Supplementary Information

A missing member of conjugated N-heterocycles: Realizing pyrido[1,2-α]azepine by reacting ruthenium alkenylcarbene complex with alkyne

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Contents

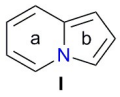
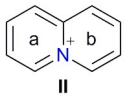
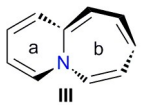
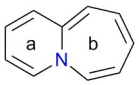
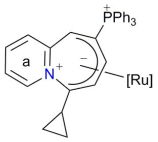
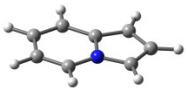
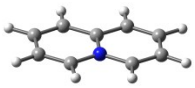
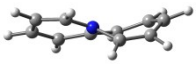
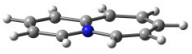
1. Density Functional Theory (DFT) Calculations

All structures were optimized at the B3LYP level of DFT.[1-3] Additionally, Frequency calculations were also performed to identify all the stationary points as minima (zero imaginary frequency) or transition states (one imaginary frequency), and to provide Gibbs free energies at 298.15 K. In the B3LYP calculations, the effective core potentials (ECPs) of Hay and Wadt with a double-ζ valence basis set (LanL2DZ)[4] were used to describe the Ru, Cl, and P atoms, whereas the standard 6-31G(d) basis set was used for the C, N, and H atoms. Polarization functions were added for Ru (ζ(f) = 1.235), Cl (ζ(d) = 0.514) and P (ζ(d) = 0.340)[5] in all calculations. All the optimizations were performed with the Gaussian 09 software package.[6] Nucleus-independent chemical shifts (NICS)[7-10] values in N-fused pyridines were calculated at the B3LYP/6-31G(d) level. The anisotropy of the induced current density (ACID) calculations were carried out with the ACID program.[11] The energies (in kcal/mol) are given including the zero-point energy corrections.

The aromaticity of the archetypal N-fused pyridines, indolizine (**I**), quinolizinium salt (**II**), and pyrido[1,2-α]azepine (**III**) were investigated by the density functional theory (DFT) calculations. It is generally believed that negative values of nucleus-independent chemical shift (NICS) calculations[7-10] indicate aromaticity while positive values suggest antiaromaticity. As shown in Table S1, the negative NICS values of indolizine (**I**) and quinolizinium salt (**II**) indicate their aromaticity. The aromaticity of **I** and **II** were further confirmed by the anisotropy of the current-induced density (ACID) calculations.[11] The ACID method is a versatile, intuitive, and generally applicable approach to investigating and visualizing electron delocalization. The clockwise current density vectors of **I** and **II** plotted on the AICD isosurfaces show diatropic ring current along the periphery of the bicycles (Figure S1a and b), further confirming the aromaticity of **I** and **II**.

The DFT geometry optimizations of pyrido[1,2-α]azepine led to a nonplanar, twisted structure **III** (Table S1, entry 3). Only when we conducted the C_s-constrained optimization, the planar counterpart pyrido[1,2-α]azepine **III-constr** can be obtained with one imaginary frequency in its Hessian matrix (Table S1, entry 4). The antiaromaticity of **III-constr** is evidenced by the large positive NICS values (Table S1, entry 4) and the counterclockwise current density vectors plotted on the ACID isosurface along the periphery of fused-ring framework (Figure S1d). Note especially that the NICS values of the nonplanar, distorted system **III** (Table S1, entry 3) are positive, however, much lower than those of planar structure **III-constr**. Furthermore, the distorted structure **III** is 3.1 kcal/mol lower in energy compared to the planar counterpart **III-constr**. The nonplanarity of the distorted form **III** might be an attempt to escape from antiaromaticity and lability of planar pyrido[1,2-α]azepine framework. Indeed, the coordination with the ruthenium twists the bicyclic pyrido[1,2-α]azepine unit in complex **2**, which results in the significant π-delocalization of pyridine ring as reflected in the crystallographic data and the calculated NICS values (Table S1, entry 5). We inferred it may be important for the stabilization of the bicyclic pyrido[1,2-α]azepine unit in **2**.

Table S1. The computed NICS(0), NICS(1), and NICS(1)$_{zz}$ values (ppm) of indolizine (**I**), quinolizinium salt (**II**), pyrido[1,2-α]azepine (**III**), the planar isomer of pyrido[1,2-α]azepine (**III-constr**), and the cation moiety of **2**. When the environments at points 1 angstrom above and below the ring centers are not equivalent, the averaged values are used for NICS(1) and NICS(1)$_{zz}$.

entry	1		2	3		4		5
compound structures	 **I**		 **II**	 **III**		 **III-constr**[a]		 [Ru] = $RuCl_2PPh_3$ **2**$^+$
Optimized structures								See, Figure S2
	Ring a	**Ring b**	**Ring a/b**	**Ring a**	**Ring b**	**Ring a**	**Ring b**	**Ring a**
NICS(0)	−6.9	−18.1	−8.6	8.8	16.3	19.9	50.9	−6.6
NICS(1)	−7.7	−14.9	−10.3	5.2	11.7	15.1	40.0	−8.5
NICS(1)$_{zz}$	−18.2	−39.3	−25.5	22.0	40.9	50.8	124.4	−18.7
[a] **III-constr** is a C_s-constrained optimization of **III**. **III-constr** has one imaginary frequency in its Hessian matrix.								

