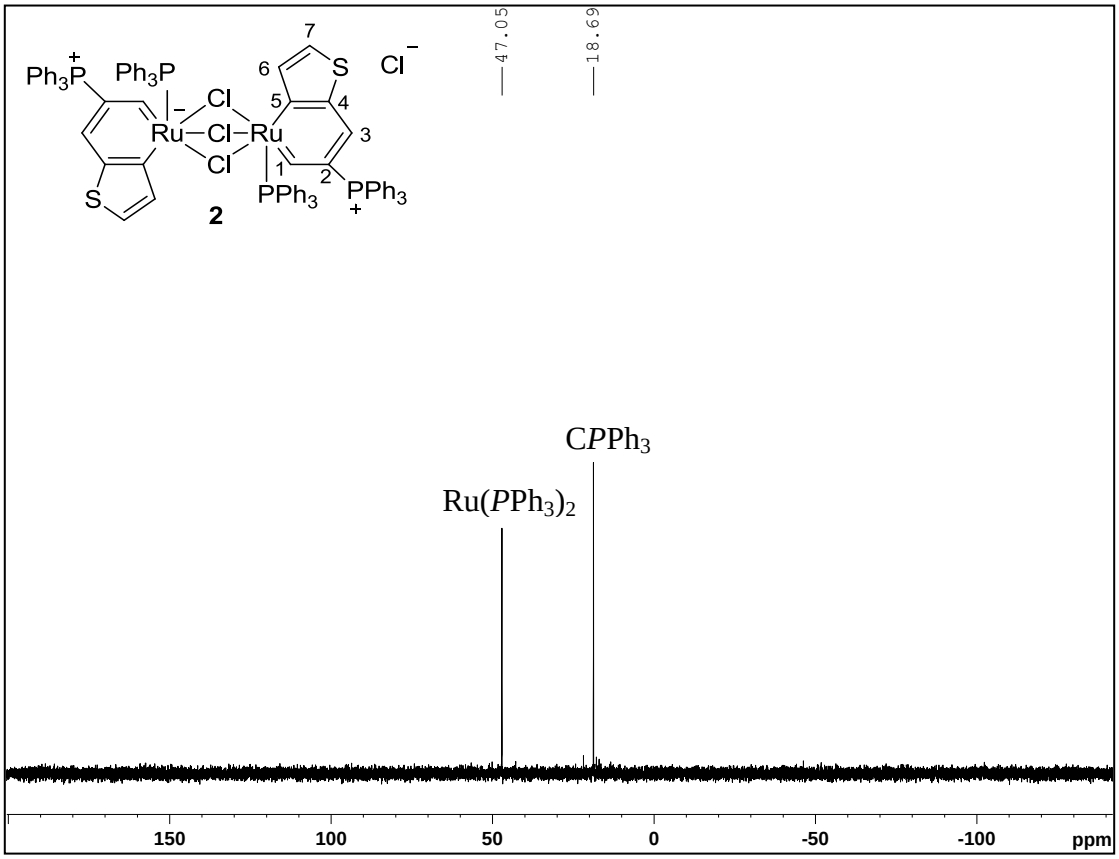


Figure S4 The $^{31}P\{^{1}H\}$ NMR (202.5 MHz, CD_2Cl_2) spectrum for complex **2.**

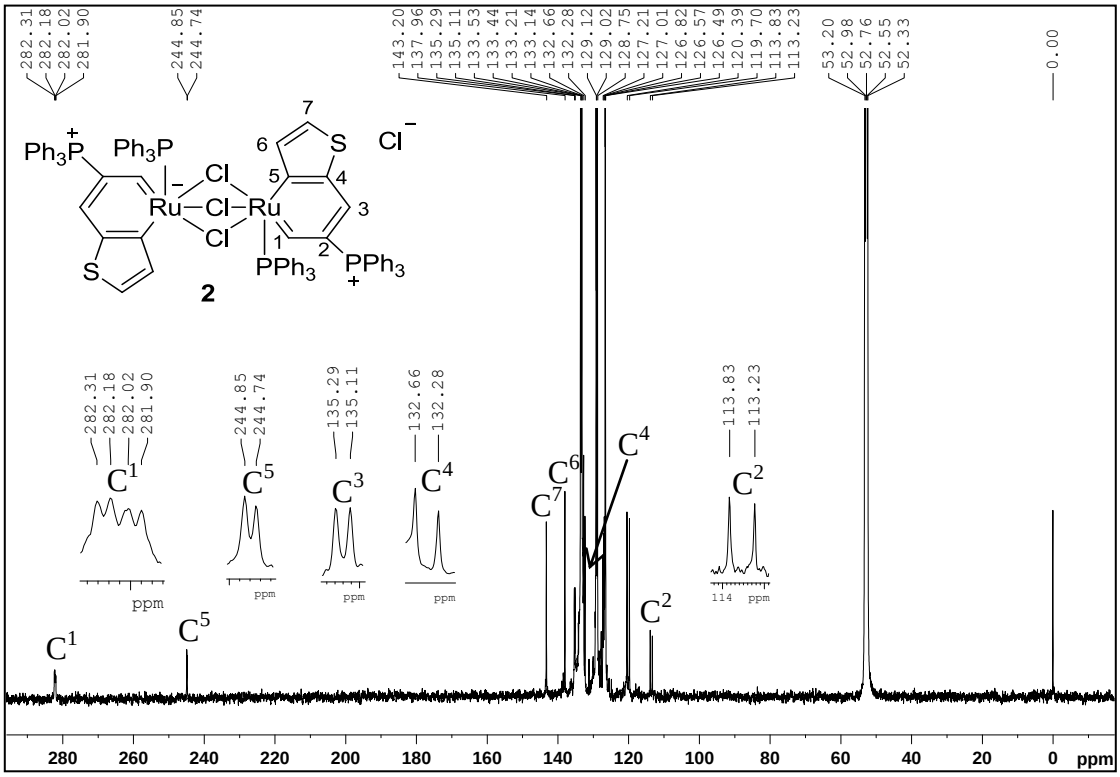


Figure S5 The $^{13}C\ \{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum for complex **2**.

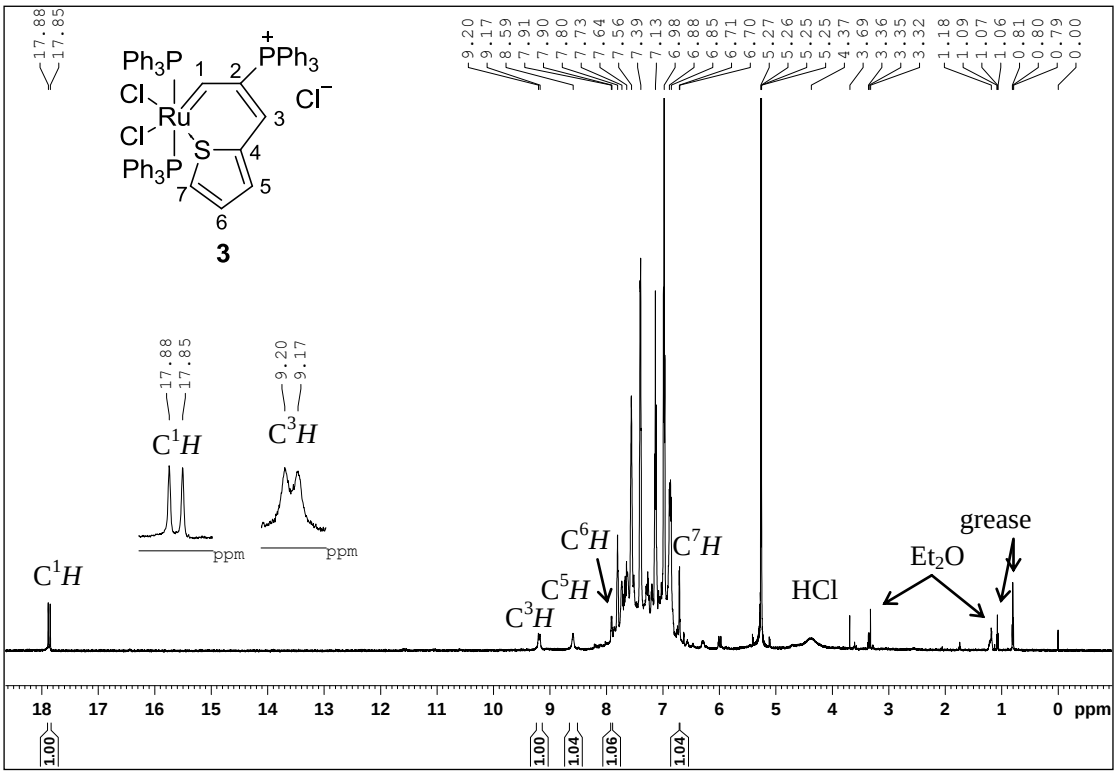


Figure S6 The ^{1}H-NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **3** at 278 K.

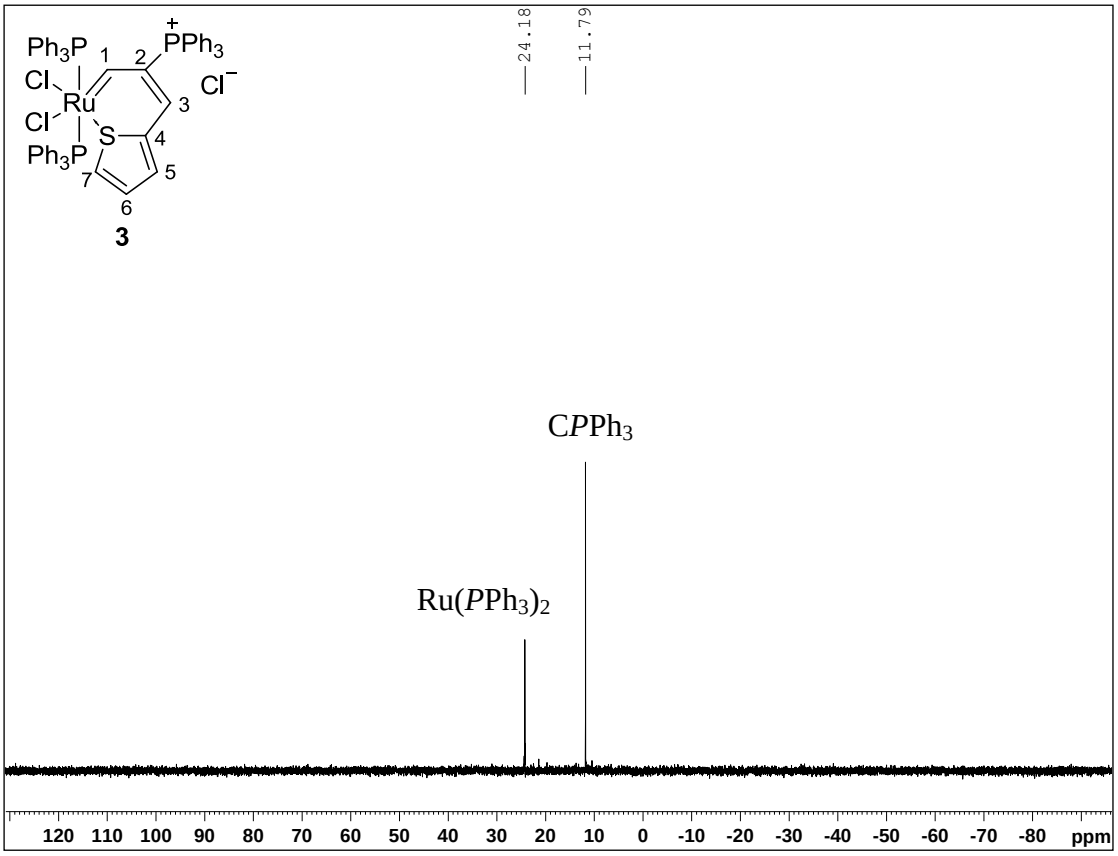


Figure S7 The ^{31}P {^{1}H} NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **3** at 278 K.