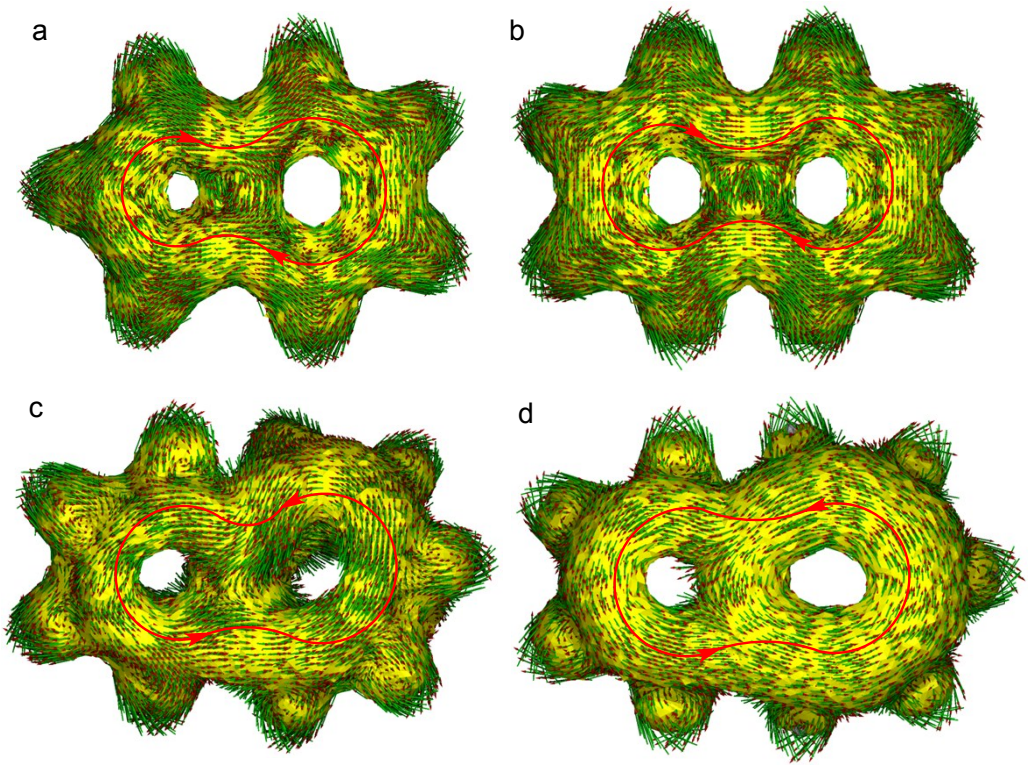


Figure S1. a) ACID isosurfaces of the indolizines (**I**); b) ACID isosurfaces of the quinolizinium salts (**II**); c) ACID isosurfaces of the pyrido[1,2-α]azepines (**III**); d) ACID isosurfaces of the planar pyrido[1,2-α]azepine (**III-constr**). Current density vectors are plotted onto the ACID isosurface of 0.025. The diatropic (clockwise) ring current indicating the aromaticity. The paratropic (counterclockwise) ring current indicating the antiaromaticity. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

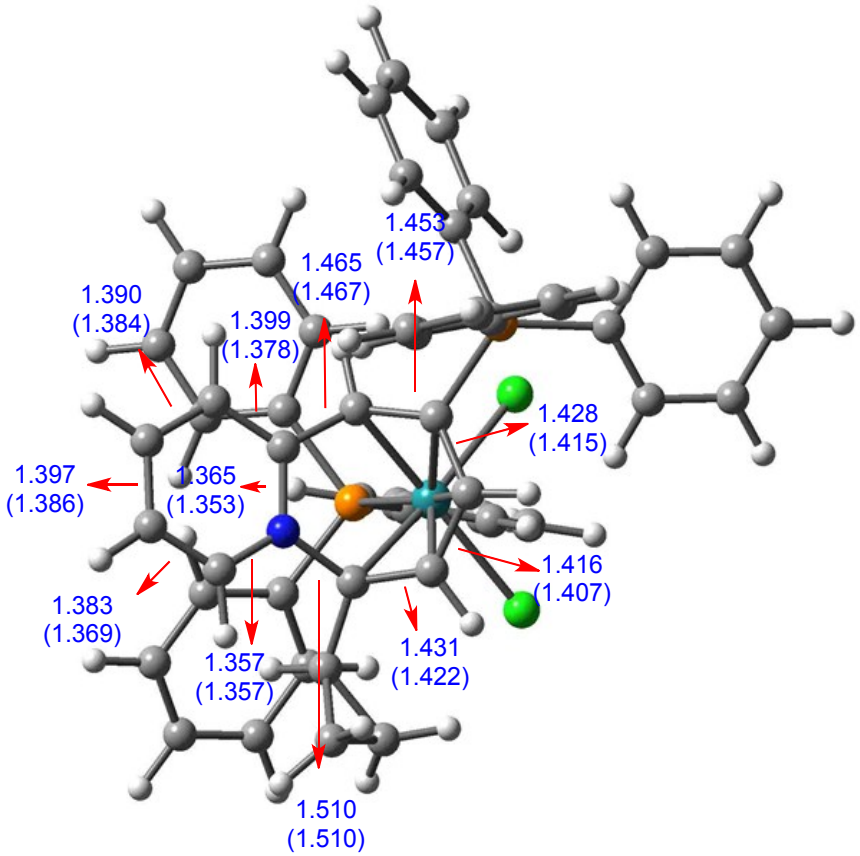
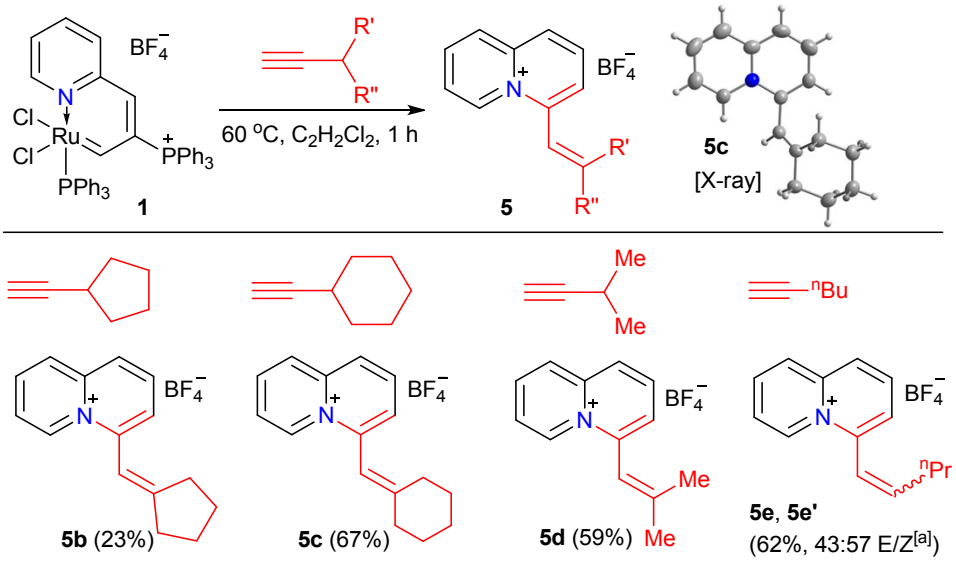


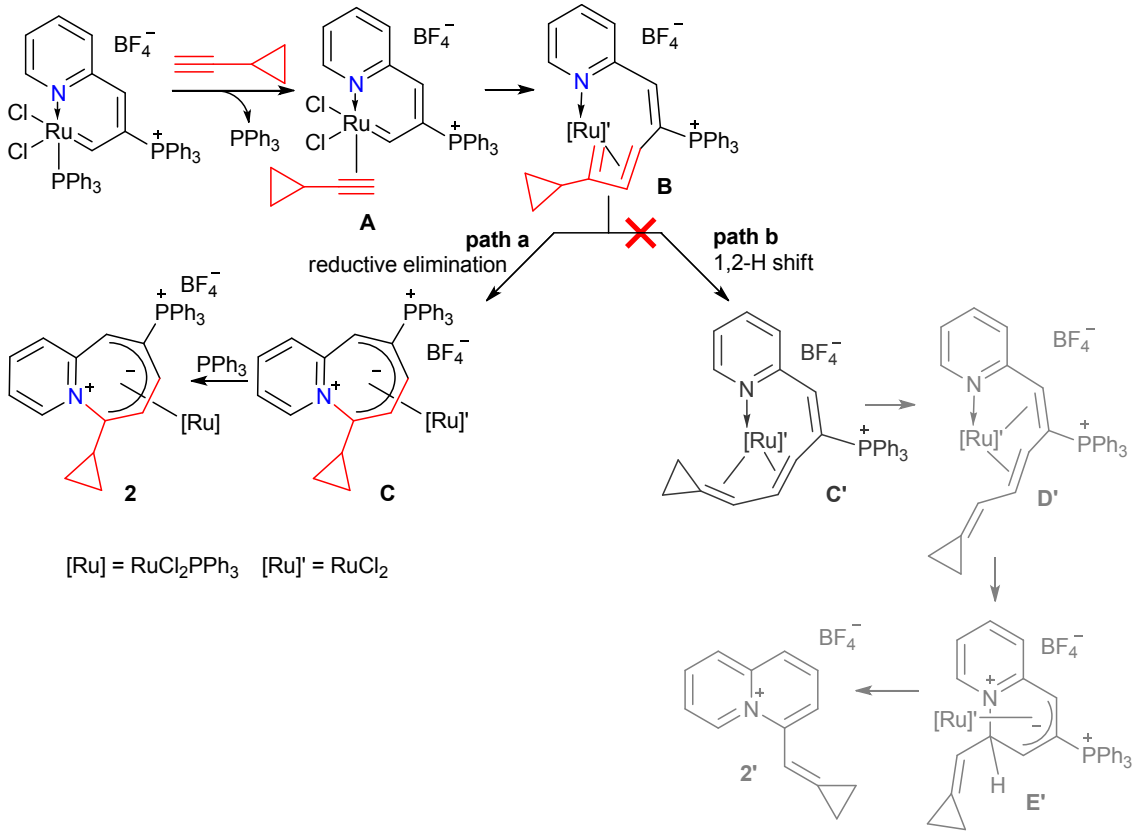
Figure S2. Comparison of the calculated and experimental (in parentheses) bond lengths (Å) for complex **2**. These calculated data for the real system and those for the model are consistent with the experimental values, indicating the reliability of the calculations performed using the model system.