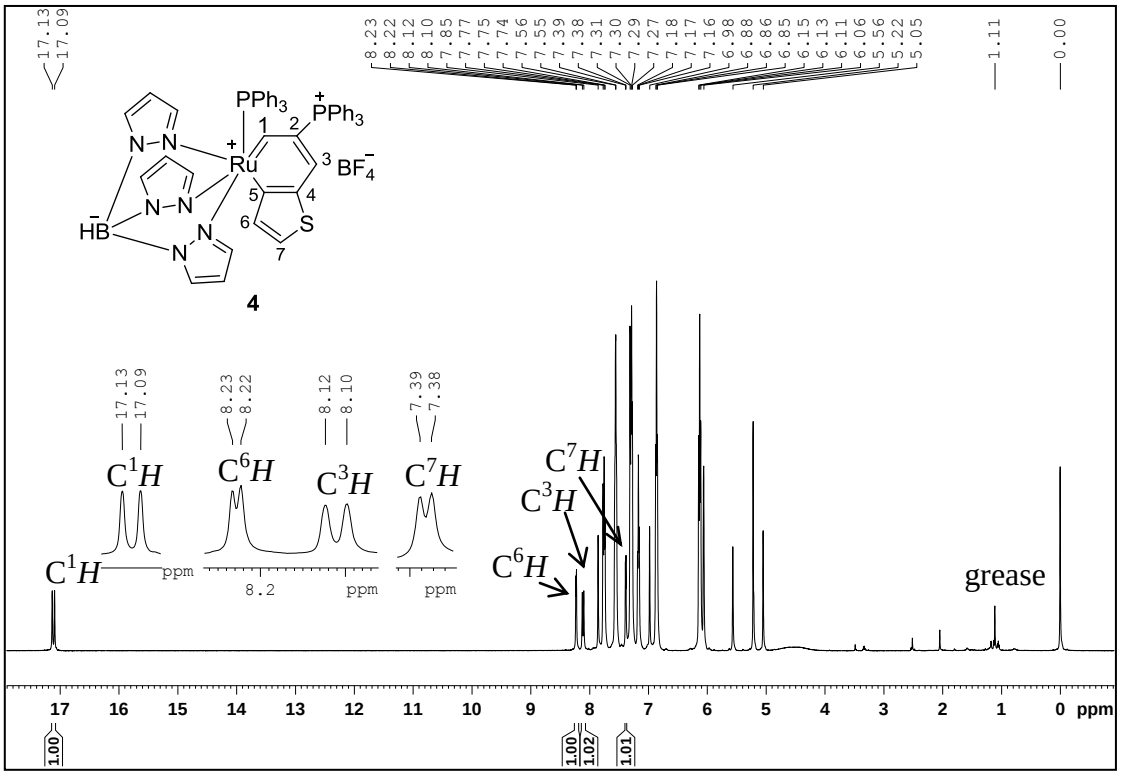


Figure S8 The ^{1}H-NMR (500.2 MHz, CD_2Cl_2) spectrum for complex **4**.

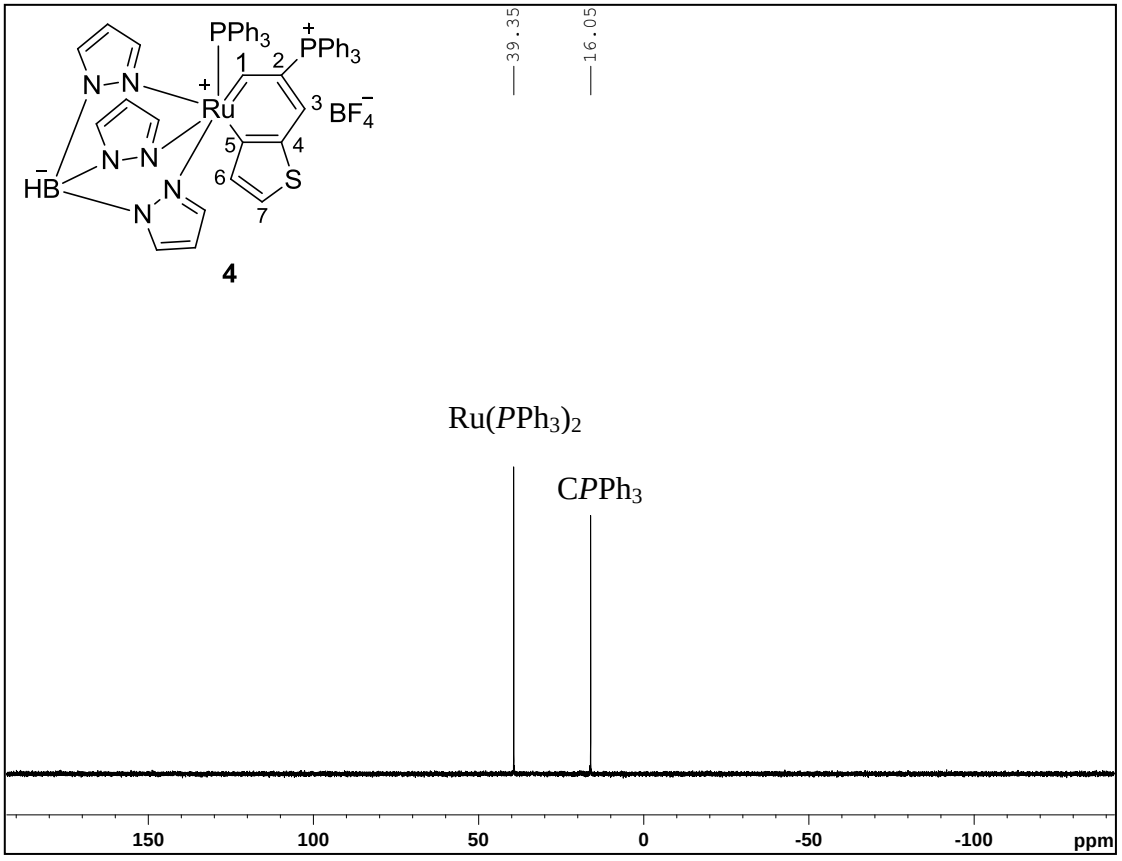


Figure S9 The ^{31}P {^{1}H} NMR (202.5 MHz, CD_2Cl_2) spectrum for complex **4**.

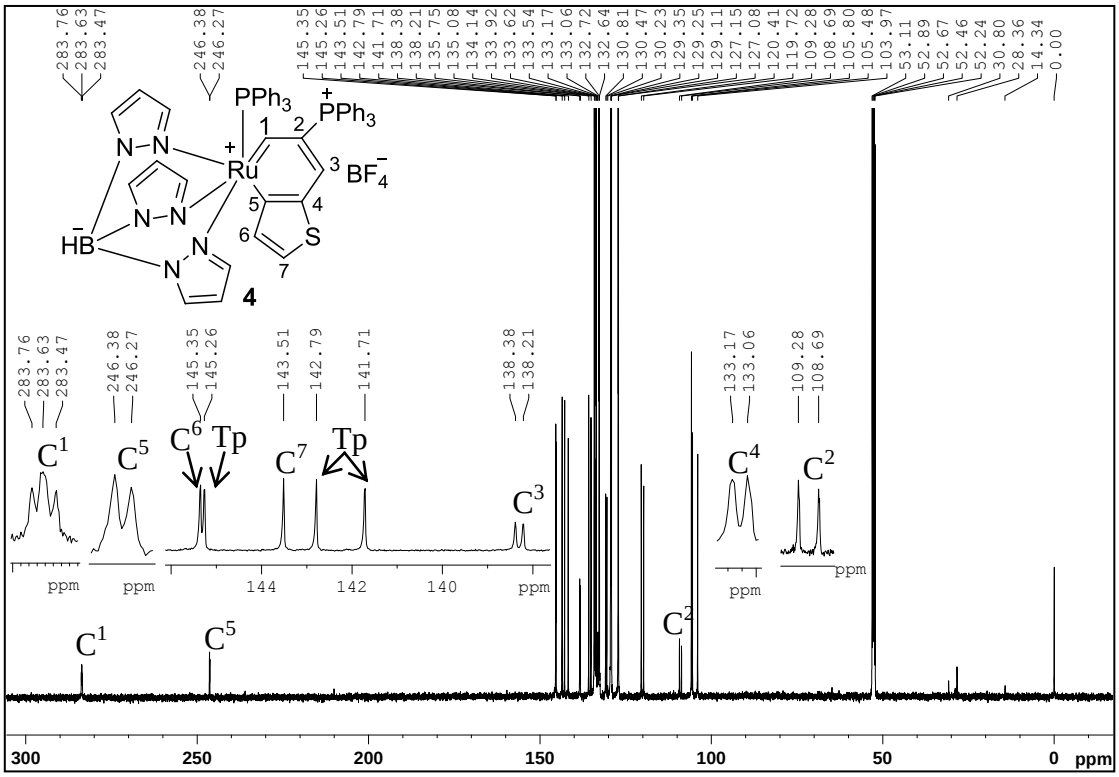


Figure S10 The ^{13}C {^{1}H} NMR (125.8 MHz, CD_2Cl_2) spectrum for complex **4**.

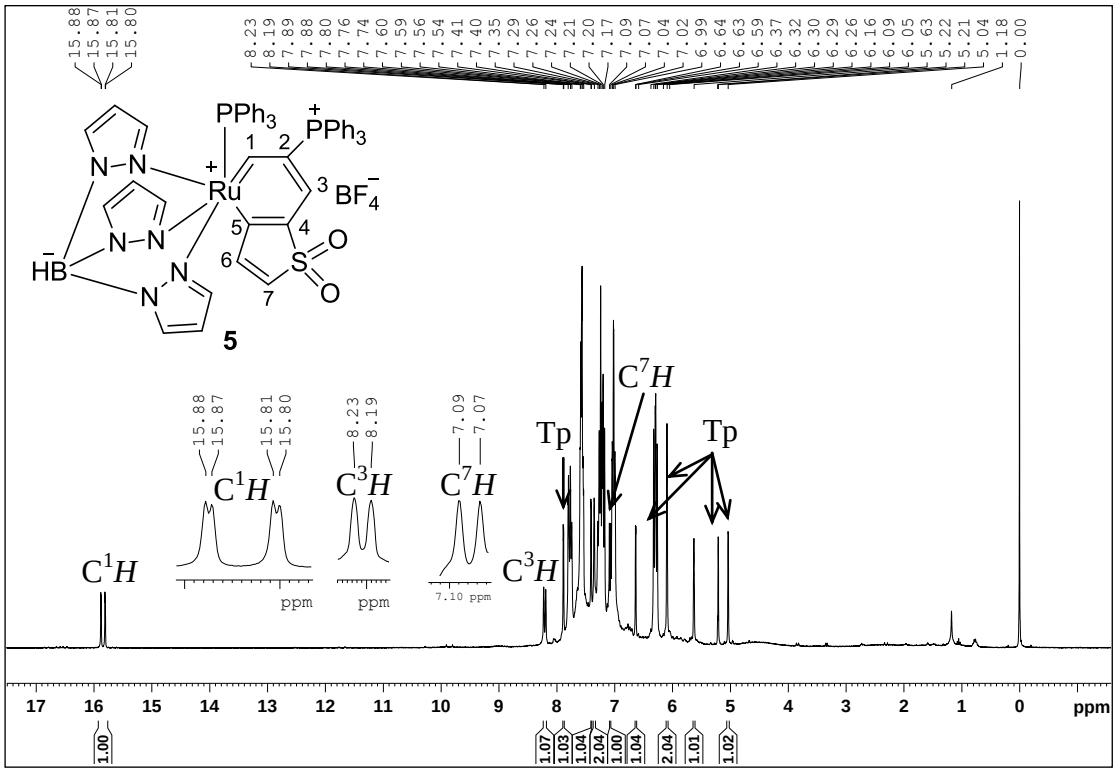


Figure S11 The ^{1}H-NMR (300.1 MHz, CD_2Cl_2) spectrum for complex **5**.

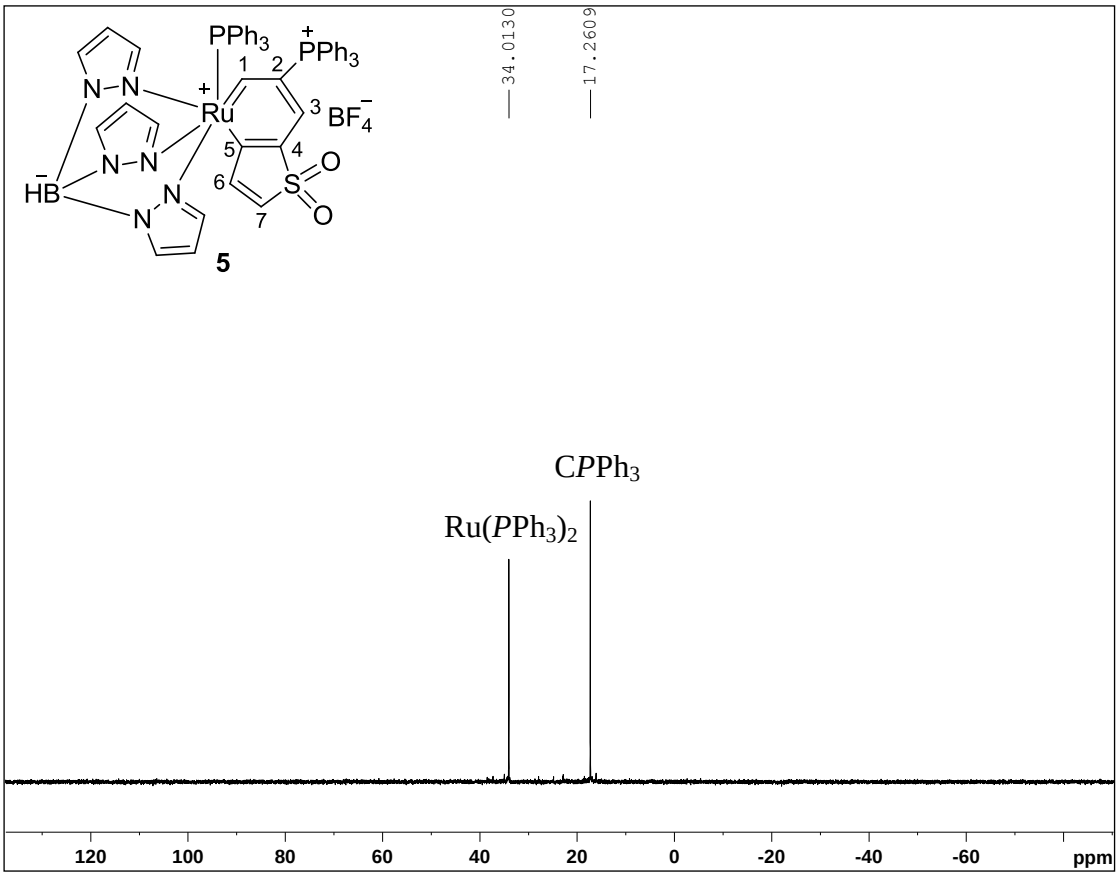


Figure S12 The ^{31}P {^{1}H} NMR (121.5 MHz, CD_2Cl_2) spectrum for complex **5**.

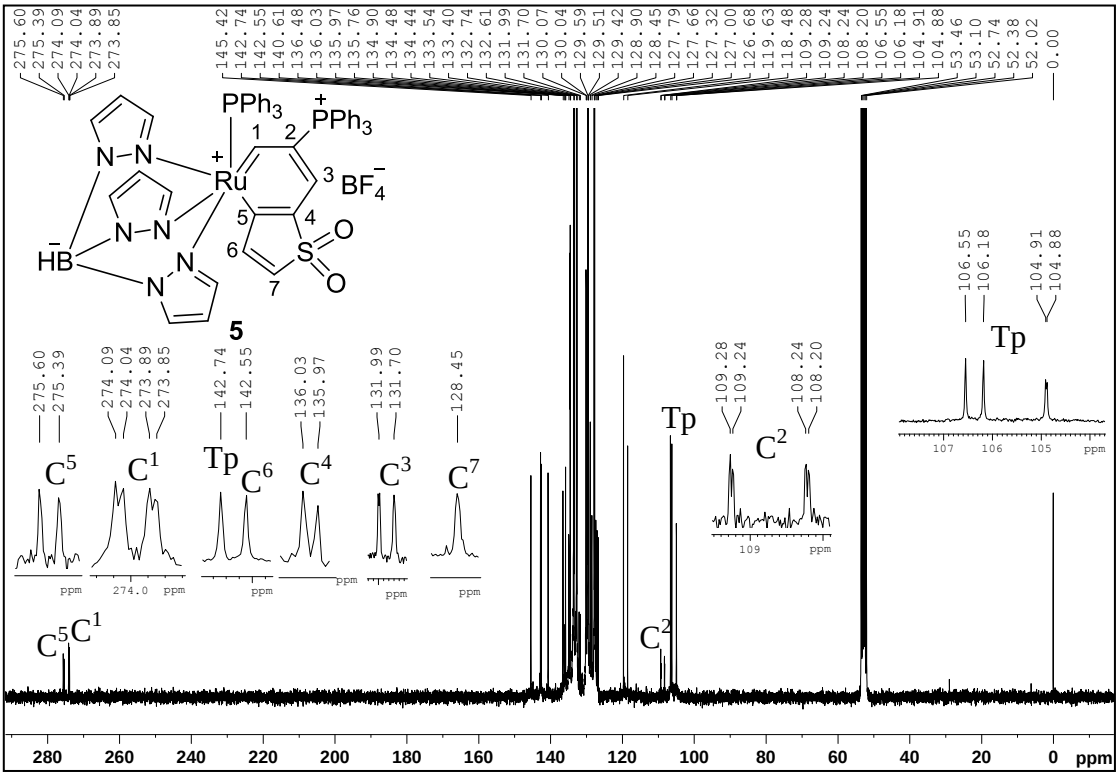


Figure S13 ^{13}C {^{1}H} NMR (75.5 MHz, CD_2Cl_2) spectrum for complex **5.**

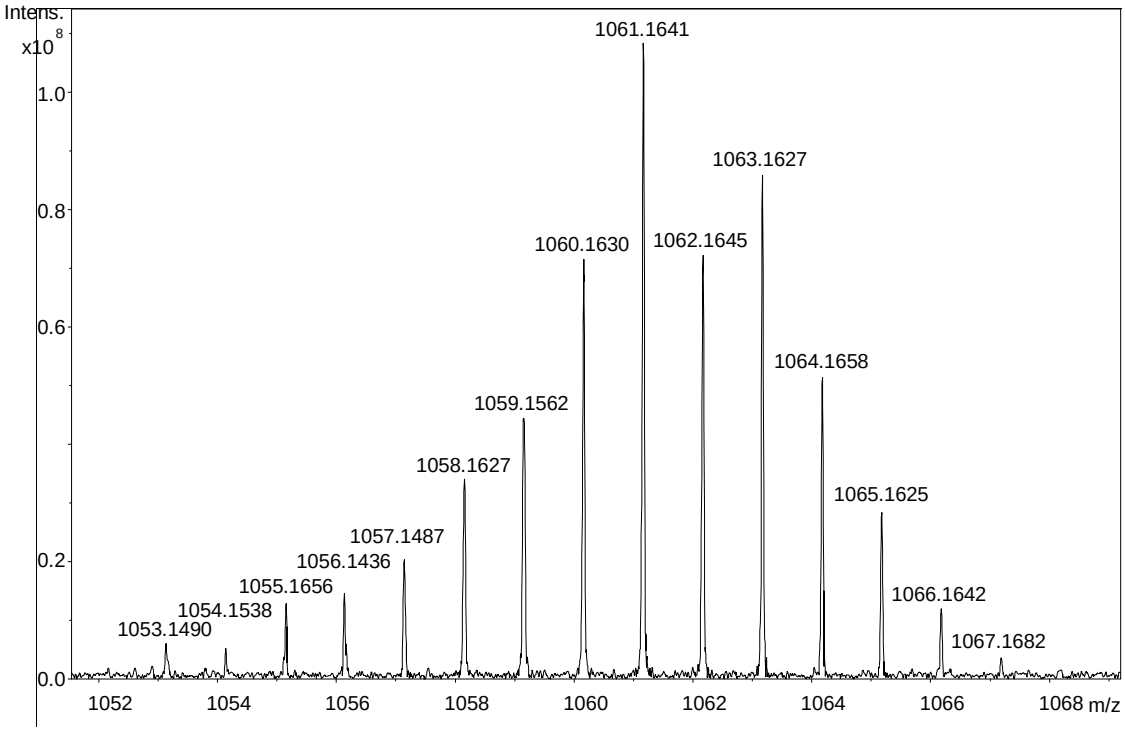


Figure S14 Positive-ion ESI-MS spectrum of [**1**–Cl]$^+$ measured in dichloromethane.

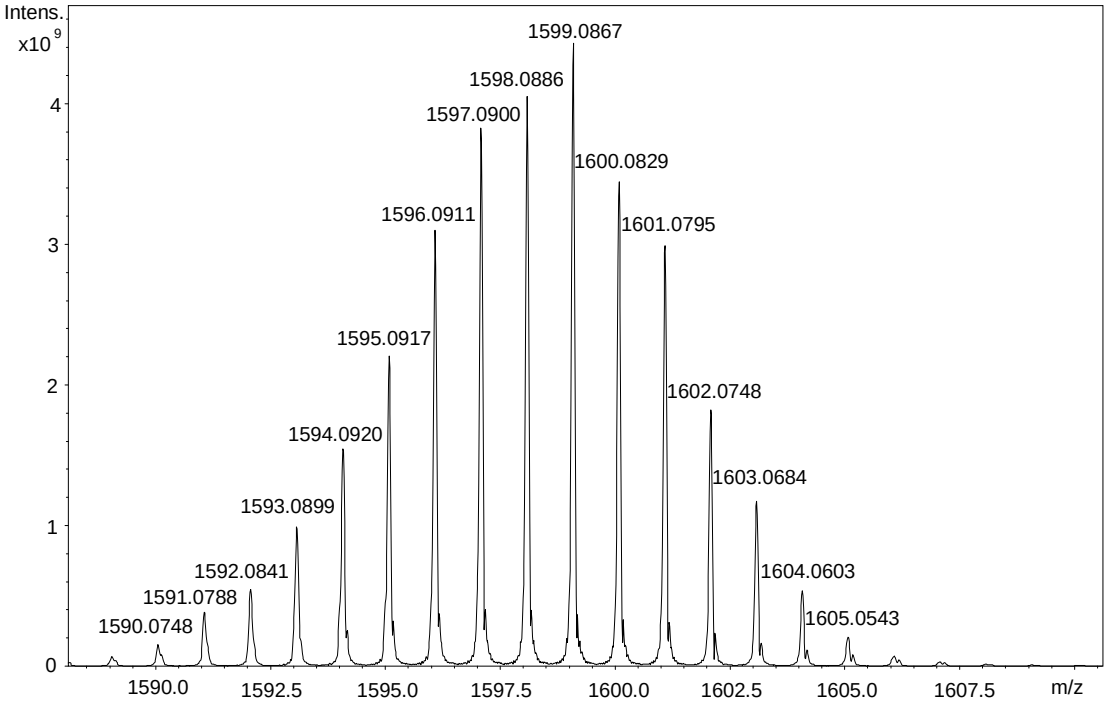


Figure S15 Positive-ion ESI-MS spectrum of [**2**–Cl]$^+$ measured in methanol.