2. The Synthesis of Quinolizinium Salts 5b-5e

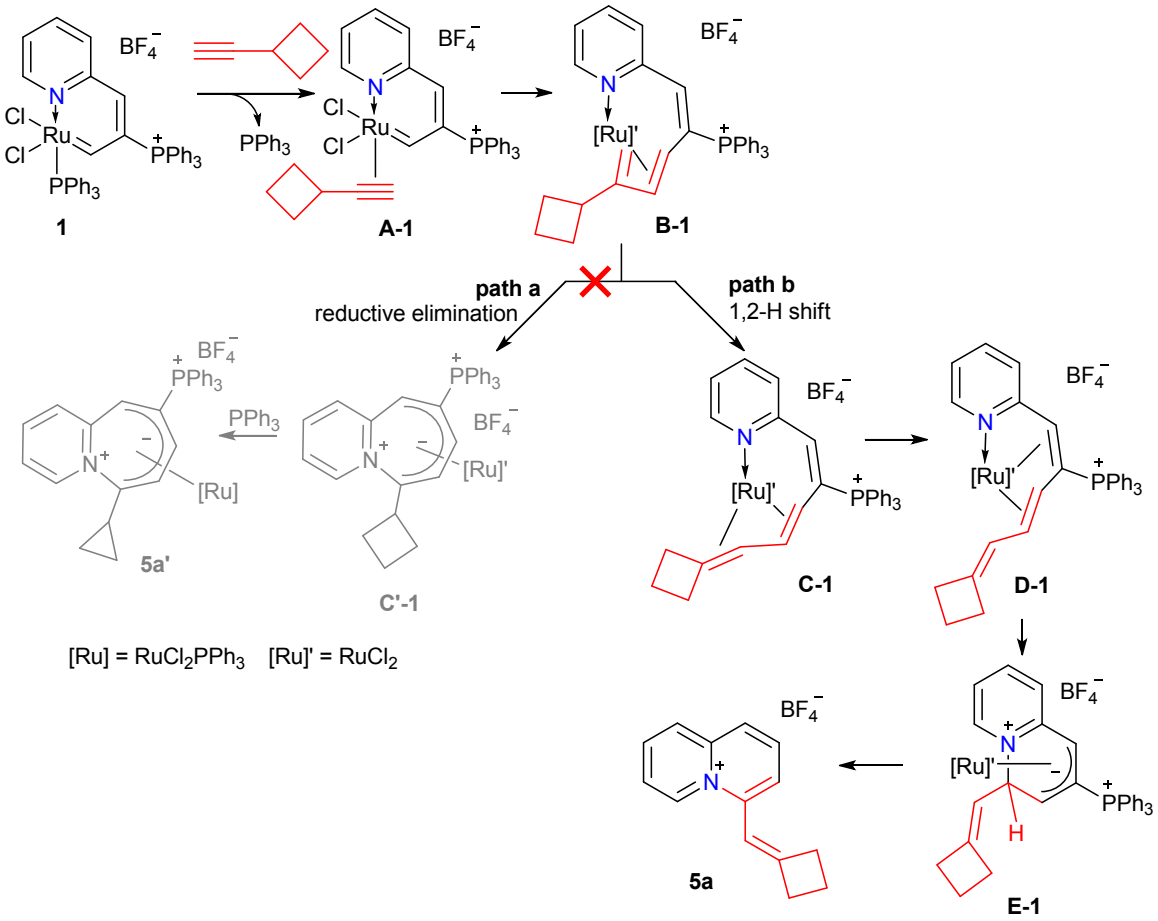


Scheme S1. Synthesis of 4-alkenyl-substituted quinolizinium salts **5b-5e**. [a] E/Z ratio was determined by ^{1}H nuclear magnetic resonance (NMR).

3. Proposed Mechanisms for the Formation of the Pyrido[1,2-α]azepine-Ruthenium Complexes or Quinolizinium Salts



Scheme S2. Plausible mechanisms for the formation of the pyrido[1,2-α]azepine-ruthenium complex **2** or the hypothetical quinolizinium salt **2′**.



Scheme S3. Plausible mechanisms for the formation of the hypothetical pyrido[1,2-α]azepine-ruthenium complex **5a′** or the quinolizinium salt **5a**.

4. Energy Profiles of the Key Intermediates with a Cyclobutyl Substituent in the Elimination or 1,2-H Shift Reaction Pathway

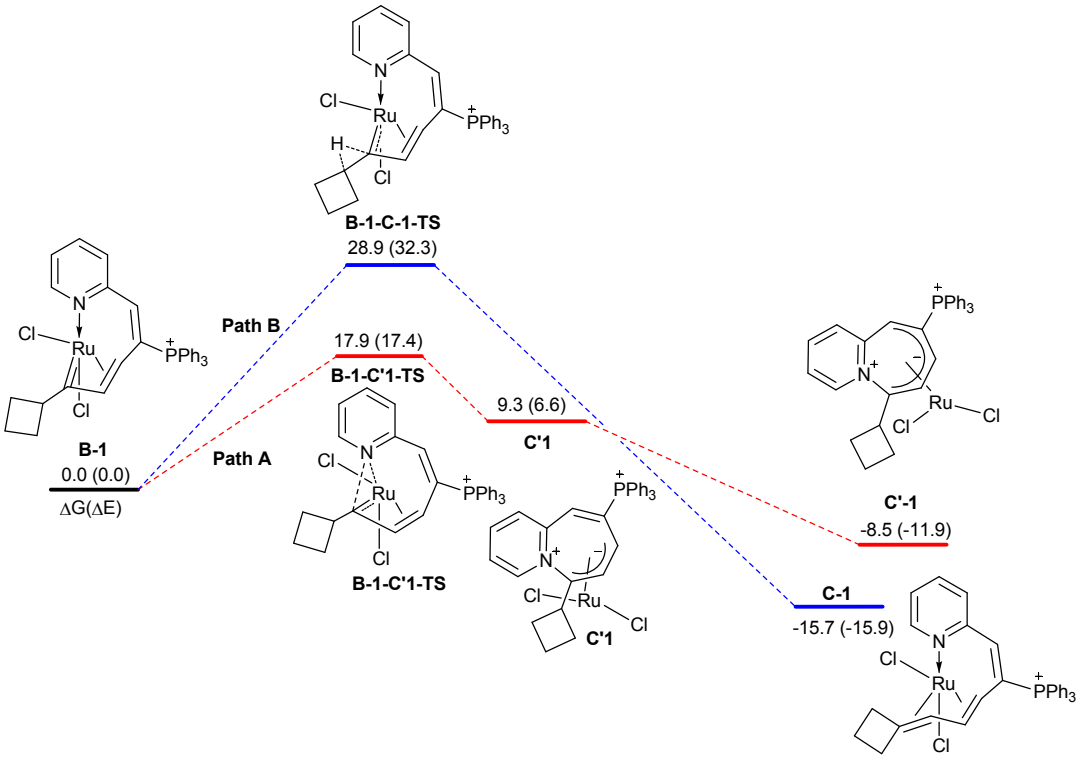
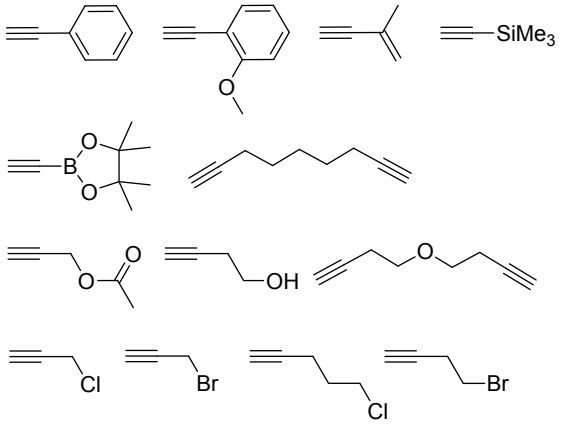
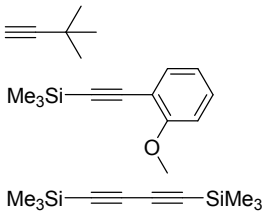


Figure S4. Energy profiles of the key intermediates with a cyclobutyl substituent in the elimination or 1,2-H shift reaction pathway (labelled in red and blue, respectively). The relative Gibbs free energies and electronic energies (in parentheses) are given in kcal/mol.

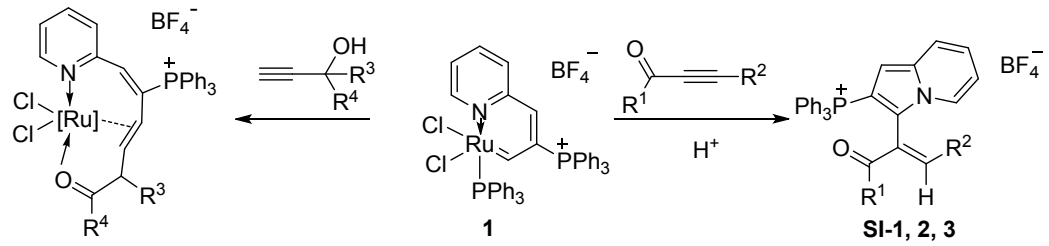
5. The Reaction Outcomes of Complex 1 with Other Alkynes

Table S2. The reaction outcomes of complex **1** with other alkynes.

A summary of alkynes failed to afford the desired product under the same conditions.

Lead to a mixture of unidentified species	Do not react with complex **1**
	

A summary of alkynes which undergo different reactions by treating with 1.[12, 13]



SI-4, 5, 6, 7, 8 | **1** | **SI-1, 2, 3**

[Ru] = $RuPPh_3$
SI-4: $R^3 = R^4 = Ph$
SI-5: $R^3 = Ph$, $R^4 = CH_3$

SI-6: $R^3 = H$, $R^4 = Ph$
SI-7: $R^3 = H$, $R^4 = CH_3$
SI-8: $R^3 = CH{=}CH_2$, $R^4 = CH_3$

SI-1: $R^1 = CH_3$, $R^2 = Ph$
SI-2: $R^1 = CH_3$, $R^2 = CH_2CH_3$
SI-3: $R^1 = OCH_3$, $R^2 = COOMe$

6. Crystallographic Details

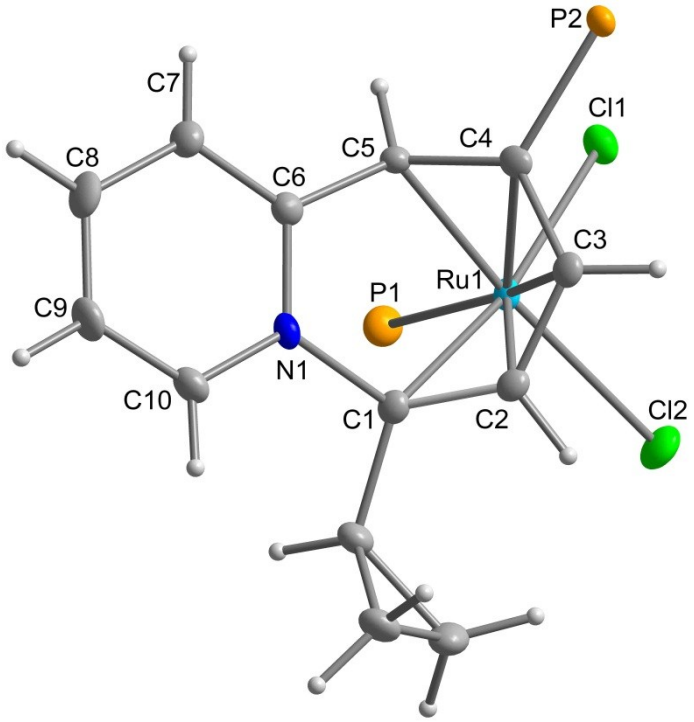


Figure S5. Single-crystal X-ray structure for cationic complex **2** with thermal ellipsoids drawn at the 50% probability level. The phenyl groups in the triphenylphosphine (PPh_3) moieties were omitted for clarity. Selected bond lengths [Å] and angles [deg]: Ru1−C1 2.188(3), Ru1−C2 2.129(3), Ru1−C3 2.225(3), Ru1−C4 2.136(3), Ru1−C5 2.105(3), N1−C1 1.510(4), C1−C2 1.422(4), C2−C3 1.407(4), C3−C4 1.415(4), C4−C5 1.457(4), C5−C6 1.467(4), N1−C6 1.353(4), C6−C7 1.378(4), C7−C8 1.384(5), C8−C9 1.386(5), C9−C10 1.369(5), N1−C10 1.357(4); C1−C2−C3 126.5(3), C2−C3−C4 121.1(3), C3−C4−C5 122.7(3), C4−C5−C6 119.3(3), C5−C6−N1 116.3(3), C6−N1−C1 118.9(2), N1−C6−C7 119.8(3), C6−C7−C8 119.8(3), C7−C8−C9 119.5(3), C8−C9−C10 119.0(3), C9−C10−N1 120.9(3), C10−N1−C6 120.7(3).