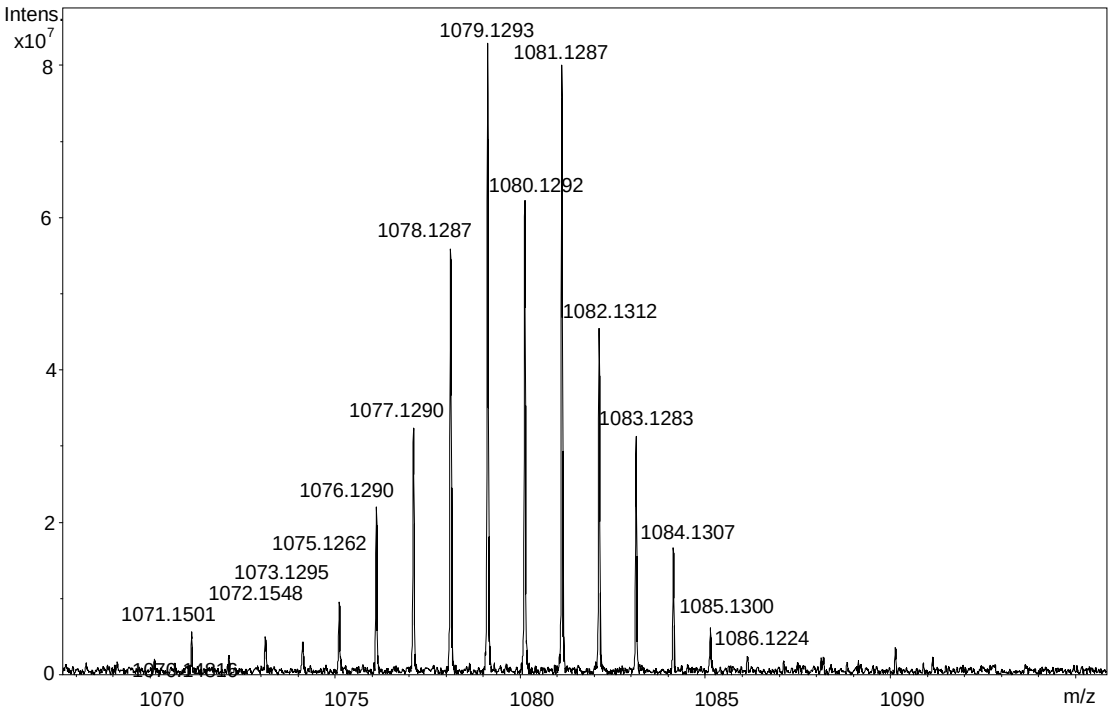


Figure S16 Positive-ion ESI-MS spectrum of [**3**–Cl]$^+$ measured in dichloromethane.

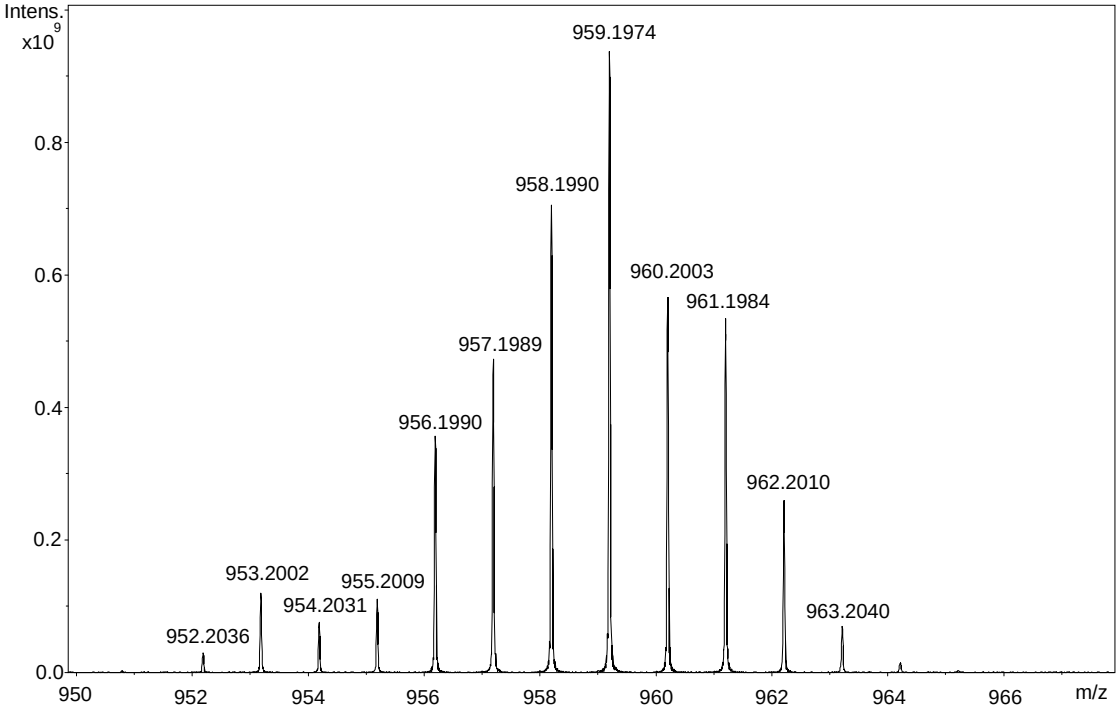


Figure S17 Positive-ion ESI-MS spectrum of [**4**–BF_4]$^+$ measured in methanol.

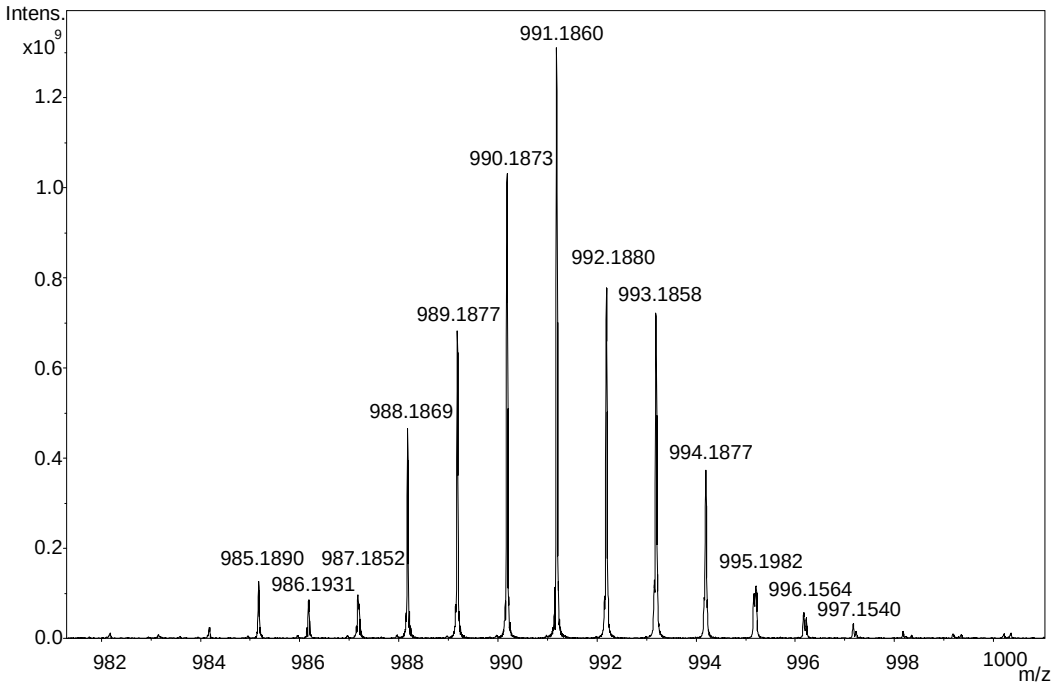


Figure S18 Positive-ion ESI-MS spectrum of $[\mathbf{5}–BF_4]^+$ measured in methanol.

3. Crystallographic details

Single-crystal X-ray diffraction data were collected on an Oxford Gemini S Ultra CCD Area Detector with graphite-monochromated Mo Ka radiation (λ = 0.71073 Å). All of the Data were corrected for absorption effects using the multi-scan technique. The structures were solved by Patterson methods, expanded by difference Fourier syntheses and refined by full matrix least-squares on F^2 using Bruker SHELXL-2013 program package. Non-H atoms were refined anisotropically unless otherwise stated. Hydrogen atoms were introduced at their geometric positions and refined as riding atoms unless otherwise stated. The crystal suitable for X-ray diffraction was grown from the CH_2Cl_2 solution layered with ether or n-hexane for complex **1**, **4** and **5**. CCDC-1048066 (**1**), CCDC-1048063 (**4**) and CCDC-1048067 (**5**), contain the supplementary crystallographic data for this paper. For further details on the crystal data, data collection, and refinements, see Table S1, These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Crystal data and structure refinement for **1**, **4** and **5**.

	1 ·2CH_2Cl_2	**4** 2CH_2Cl_2	**5** ·1CH_2Cl_2 2.5H_2O 0.5 C_6H_6
formula	$C_{63}H_{55}Cl_6$ $ORuP_3S$	$C_{54}H_{48}B_2Cl_4$ $F_4N_6RuP_2S$	$C_{56}H_{54}B_2Cl_2$ $F_4N_6O_{4.5}RuP_2S$
Mr	1266.81	1215.47	1236.63
T [K]	123(2)	173.05(10)	173.00(14)

λ [Å] (MoKα radiation)	0.71073	0.71073	0.71073
crystal system	Monoclinic	Monoclinic	Monoclinic
space group	*Cc*	P2(1)/c	C2/c
a [Å]	13.1210(3)	16.2188(7)	42.420(2)
b [Å]	21.3650(4)	15.6604(6)	16.0779(8)
c [Å]	20.9552(4)	21.8580(9)	19.2499(8)
α [°]	90	90	90
β [°]	101.630(2)	98.260(4)	113.694(6)
γ [°]	90	90	90
V [$Å^3$]	5753.8(2)	5494.2(4)	12022.2(11)
Z	4	4	8
ρ_{calcd} [gcm^{-3}]	1.462	1.469	1.378
μ [mm^{-1}]	0.713	0.633	0.500
F(000)	2592	2472	5104
crystal size [mm^3]	0.30×0.20 ×0.10	0.30×0.20 ×0.20	0.20×0.15 ×0.15
θ range [°]	2.75 to 29.32	2.89 to 25.00	2.91 to 25.00
reflns collected	17746	26396	56423
independent reflns	10022	9641	10556
observed reflns [$I \geq 2\sigma(I)$]	8390	7347	7860
data/restraints /params	10022/17/688	9641/0/667	10556/ 18 / 789
GOF on F^2	1.034	1.036	1.077
R_1/wR_2 [$I \geq 2\sigma(I)$]	0.0387/0.0879	0.0518/0.1004	0.0682/0.1620
R_1/wR_2 (all data)	0.0510/0.1153	0.0744/0.11095	0.0973/0.1759
largest peak/hole [e $Å^{-3}$]	0.78/-0.59	1.10/−0.58	0.81/−0.68