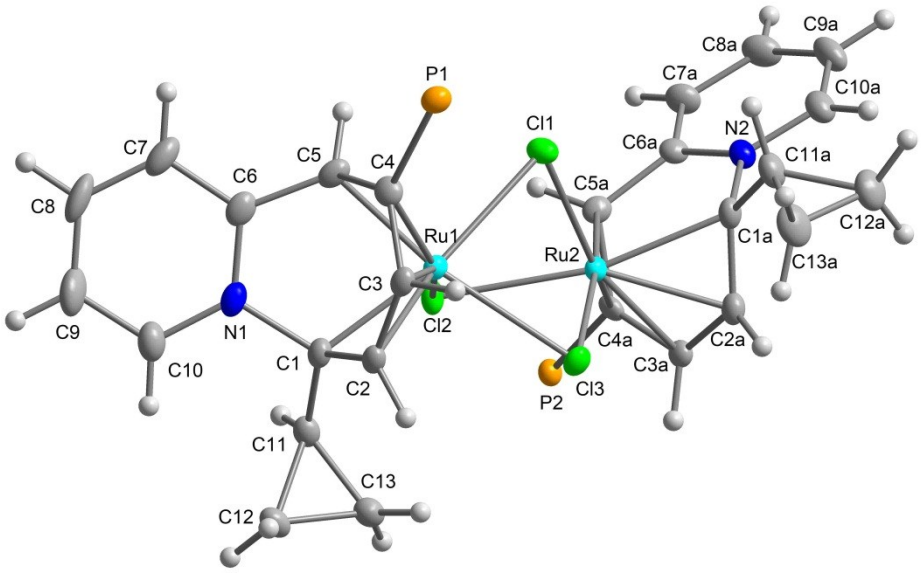


Figure S6. Single-crystal X-ray structure for cationic complex **3** with thermal ellipsoids drawn at the 50% probability level. The phenyl groups in the triphenylphosphine (PPh_3) moieties were omitted for clarity. Selected bond lengths [Å] and angles [deg]: Ru1−C1 2.130(4), Ru1−C2 2.127(4), Ru1−C3 2.169(4), Ru1−C4 2.106(4), Ru1−C5 2.087(4), C1−C2 1.419(6), C2−C3 1.425(6), C3−C4 1.426(6), C4−C5 1.479(6), C5−C6 1.468(6), N1−C6 1.342(6), N1−C1 1.497(5), C6−C7 1.392(6), C7−C8 1.373(7), C8−C9 1.388(8), C9−C10 1.374(7), C10−N1 1.361(6); C1−C2−C3 122.7(4), C2−C3−C4 122.7(4), C3−C4−C5 120.8(4), C4−C5−C6 118.7(3), C5−C6−N1 115.7(4), C6−N1−C1 117.5(3), N1−C1−C2 118.3(3), N1−C6−C7 119.1(4), C6−C7−C8 119.6(4), C7−C8−C9 120.5(4), C8−C9−C10 118.6(5), C9−C10−N1 120.2(5), C10−N1−C6 122.0(4).

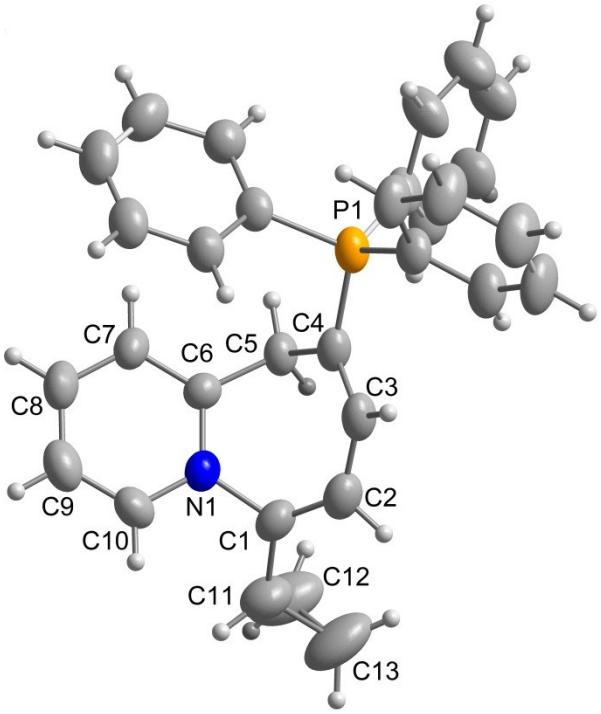


Figure S7. Single-crystal X-ray structure for cationic complex **4** with thermal ellipsoids drawn at the 50% probability level. Selected bond lengths [Å] and angles [deg]: N1−C1 1.464(6), C1−C2 1.330(6), C2−C3 1.444(7), C3−C4 1.328(6), C4−C5 1.543(5), C5−C6 1.489(5), C6−N1 1.367(5), C6−C7 1.377(6), C7−C8 1.381(6), C8−C9 1.375(7), C9−C10 1.374(7), C10−N1 1.351(5); N1−C1−C2 120.0(4), C1−C2−C3 127.5(4), C2−C3−C4 122.5(4), C3−C4−C5 119.7(4), C4−C5−C6 107.3(3), C5−C6−N1 118.0(4), C6−N1−C1 122.0(3), N1−C6−C7 118.5(4), C6−C7−C8 121.0(4), C7−C8−C9 119.1(4), C8−C9−C10 119.4(4), C9−C10−N1 120.8(4), C10−N1−C6 121.1(4).