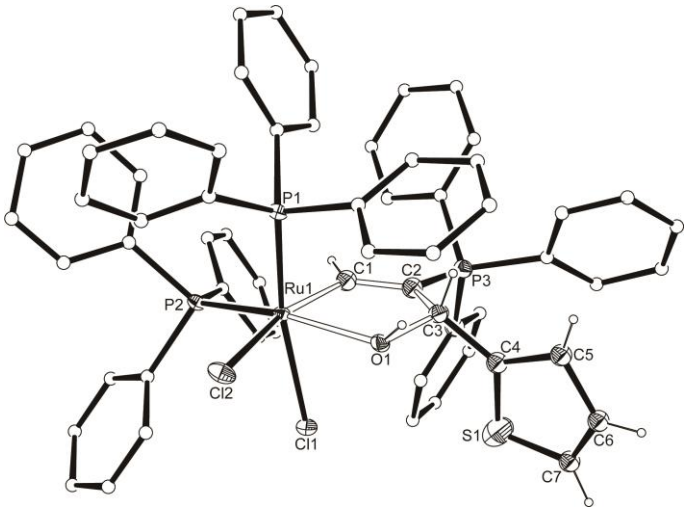
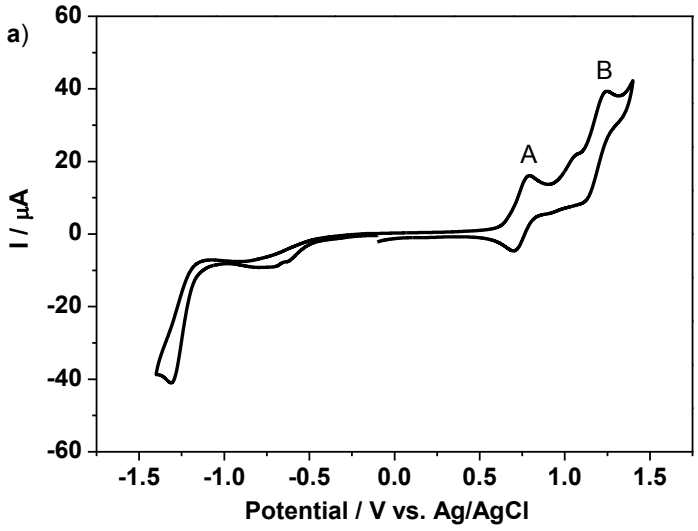


Figure S19 X-ray structure of compound **1** (ellipsoids at the 50% probability level), hydrogen atoms in PPh_3 have been omitted for clarity. Selected bond distances [Å] and angles [º]: Ru1−C1 1.959(6), Ru1−O1 2.214(4), C1−C2 1.359(9), C2−C3 1.514(10) C3−O1 1.457(8); O1−Ru1−C1 77.8(2), Ru1−C1−C2 120.2(5), C1−C2−C3 118.9(5), C2−C3−O1 107.1(5), C3−O1−Ru1 114.0(4).

4. Cyclic voltammogram of complex 2 and 4



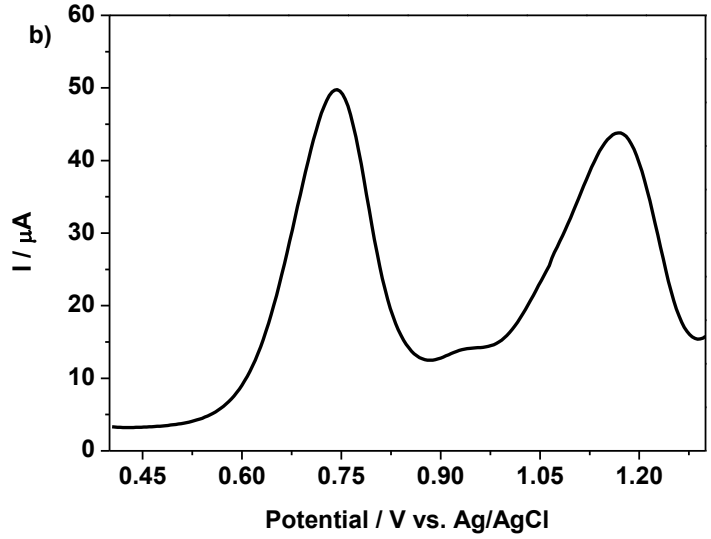


Figure S20 Cyclic (a) and differential pulse voltammogram (b) of compound **2** scanning in the positive direction, measured in CH_2Cl_2 with 0.10 M Bu_4NPF_6 as supporting electrolyte at a scan rate of 0.10 V/s.

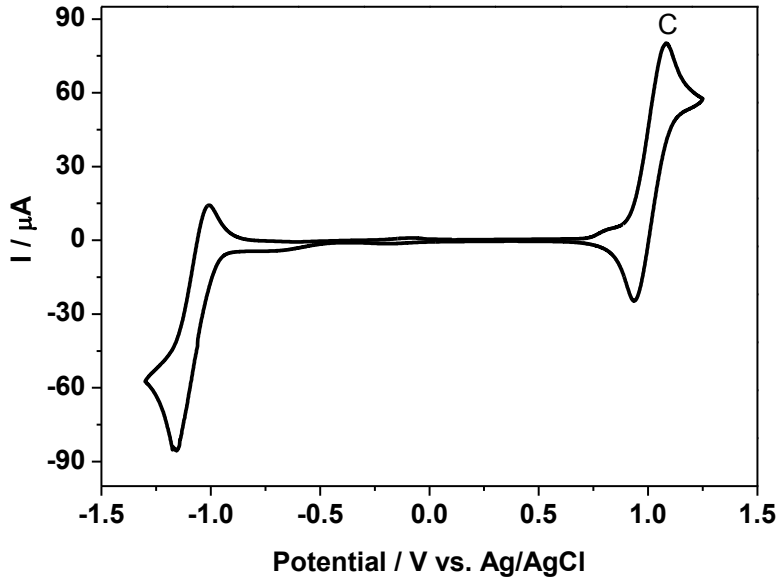


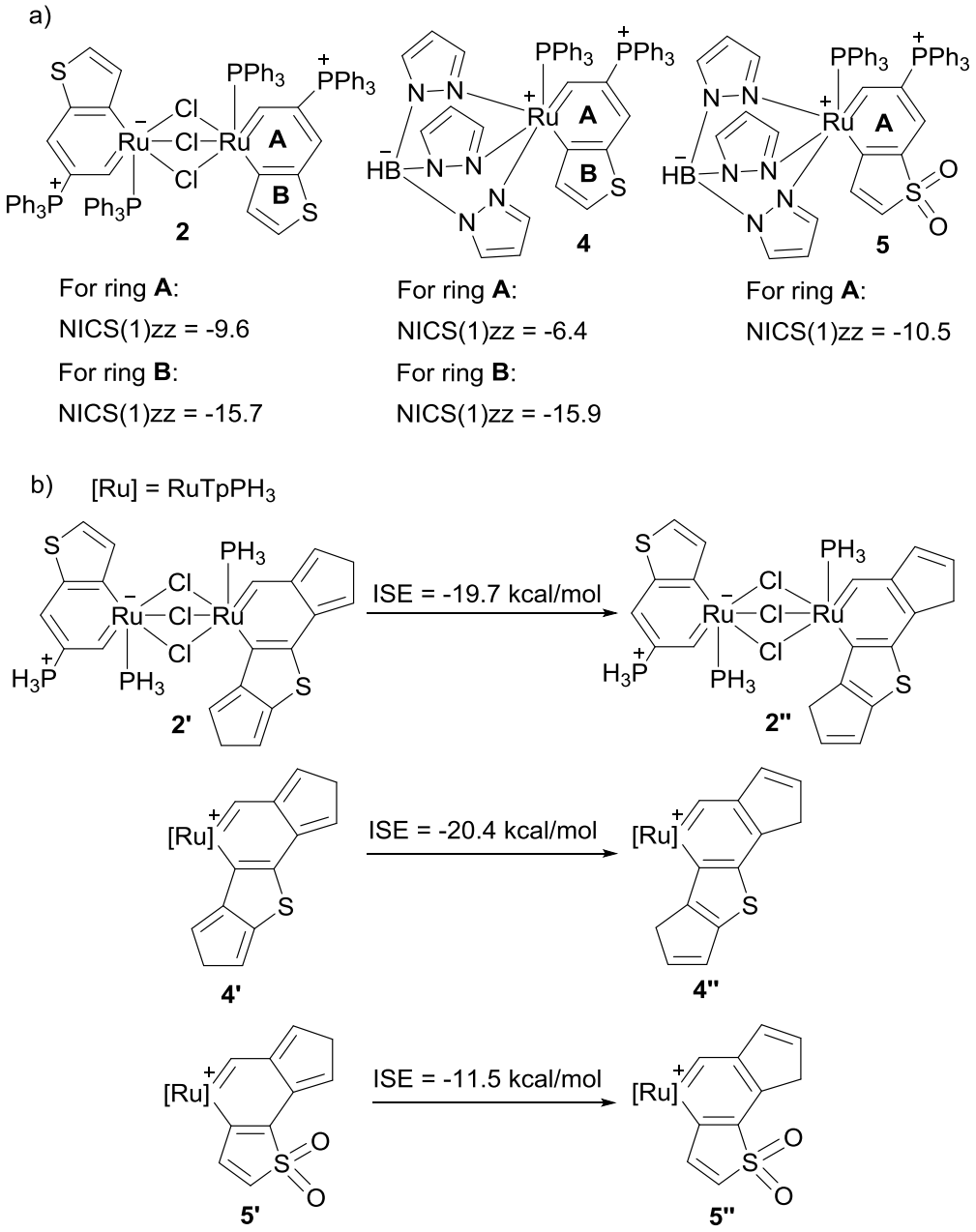
Figure S21 Cyclic voltammogram of 3 mM complex **4** measured in CH_2Cl_2 with 0.10 M Bu_4NPF_6 as supporting electrolyte at a scan rate of 0.10 V/s.

5. Theoretical calculations

Computational details

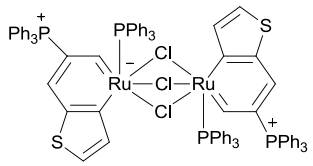
All structures were optimized at the B3LYP level of density functional theory. [1-3] In addition, the frequency calculations were performed to confirm the characteristics

of the calculated structures as minima. In the B3LYP calculations, the effective core potentials (ECPs) of Hay and Wadt with a double-ζ valence basis set (LanL2DZ) were used to describe the Ru, P, Cl and S atoms, whereas the standard 6-311++G(d,p) basis set was used for the C, H, O, N, and B atoms.[4] Polarization functions were added for Ru (ζ(f) = 1.235), P (ζ(d) = 0.34), Cl (ζ(d) = 0.514) and S (ζ(d) = 0.421)[5] in all the calculations. Nucleus-independent chemical shifts (NICS) values were calculated at the B3LYP/6-311++G(d,p) level. All the optimizations were performed with the Gaussian 09 software package.[6]



Scheme S1. Theoretical evaluations of the aromaticity of **2**, **4** and **5**. a) Computed NICS(1)$_{zz}$ values (in ppm) of **2**, **4** and **5**. b) The aromaticity in model complexes **2′**, **4′** and **5′** computed by the strain-balanced ISE methods.

Cartesian coordinates and electronic energies for all the species calculated in this study



2

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Cl	0.68907400	-3.84306800	1.59147000
C	1.47555000	0.28086400	-0.07743700
H	2.52574200	0.54233700	-0.25830600
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C	-0.82995000	1.21030800	-0.07743700
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C	0.78543000	-3.29452800	4.82329000
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H	0.73171000	-7.29718300	-1.03399400
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H	6.49313000	-1.19812900	-1.62208400
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C	-1.10441200	5.72606400	-2.14724000
H	-1.17124800	6.12536200	-3.15494000
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C	0.07584100	-5.17909600	7.85611700
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S	3.30921700	0.18644900	6.82479300
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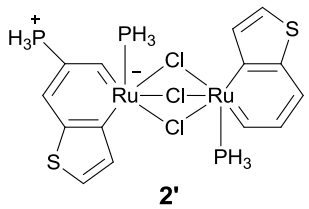

2'

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C	3.77749900	0.32434600	-1.18050100
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H	2.13118200	4.72461000	-0.39425300
P	2.29057400	-1.39552300	2.51559200
H	1.30888700	-2.08351900	3.27426200
H	3.24054800	-2.44465800	2.33234600
H	2.95848800	-0.69806400	3.56741000
H	-3.93414900	-2.08191700	-3.04383200
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H	-2.32068800	2.33479100	1.10824300
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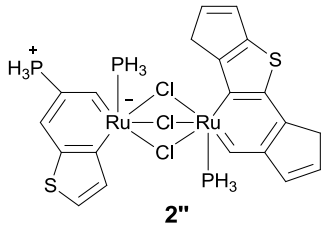

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C	3.66467900	-2.38273300	-0.61340600
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H	4.87032200	-3.70186300	-1.88480200
S	5.13066000	-1.34109300	-2.51522500
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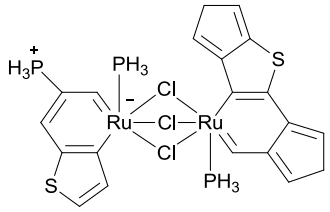
H	4.93232900	4.22998900	-1.48742900
H	2.77729200	4.28317300	-1.96877800
H	2.17873400	-1.01666200	3.73623700
H	3.89540500	0.26128700	3.35102200
H	3.94374500	-1.80280300	2.72563900
Cl	0.19100700	0.95604000	2.17899700
Cl	0.46220500	0.21464200	-1.26050300
Cl	0.73462700	-2.34470600	1.09672300
C	-2.70459400	0.64105600	-0.08875300
C	-3.98614200	0.21621900	-0.55490900
C	-4.30737500	-1.06904900	-0.97708100
C	-3.37842900	-2.14144100	-1.02083400
C	-2.05513900	-2.02698300	-0.60885100
Ru	-1.24277700	-0.62875000	0.44038400
H	-1.38622600	-2.84880500	-0.88810900

P	-2.54096700	-1.24926700	2.21611100
H	-2.82013800	-0.27880900	3.22330900
H	-2.09214600	-2.31281100	3.05550800
H	-3.86991100	-1.70508500	1.96826700
S	-5.13457800	1.58698900	-0.83845500
C	-2.67740600	2.06298400	-0.06216000
C	-3.86095100	2.69238400	-0.40738400
C	-5.60754300	-1.53139700	-1.59912000
C	-1.67419000	3.13555100	0.26711000
C	-4.04819500	-3.27506800	-1.67898500
C	-3.72905300	4.13188500	-0.32157800
C	-5.31237700	-2.95755200	-2.00327100
C	-2.45925200	4.40700900	0.06071000
H	-3.56582300	-4.22862500	-1.85664200
H	-6.03825400	-3.60252500	-2.48016000
H	-6.43810000	-1.46271900	-0.88388600
H	-5.88958000	-0.90486600	-2.45457300
H	-4.50954300	4.85083100	-0.53200300
H	-2.05026300	5.39868200	0.20853000
H	-1.28522600	3.04026000	1.28648900
H	-0.79656000	3.07573300	-0.38838800

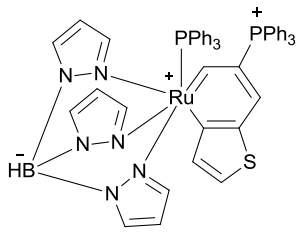


2'''

E = -1047.97843205 a.u.

Ru	2.08084600	-0.13604300	0.68681600
P	3.28387200	3.81377200	-1.09301800
P	3.18075500	-0.65804300	2.66925000
C	2.72918000	1.63842300	0.41808900
H	2.45545400	2.40822400	1.14937500
C	3.38812200	2.07705400	-0.74407900
C	4.02436400	1.23174000	-1.69193400
H	4.57107900	1.68213700	-2.51648100
C	4.05932200	-0.13710900	-1.55596400
C	3.41273700	-0.90903600	-0.53637700
C	3.80497900	-2.28201300	-0.64823800
H	3.41425800	-3.05371100	0.00058200
C	4.64455100	-2.55229200	-1.68958700
H	5.03138100	-3.51906400	-1.98186400
S	5.07683700	-1.15150200	-2.63652200

H	3.12318100	4.56139000	0.09532700
H	4.39253000	4.40317300	-1.76278100
H	2.18841200	4.22993600	-1.90156600
H	2.34353500	-1.08408900	3.73251900
H	3.94955900	0.33199900	3.35232800
H	4.14746600	-1.70780800	2.68097100
Cl	0.22693200	0.85198300	2.25565800
Cl	0.46434500	0.21537600	-1.20780100
Cl	0.82913700	-2.37176700	1.08329600
C	-2.72125300	0.59378200	-0.12507000
C	-3.90295300	0.20785600	-0.70245400
C	-4.27665600	-1.13012600	-1.08511000
C	-3.28893900	-2.23478600	-1.02729700
C	-1.94915500	-2.08489100	-0.53220100
Ru	-1.20640600	-0.68850100	0.45104600
H	-1.28044300	-2.92790300	-0.74679400
P	-2.56021600	-1.14517500	2.25630700
H	-2.83908900	-0.05571200	3.12739600
H	-2.15254900	-2.11426100	3.22197800
H	-3.88849000	-1.60348400	2.02080600
S	-5.08508700	1.55464200	-1.08093400
C	-2.69652800	2.04610100	0.03642400
C	-3.92606600	2.71919400	-0.43787600
C	-5.43424600	-1.61447000	-1.60515300
C	-1.85701000	3.00070500	0.50982000
C	-3.86397300	-3.36585500	-1.52218200
C	-3.85646200	4.05274900	-0.26255000
C	-5.27899600	-3.07739900	-1.92142700
C	-2.51588900	4.34945900	0.36759200
H	-3.38415900	-4.33213000	-1.61260600
H	-6.33669100	-1.05235600	-1.80219400
H	-5.99279700	-3.71407600	-1.37800800
H	-5.44303900	-3.29670200	-2.98710400
H	-4.59632700	4.79996100	-0.51135900
H	-0.88853500	2.83728500	0.95619100
H	-2.62515700	4.84449100	1.34380600
H	-1.91696300	5.03450800	-0.25135900



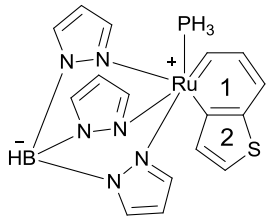
4

E = -2477.96757261 a.u.

Ru	1.05739700	-1.63784000	0.25862500
P	-3.21500500	0.05924000	-0.59422500
P	0.91264500	-1.38324500	2.59927000
N	0.55600800	-3.74722100	0.38158800
N	1.35270300	-4.65648500	-0.27664900
N	1.35255000	-2.08416200	-1.78087900
N	2.01950200	-3.21384000	-2.18348700
N	3.16163000	-2.24737300	0.43589300
N	3.55415900	-3.39726900	-0.21633600
C	-0.81195800	-1.22165900	-0.04767500
H	-1.35137400	-1.96962200	-0.16512700
C	-1.49657500	-0.00562600	-0.12430500
C	-0.81195800	1.23868300	-0.04767500
H	-1.31680000	2.01974600	-0.03414500
C	0.56141200	1.34962500	0.00870400
C	1.50168200	0.27681700	-0.04767500
C	2.78282200	0.83556100	-0.36438300
H	3.53430500	0.30906200	-0.52269700
C	2.81657200	2.19916600	-0.41326600
H	3.59463600	2.67903500	-0.58075200
S	1.31494900	2.93864800	-0.14190800
C	2.21275300	-0.38902900	3.43618400
C	-3.41380300	0.13297800	-2.38006000
C	-0.65047400	0.55027800	3.97411900
H	0.12609900	1.05675800	4.02811800
C	4.27844900	-1.75629800	0.99727100
H	4.30937700	-0.98211000	1.51169200
C	-4.32912900	-3.81178000	-0.16900800
H	-4.15185700	-4.61656000	-0.60009200
C	0.92956100	-1.49293200	-2.90451300
H	0.43562100	-0.70570800	-2.93342800
C	-2.96658500	0.26846400	4.52041800
H	-3.73770700	0.56692100	4.94441100
C	1.32942900	-2.21912800	-4.02010900
H	1.16665100	-2.01695700	-4.91272900
C	-4.63992800	2.46808600	-0.63944800

H	-4.77675800	2.32394800	-1.54739000
C	3.46382800	1.67100200	3.61253200
H	3.63162200	2.53437200	3.30794500
C	-1.81312100	-1.38215100	3.21242200
H	-1.83585800	-2.17339500	2.72184600
C	-3.74914900	1.77518400	1.47817000
H	-3.27239800	1.16148600	1.98862800
C	-0.46908400	-4.44615900	0.88130200
H	-1.16314800	-4.08038700	1.38222600
C	-2.96393800	-0.94277300	3.83696400
H	-3.73723200	-1.45729800	3.80167600
C	2.00676600	-3.28722500	-3.52406000
H	2.39758100	-3.96032000	-4.03230000
C	-1.81502200	1.02081100	4.56284700
H	-1.81796000	1.84852700	4.98802600
C	-3.94374500	1.53391600	0.12288000
C	-4.07076900	-1.42190000	-0.02542000
C	-2.38992800	0.61151600	-3.18086500
H	-1.58351500	0.86550500	-2.79457500
C	-0.63060600	-0.67498100	3.29978900
C	-4.25071900	2.90954700	2.08022500
H	-4.12562100	3.05511900	2.99020900
C	0.78918800	-5.88254500	-0.18171300
H	1.12961000	-6.66321500	-0.55650800
C	2.11375700	-3.84225400	3.15496400
H	2.62077400	-3.65573800	2.39817200
C	1.08132700	-2.97253300	3.51541100
C	2.50007900	0.89496900	2.99177600
H	2.03529000	1.24005100	2.26386000
C	4.87535500	-3.57570900	-0.04662900
H	5.37216400	-4.28157400	-0.38967800
C	-3.81770500	-2.62347600	-0.67212700
H	-3.30213100	-2.63269200	-1.44573000
C	-0.36174900	-5.79070100	0.55393800
H	-0.94401200	-6.47705100	0.78314500
C	-4.94875200	3.83210200	1.30911400
H	-5.29652800	4.59947400	1.70575800
C	4.17597600	1.16911600	4.67857500
H	4.83428300	1.68308800	5.08614200
C	2.93562300	-0.88369700	4.52827200
H	2.76599500	-1.74021200	4.84667000
C	3.90537100	-0.09833900	5.13286900
H	4.37791400	-0.43611400	5.85853600
C	0.60198700	-4.43978500	5.37037900

H	0.08694000	-4.64384500	6.11645300
C	2.39877300	-4.97230300	3.89278800
H	3.10221800	-5.52528800	3.64393600
C	-4.87956400	-1.40672400	1.08872700
H	-5.08305900	-0.60138400	1.50669400
C	-2.55621200	0.71520300	-4.55051200
H	-1.86188000	1.04165500	-5.07743800
C	0.33375700	-3.29955200	4.63835500
H	-0.36293500	-2.74240700	4.90093200
C	5.37666100	-2.54775600	0.71294100
H	6.25789700	-2.41332500	0.97536500
C	-5.39556800	-2.60094700	1.59269900
H	-5.93756100	-2.58857500	2.34833600
B	2.55056000	-4.17776400	-1.10321400
H	2.99562300	-4.94248200	-1.52468500
C	-5.12488300	3.61357900	-0.03566000
H	-5.57834300	4.24468800	-0.54814900
C	-4.62271500	-0.24732400	-2.97326900
H	-5.31809500	-0.56860200	-2.44663600
C	-3.73681500	0.34233400	-5.13304300
H	-3.84487600	0.41202200	-6.05465800
C	-4.77959100	-0.14097600	-4.34382900
H	-5.58135500	-0.39410400	-4.73880300
C	-5.10431800	-3.79515800	0.97722500
H	-5.42890400	-4.59240000	1.33114200
C	1.63706200	-5.27514300	4.99837100
H	1.81899600	-6.04164100	5.49421900

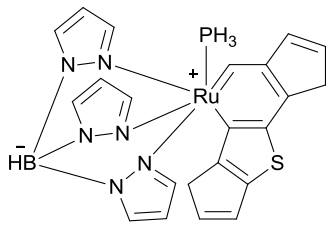


4'

E = -1084.74398568 a.u.