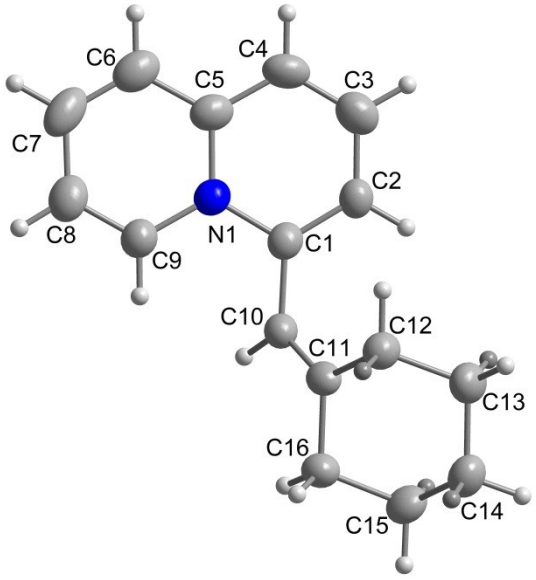


Figure S8. Single-crystal X-ray structure for cationic complex **5c** with thermal ellipsoids drawn at the 50% probability level. Selected bond lengths [Å] and angles [deg]: C1−C2 1.364(5), C2−C3 1.394(5), C3−C4 1.354(5), C4−C5 1.402(6), C5−C6 1.410(5), C6−C7 1.354(6), C7−C8 1.422(6), C8−C9 1.337(5), C9−N1 1.394(5), N1−C1 1.400(4), N1−C5 1.388(5), C1−C10 1.474(5), C10−C11 1.322(5); N1−C1−C2 118.4(3), C1−C2−C3 121.6(3), C2−C3−C4 119.8(4), C3−C4−C5 120.5(4), C4−C5−N1 118.9(3), C5−N1−C1 120.7(3), N1−C5−C6 118.7(4), C5−C6−C7 121.5(4), C6−C7−C8 118.5(4), C7−C8−C9 120.5(4), C8−C9−N1 121.5(4), C9−N1−C5 119.3(3), C1−C10−C11 125.1(3), C10−C11−C12 126.2(3), C10−C11−C16 121.2(3).

Crystallographic analysis

A crystal of **2** suitable for X-ray diffraction was grown from a dichloroethane solution layered with hexane. A crystal suitable for X-ray diffraction of **3** was grown from a dichloroethane/methanol solution layered with hexane. Single crystals of **4** and **5c** suitable for X-ray diffraction were grown from a dichloromethane solution layered with hexane. Single-crystal X-ray diffraction data were collected on an Agilent SuperNova diffractometer or a Rigaku R-AXIS SPIDER IP CCD area detector with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) or Cu-Kα radiation (λ = 1.54178 Å). All the data were corrected for absorption effects using a multi-scan technique. All the structures were solved by the Patterson function, completed by subsequent difference Fourier map calculations, and refined by a full-matrix least-squares method on F^2 using the SHELXTL program package. All non-hydrogen atoms were refined anisotropically unless otherwise stated. The hydrogen atoms were placed at their idealized positions and assumed the riding model unless otherwise stated. The water (H_2O) solvent molecules in **3** and **4** were refined without the addition of H atoms. X-ray crystal structure information is available at the Cambridge Crystallographic Data Centre (CCDC) under deposition numbers CCDC 1548362 (**2**), CCDC 1548363 (**3**), CCDC 1548364 (**4**), and CCDC 1548359 (**5c**). For further details on the crystal data, data collection, and refinements, see Table S2.

Table S3 Crystal data and structure refinement for **2**, **3**, **4**, and **5c**.

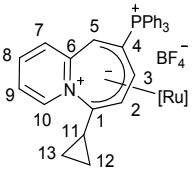
	2·$C_2H_4Cl_2$	**3**·$C_2H_4Cl_2$·0.5CH_3OH·1.5H_2O	**4**·0.25H_2O·0.5CH_2Cl_2	**5c**
Formular	$C_{51}H_{46}BCl_4F_4NP_2Ru$	$C_{64.50}H_{60}B_3Cl_5F_{12}N_2O_2P_2Ru_2$	$C_{31.5}H_{28}B_2ClF_8NO_{0.25}P$	$C_{16}H_{18}BF_4N$
Mr	1064.51	1596.90	664.59	311.12
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	*P-1*	*P-1*	$P2_1/n$
a [Å]	10.2733(2)	13.9016(3)	9.2290(7)	12.9618(6)
b [Å]	16.5521(3)	15.3374(4)	12.4861(7)	9.9513(4)
c [Å]	27.6804(6)	17.6017(5)	15.3456(7)	13.2243(7)
α [°]	90.00	84.684(2)	107.395(2)	90.00
β [°]	98.924(2)	67.829(2)	100.184(2)	118.4200(10)
γ [°]	90.00	74.648(2)	106.684(2)	90.00
V [Å^3]	4649.93(16)	3351.33(16)	1548.27(16)	1500.19(12)
Z	4	2	2	4
ρ_{calcd} [gcm^{-3}]	1.521	1.582	1.426	1.378
μ [mm^{-1}]	0.690	0.776	0.248	0.114
F (000)	2168	1606	680.0	648
2θ range [°]	6.65 to 49.986	6.61 to 50.00	6.294 to 54.966	6.08 to 54.954
Reflns collected	26520	26045	15215	14337
Independent reflns	8173	11764	7031	3431
Obserbed reflns [$I \geq 2\sigma(I)$]	6798	9943	3543	1664
Data/restrains/params	8173/0/577	11764/7/849	7031/12/511	3431/0/209
GOF on F^2	1.045	1.093	1.146	1.072
R_1/wR_2 [$I \geq 2\sigma(I)$]	0.0391/0.0888	0.0469/0.1280	0.0838/0.2123	0.0982/0.2778
R_1/wR_2 (all data)	0.0514/0.0940	0.0576/0.1363	0.1568/0.3042	0.1653/0.3401
Largest peak/hole [e Å^{-3}]	0.95/−0.71	1.91/−1.25	0.48/−0.81	0.79/−0.72
CCDC No.	1548362	1548363	1548364	1548359