Ru	-0.15344600	0.51427000	-0.09290300
N	1.91295400	1.38005000	-0.08986400
N	2.95984700	0.54918100	0.13934400
N	0.53220700	-0.60050100	1.59358800
N	1.77959800	-1.13411600	1.59481100
N	0.83840800	-1.16086800	-1.28662200
N	2.05956300	-1.58211700	-0.87039700
C	-0.84592400	2.02777200	0.91740700

H	-0.11120500	2.65402600	1.44080600
C	-2.16517500	2.47558300	1.05614500
C	-3.26924700	1.69567700	0.70712400
H	-4.25894300	2.09085600	0.92364200
C	-3.18062900	0.38992200	0.20667100
C	-1.99436100	-0.33254900	-0.05246900
C	-2.31225500	-1.70961000	-0.29459200
H	-1.56111500	-2.46337500	-0.49075100
C	-3.64823800	-2.00931200	-0.27737400
H	-4.10948600	-2.97089800	-0.45547000
S	-4.65092200	-0.63204300	0.07113100
C	0.54094700	-1.87327500	-2.37776400
H	-0.39835300	-1.72018800	-2.88605600
C	-0.03626100	-0.91880900	2.75950000
H	-1.04120100	-0.59393400	2.97481700
C	0.85253900	-1.67179300	3.53949200
H	0.68807400	-2.07325400	4.52547900
C	2.42194400	2.60602900	-0.24156300
H	1.77073200	3.44629900	-0.42697600
C	1.99215500	-1.78472700	2.75969700
H	2.93229500	-2.27751400	2.94743300
C	4.11611200	1.24779000	0.13151600
H	5.05896600	0.75298100	0.30039500
C	2.52147200	-2.54968200	-1.69093100
H	3.47995000	-3.01049100	-1.51373000
C	3.81860800	2.57916000	-0.11198300
H	4.50684000	3.40506900	-0.18220100
C	1.57560600	-2.77053200	-2.68004900
H	1.62599400	-3.47546400	-3.49325900
B	2.72731600	-0.96198100	0.38216500
H	3.77130900	-1.50653400	0.59941400
P	-0.81842300	1.61424900	-2.03833200
H	-0.04841700	2.70262000	-2.55659200
H	-0.93558100	0.87988000	-3.25850400
H	-2.09697900	2.24455100	-2.05376300
H	-2.36854200	3.42510100	1.54810900

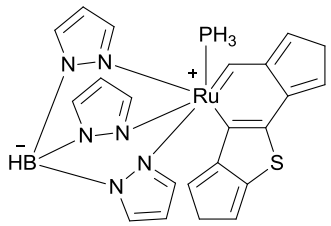


4"

E = -1315.82067855 a.u.

Ru	0.27553600	-0.50812300	-0.23878600
P	-0.32931300	-1.24835800	-2.36194800
N	2.22660200	-1.61041600	-0.23253200
N	3.33229200	-0.96063100	0.20892100
N	0.93563700	0.24475600	1.64751400
N	2.22364600	0.64303200	1.80312200
N	1.56565700	1.15047200	-1.12940100
N	2.77511800	1.37192900	-0.55617800
C	-0.64588200	-2.09730400	0.45491000
H	-0.03343300	-2.88061500	0.92086900
C	-1.99887200	-2.39995600	0.37162000
C	-3.00267100	-1.44263700	0.03738500
C	-2.75314300	-0.09475600	-0.18470700
C	-1.46671100	0.53353200	-0.14057900
C	-1.65930800	1.93712300	-0.01210900
C	-2.97460300	2.37458800	-0.05080300
S	-4.13062700	1.08608600	-0.21345300
C	1.48628200	1.97245300	-2.18059400
H	0.59909800	1.98348400	-2.79473300
C	0.31555100	0.44642400	2.81321700
H	-0.72757600	0.19551900	2.91843100
C	1.20986700	0.98696900	3.74857500
H	1.01152000	1.25609100	4.77266400
C	2.60521200	-2.85848400	-0.52122600
H	1.88513400	-3.57472400	-0.88546600
C	2.40964500	1.09350200	3.06367600
H	3.37584600	1.45210700	3.37965100
C	4.39588900	-1.79377700	0.19648200
H	5.36648000	-1.45218100	0.51835500
C	3.44556200	2.32542100	-1.23843600
H	4.43108200	2.63410700	-0.92877000
C	3.97485600	-3.02914600	-0.26860400
H	4.56754200	-3.91883200	-0.40228400
C	2.65214900	2.74382900	-2.29552000
H	2.88211300	3.49308900	-3.03482000
B	3.24853200	0.52052200	0.64908500
H	4.32288200	0.90002200	1.01775500
H	0.36026000	-2.35715400	-2.94663000
H	-1.66173000	-1.70727400	-2.57832700
H	-0.23214900	-0.37232100	-3.48820800
C	-2.69311900	-3.65288600	0.71550100
C	-4.35812700	-2.11048800	0.14301800
C	-0.79139000	3.15355700	0.19617500

C	-3.05385100	3.81289800	0.09277500
C	-4.02192200	-3.51692900	0.58117500
C	-1.79276800	4.28023000	0.24884600
H	-2.17466900	-4.55280700	1.02432500
H	-4.76959900	-4.27996200	0.75166500
H	-4.88805300	-2.08805800	-0.81864700
H	-5.00830400	-1.59383000	0.85981400
H	-3.96286700	4.39889200	0.08961200
H	-1.51891100	5.31717600	0.39479600
H	-0.20991300	3.08768700	1.12447500
H	-0.05980700	3.30340900	-0.60370200

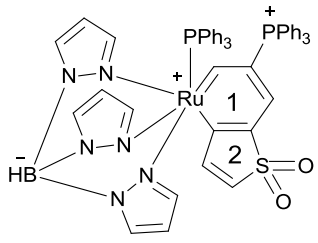


4'''

E = -1315.78742409 a.u.

Ru	0.28978700	-0.53110400	-0.20061800
P	-0.40286900	-1.11273900	-2.36259300
N	2.25871600	-1.59093000	-0.23398300
N	3.35949900	-0.94101200	0.21399700
N	0.94713000	0.29855600	1.64802400
N	2.24351300	0.67277300	1.80077200
N	1.56240900	1.17177400	-1.11711800
N	2.78488800	1.38032400	-0.56253000
C	-0.52736100	-2.09219700	0.47383100
H	0.10854800	-2.85731400	0.94153000
C	-1.91222000	-2.47370600	0.40558600
C	-3.01676700	-1.53052500	0.08990200
C	-2.76410300	-0.11584300	-0.04713100
C	-1.53528600	0.49188100	-0.08421600
C	-1.70397000	1.94273900	-0.04454200
C	-3.11669000	2.38441800	-0.02738900
S	-4.21651400	1.00314400	-0.04483200
C	1.46544400	2.01376100	-2.15058600
H	0.56012800	2.05508300	-2.73506600
C	0.31697600	0.56866900	2.79443000
H	-0.73569100	0.35873900	2.89273300
C	1.21332700	1.12373000	3.71610200
H	1.00893600	1.44440700	4.72388800
C	2.64871100	-2.82657700	-0.56084700

H	1.93520700	-3.53951600	-0.94430500
C	2.42323900	1.17432700	3.04109000
H	3.39186200	1.53160800	3.35112800
C	4.43339500	-1.75977900	0.16830600
H	5.40349100	-1.41329400	0.48621600
C	3.44405400	2.34294700	-1.24189800
H	4.43405800	2.64769500	-0.94274100
C	4.02251200	-2.98762300	-0.32449700
H	4.62455300	-3.86587200	-0.48830100
C	2.63223700	2.78015600	-2.27711300
H	2.84856100	3.54333000	-3.00609000
B	3.26745800	0.54083200	0.64628500
H	4.34022300	0.92840700	1.01023900
H	0.38522800	-1.98897200	-3.17396000
H	-1.66514200	-1.74773800	-2.53573500
H	-0.56314100	-0.06528200	-3.31566800
C	-2.44007300	-3.71500600	0.60380600
C	-4.18562100	-2.22277000	0.09235700
C	-0.92454000	3.05165200	0.03082200
C	-3.21245600	3.72602200	0.03764800
C	-3.92398000	-3.66964900	0.40935000
C	-1.80538800	4.27270800	0.08509800
H	-1.88054700	-4.60717300	0.85598900
H	-5.17432300	-1.81528000	-0.06744200
H	-4.45191000	-4.00194400	1.31579100
H	-4.25282700	-4.35388800	-0.38674100
H	-4.10597800	4.33242700	0.07283400
H	0.15290400	3.08969100	0.06251400
H	-1.59914600	4.95790400	-0.75003700
H	-1.62739600	4.85574000	1.00042400



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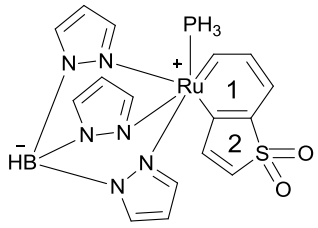
S	0.45583500	3.14230900	0.31692800
P	2.79356700	-1.64942400	0.36088300
N	-2.00001500	-0.88334700	2.07955800

C	-1.89236400	2.21133000	0.56657500
H	-2.80762600	2.15466300	0.72447000
O	1.29822000	3.32313000	1.47044400
C	1.27214900	-0.79033300	-0.02601000
C	-1.11205800	1.01693200	0.12690600
O	0.75857900	3.90858100	-0.86144800
C	-2.49738300	0.84387900	-3.06426400
C	-1.23977800	3.35757800	0.72267000
H	-1.62228500	4.15676700	1.00539900
C	-3.52757800	3.29712300	-3.89032700
H	-3.88173800	4.11622300	-4.14777900
C	1.87674100	-4.21925700	0.86686300
H	1.52739800	-3.88204900	1.65981300
C	-2.88373800	-2.01890800	-3.16247200
C	2.88333600	-5.23542100	-1.49321100
H	3.22278900	-5.57855300	-2.28852800
C	-3.65066800	0.90358200	-3.83044700
H	-4.07907400	0.11654500	-4.08089700
C	2.63508500	-3.40169200	0.04086000
C	1.38324100	-0.27692500	-4.92899800
H	1.72122400	0.37700100	-5.49524700
C	1.35049500	0.59660400	-0.09593800
H	2.19094400	0.98633600	-0.19608600
C	0.03928800	-1.45515300	0.04706100
H	0.10662500	-2.37668400	0.15001900
C	-0.23905000	-0.94929100	-3.28283100
C	2.77222000	-0.20024500	2.70943100
H	2.30515000	0.43598200	2.21893700
C	3.08112800	0.05085800	4.04906500
H	2.82171700	0.85011500	4.44847800
C	3.14735900	-1.37396800	2.10897000
C	0.45159500	-2.15461600	-3.12833900
H	0.16806200	-2.76964900	-2.49093200
C	-1.85215100	2.03643700	-2.75630000
H	-1.06575500	2.01530500	-2.26103800
C	-4.52810300	-3.95365500	-4.32663500
H	-5.07098600	-4.61510500	-4.69231500
C	1.63529600	-5.54088300	0.51215600
H	1.14940700	-6.09658100	1.07697900
C	-4.17339800	2.12421200	-4.22735200
H	-4.96070200	2.15327500	-4.72210600
C	0.22585300	-0.02417200	-4.18542800
H	-0.23294500	0.77565500	-4.30399000
C	0.24551800	1.42228300	-0.02601000

C	3.89846000	-0.66398500	-1.95851900
H	3.03012000	-0.66897200	-2.29497500
C	-2.35713900	3.24376000	-3.16724500
H	-1.90628200	4.03125200	-2.95930300
C	4.13386200	-0.99603100	-0.63239400
C	-3.27378900	-3.76533800	-4.79651600
H	-2.95884400	-4.29095500	-5.49504500
C	-2.46083600	-2.79318000	-4.24184900
H	-1.61346800	-2.65394200	-4.59618300
C	3.77072400	-0.88780300	4.77146800
H	3.99700000	-0.71910000	5.65647700
C	3.15785700	-3.93242100	-1.14286600
H	3.68932600	-3.40494700	-1.69255000
C	2.02262600	-1.49800200	-4.82337500
H	2.76256200	-1.68897700	-5.35392100
C	1.54946700	-2.43576900	-3.91442700
H	1.97388000	-3.25822000	-3.83479800
C	-4.19393100	-2.23365400	-2.68381400
H	-4.50636400	-1.74868000	-1.95408500
C	4.95766300	-0.32508300	-2.77251300
H	4.81709500	-0.11834900	-3.66869300
C	6.25635400	-0.29696600	-2.23073500
H	6.97945900	-0.07541000	-2.77599500
C	-5.00159700	-3.15485900	-3.29071500
H	-5.88337000	-3.24822400	-3.00549900
C	3.83720800	-2.31810800	2.84177500
H	4.10940200	-3.11422200	2.44135800
C	5.43278000	-0.94886400	-0.11048800
H	5.58444100	-1.16053600	0.78184100
C	4.12347100	-2.07459400	4.18538600
H	4.55858600	-2.72507100	4.68846200
C	2.12368000	-6.02264000	-0.68824000
H	1.93304200	-6.89550800	-0.94647000
C	6.47115100	-0.59031800	-0.91415700
H	7.33486700	-0.54605000	-0.56622200
N	-4.76415900	-0.96780000	0.85971300
N	-3.54374800	-3.17097200	0.88245400
N	-3.11650000	-1.44962800	2.64551100
N	-2.49876300	-2.85563300	0.05662100
N	-3.93367000	-0.20980000	0.05657200
C	-3.03882200	-1.32542900	3.98298500
H	-3.67731900	-1.62875300	4.58933000
C	-4.71617700	0.73507800	-0.49927200
H	-4.41894600	1.38611200	-1.09324000

C	-2.09354600	-4.01233000	-0.45044300
H	-1.38304800	-4.10708200	-1.04312600
C	-1.87333000	-0.68424000	4.31092200
H	-1.56384900	-0.46648200	5.15991900
C	-6.01940400	-0.47315500	0.79197000
H	-6.75896700	-0.80442000	1.24917900
C	-3.76286800	-4.49493200	0.85748100
H	-4.42138200	-4.94324900	1.33614200
C	-2.86957700	-5.06719000	0.02250500
H	-2.79273300	-5.96915200	-0.18966200
C	-6.02457800	0.60450400	-0.06708800
H	-6.75232300	1.13163300	-0.30632900
C	-1.25106800	-0.42926000	3.08900400
H	-0.43184100	-0.00159500	2.99168800
B	-4.19697900	-2.07706600	1.74973800
H	-4.90959300	-2.46480700	2.30071200



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Ru	0.18890800	0.53413800	-0.05797500
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N	0.86856000	-0.65089500	1.58134900
C	-1.98961800	-1.62440200	-0.24146000
H	-1.21184400	-2.36448900	-0.38161700
O	-5.08997200	-0.56395000	1.24803200
C	-1.71645900	2.54958900	1.18657900
C	-1.63951500	-0.19817500	-0.01775600
O	-5.01122200	-0.08021600	-1.28079600
C	-3.29134100	-1.92581000	-0.28496100
H	-3.78602500	-2.86965700	-0.46394500
C	-2.85416300	1.83110000	0.78405000
H	-3.83488900	2.23855300	1.01531300
C	-0.42608700	2.05461700	1.02489200
H	0.34331800	2.61916700	1.56483000
C	-2.78956900	0.56423900	0.21933500
N	2.29221200	-1.61963800	-0.95743600
N	3.31088800	0.42868000	0.10722500
N	2.08613100	-1.24741500	1.52990100

N	2.29790300	1.31498000	-0.06263800
N	1.08739900	-1.12153900	-1.33505600
C	2.30244100	-1.92950700	2.67569000
H	3.22210000	-2.47189700	2.82375900
C	0.74261700	-1.76503800	-2.45612800
H	-0.19280900	-1.54346600	-2.94666300
C	2.85862900	2.52438200	-0.16391900
H	2.24363600	3.40138300	-0.29457200
C	1.19636900	-1.77452200	3.49551600
H	1.04324600	-2.18679100	4.47873400
C	2.69630400	-2.56647300	-1.83054300
H	3.63449600	-3.07915300	-1.69137500
C	4.49526700	1.07626100	0.11222800
H	5.41826100	0.53423100	0.24126300
C	4.25323200	2.43019200	-0.06179600
H	4.97611400	3.22775200	-0.10447700
C	1.72843100	-2.69449300	-2.81482200
H	1.73443400	-3.36102700	-3.66111300
C	0.32306600	-0.96120900	2.76146600
H	-0.65501100	-0.58838100	3.01988000
B	3.01429900	-1.07886200	0.30101500
H	4.03521700	-1.67798200	0.47530500
P	-0.41302900	1.79851900	-1.94383400
H	0.35809800	2.95103300	-2.28038400
H	-0.42044400	1.18581300	-3.23279000
H	-1.70991800	2.38461700	-1.97134700
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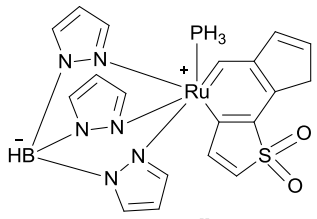

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C	-1.31994900	-2.19976700	0.22419500
H	-0.40424300	-2.76512700	0.34356400
O	-4.66401800	-1.40786600	1.25984600
C	-1.93914600	2.17700000	0.20683200
C	-1.27142200	-0.73562100	-0.02022000
O	-4.50344800	-1.73211000	-1.28959100

C	-2.52872800	-2.77089500	0.26041900
H	-2.81396900	-3.80468700	0.39107900
C	-2.90281300	1.14196300	0.03433700
C	-0.56951300	1.94214000	0.25512200
H	0.02656300	2.79654500	0.59960300
C	-2.56411700	-0.19973700	-0.06568900
N	2.91834200	-1.56358600	-0.35630500
N	3.45873800	0.87353900	0.01148400
N	2.43643600	-0.48073200	1.87072800
N	2.32278500	1.44067600	-0.46596500
N	1.67986700	-1.45903000	-0.90164100
C	2.66965400	-0.72284900	3.17924000
H	3.65525300	-0.99963100	3.51674900
C	1.55256600	-2.47868000	-1.75811300
H	0.63698000	-2.61292500	-2.31334600
C	2.66513400	2.63959600	-0.94793000
H	1.91719100	3.28817900	-1.37739600
C	1.48542200	-0.54803200	3.87667200
H	1.32235400	-0.66188300	4.93526800
C	3.55884000	-2.63815800	-0.86365900
H	4.55884100	-2.88392700	-0.54437300
C	4.50370400	1.70903100	-0.16911200
H	5.49362000	1.43006700	0.15426500
C	4.04001700	2.86034300	-0.78644500
H	4.60986800	3.72861900	-1.07260900
C	2.71656300	-3.25946100	-1.77274700
H	2.91374500	-4.14417600	-2.35495500
C	0.54847200	-0.18878600	2.89853100
H	-0.49965900	0.04328500	2.99877100
B	3.42124600	-0.52403400	0.67623400
H	4.51459300	-0.82519100	1.05825900
P	-0.25030600	0.75087100	-2.46374500
H	0.35170900	1.84128900	-3.16148600
H	-0.06257800	-0.24615300	-3.46807000
H	-1.61710200	1.05929800	-2.71763300
C	-2.68683500	3.42293100	0.44905600
C	-4.28510900	1.73554100	0.14861000
C	-4.00993000	3.19578500	0.40668000
H	-4.85551500	1.25542000	0.95356000
H	-4.86767500	1.56544400	-0.76643800
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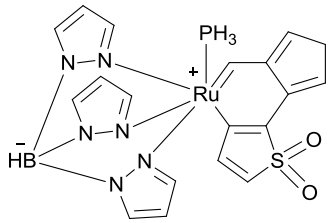
H	-2.20963900	4.37883000	0.62707400



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C	-1.35774200	-2.22592700	-0.09268200
H	-0.43586600	-2.79302500	-0.11670900
O	-4.54422700	-1.56808400	1.35072600
C	-1.90821800	2.19534000	0.31317300
C	-1.33065300	-0.73258100	-0.12242400
O	-4.67375200	-1.57483500	-1.22049200
C	-2.55507300	-2.81192000	-0.02778300
H	-2.83591000	-3.85374500	0.00443600
C	-2.95899600	1.16772400	0.08919900
C	-0.49761000	1.92033900	0.32017600
H	0.09885500	2.76542500	0.69198100
C	-2.58315300	-0.21364400	-0.04136900
N	2.94472600	-1.51086000	-0.42405700
N	3.45221900	0.88403000	0.18405000
N	2.35271700	-0.64305900	1.86469700
N	2.34003100	1.48370300	-0.30639900
N	1.72262800	-1.37954200	-1.00118900
C	2.51849700	-1.04753200	3.14170600
H	3.49118800	-1.34420300	3.49920900
C	1.64173400	-2.32895400	-1.94017100
H	0.74747600	-2.43408200	-2.53473500
C	2.70452100	2.70870700	-0.69707800
H	1.97886000	3.38371900	-1.12393600
C	1.29039600	-0.99673000	3.78285300
H	1.07131800	-1.25211100	4.80601900
C	3.61937500	-2.53157000	-0.99396000
H	4.61094000	-2.79044500	-0.65913300
C	4.50651700	1.72510100	0.10184100
H	5.48140900	1.42074300	0.44695600
C	4.07182900	2.91422300	-0.46025800
H	4.65481100	3.79615800	-0.66717500
C	2.81887200	-3.08838300	-1.97925800
H	3.04961300	-3.92052600	-2.62327900

C	0.39799600	-0.54350600	2.80369800
H	-0.66339800	-0.36419500	2.86633100
B	3.39305700	-0.56541200	0.71975700
H	4.46986200	-0.89591600	1.12373500
P	-0.23617700	0.83439700	-2.46678400
H	0.39096600	1.88298700	-3.20840500
H	-0.09922900	-0.19727000	-3.44121300
H	-1.59545300	1.17989000	-2.70944100
C	-2.51820400	3.40027200	0.50875200
C	-4.17470700	1.76626400	0.14121700
C	-4.00236800	3.23657100	0.40593900
H	-5.13549800	1.28136700	0.04408600
H	-2.01580400	4.33947800	0.70394100
H	-4.50070400	3.55458700	1.33378400
H	-4.42937100	3.87027400	-0.38509000

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