7. Experimental Procedures

General comments

All syntheses were performed under an inert atmosphere (N_2) using standard Schlenk techniques, unless otherwise stated. Reagents and solvents were used as received from commercial sources without further purification. The starting material [Ru{CHC(PPh_3)CH(2-Py)}Cl_2PPh_3]BF_4 (**1**) was synthesized according to a previously published procedure.[12] Cyclobutylethyne was prepared according to the literature.[14] Nuclear magnetic resonance (NMR) spectroscopic experiments were performed on a Bruker AV-500 spectrometer (^{1}H, 500.2 MHz; ^{13}C, 125.8 MHz; ^{31}P, 202.5 MHz) at room temperature. The ^{1}H and ^{13}C NMR chemical shifts (δ) are relative to tetramethylsilane, and the ^{31}P NMR chemical shifts 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), quartet (q), quintet (quint) and broad (br). High-resolution mass spectra (HRMS) experiments were recorded on a Bruker En Apex Ultra 7.0T Fourier Transform Mass Spectrometer. The theoretical molecular ion peak was calculated by Compass Isotope Pattern software supplied by Bruker Co. Elemental analysis data were obtained on an Elementar Analysensysteme GmbH Vario EL III instrument. Infrared (IR) spectra were obtained using a Thermo Nicolet Avatar 330 FT-IR Spectrometer using thin-film samples.

Preparation and characterization of complex 2



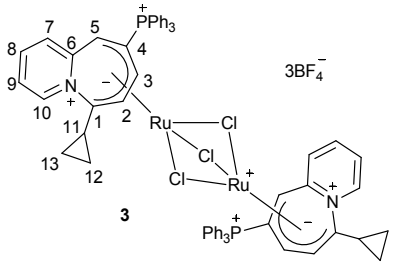
2

[Ru] = $RuCl_2PPh_3$

2: A mixture of **1** (200 mg, 0.22 mmol) and cyclopropylethyne (44 mg, 0.66 mmol) in DCM (10 mL) was stirred at room temperature (RT) for 30 min to give an orange solution. The solution was evaporated under vacuum to approximately 5 mL. The addition of diethyl ether (15 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. The precipitate was dissolved in 2 mL of DCM, and 20 mL of diethyl ether was added to obtain **2** as an orange solid. Yield: 139 mg, 65%.

Diagnostic peaks for **2** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2): δ = 9.01 (d, $^{3}J_{HH}$ = 6.0 Hz, 1H, C^{10}H), 7.79–7.12 (32H, other aromatic protons), 6.67 (dd, apparent t, $^{3}J_{HH}$ = 7.0 Hz, $^{3}J_{PH}$ = 7.0 Hz, 1H, C^{3}H), 6.46 (d, $^{3}J_{HH}$ = 7.6 Hz, 1H, C^{7}H), 4.80 (d, $^{3}J_{HH}$ = 7.0 Hz, 1H, C^{2}H), 2.60 (d, $^{3}J_{PH}$ = 10.2 Hz, 1H, C^{5}H), 1.29 (m, 1H, C^{12}H), 1.21 (m, 1H, C^{13}H, overlapped with grease, confirmed by ^{1}H-^{13}C HSQC), 0.71 (m, 1H, C^{13}H), and 0.64 ppm (m, 2H, C^{11}H and C^{12}H). ^{31}P NMR (202.5 MHz, CD_2Cl_2): δ = 15.67 (d, $^{3}J_{PP}$ = 5.9 Hz, C*P*Ph$_3$), and 28.98 ppm (s, $^{3}J_{PP}$ = 5.9 Hz, Ru*P*Ph$_3$). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 159.28 (d, $^{3}J_{PC}$ = 5.7 Hz, C6), 142.71 (s, C8), 141.11 (s, C10), 127.12-135.25 (other aromatic carbons), 125.77 (s, C7), 124.83 (s, C9), 98.65 (dd, apparent t, $^{2}J_{PC}$ = 15.0 Hz, $^{2}J_{PC}$ = 15.0 Hz, C3), 91.20 (dd, $^{2}J_{PC}$ = 5.7 Hz, $^{1}J_{PC}$ = 68.3 Hz, C4), 89.52 (d, $^{2}J_{PC}$ = 8.7 Hz, C1), 78.47 (d, $^{2}J_{PC}$ = 9.9 Hz, C2), 46.74 (br, C5), 17.15 (s, C11), 14.77 (s, C13), and 8.03 ppm (s, C12). Elemental analysis calcd (%) for $C_{49}H_{42}BCl_2F_4NP_2Ru$: C 60.95, H 4.38, N 1.45; found: C 60.78, H 4.66, N 1.61.

Preparation and characterization of complex 3

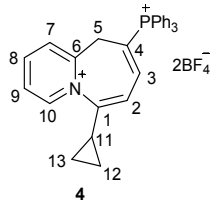


3

3: A mixture of **2** (100 mg, 0.10 mmol) and a tetrafluoroboric acid-diethyl ether complex (50 wt% solution in diethyl ether, 27 μL, 0.10 mmol) was stirred at RT for 5 h in DCM/benzene (4 mL:1 mL) to give a brown suspension. An orange solid was separated by filtration and washed with DCM (3 × 1 mL) to obtain complex **3** as an orange solid. Yield: 56 mg, 77%.

Due to its poor solubility in common organic solvents, complex **3** was only characterized by ^{1}H NMR and ^{31}P NMR. Diagnostic peaks for **3** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2/CD_3OH): δ = 9.03 (br, 2H, C^{10}H), 7.92–7.25 (36H, other aromatic protons), 6.10 (br, 2H, C^{3}H), 4.51 (br, 2H, C^{2}H), 4.31 (br, 2H, C^{5}H), 1.71-0.53 ppm (10H, C^{11}H, C^{12}H, C^{13}H). ^{31}P NMR (202.5 MHz, CD_2Cl_2/CD_3OH): δ = 28.94 ppm (s, C*P*Ph$_3$). Elemental analysis calcd (%) for $C_{62}H_{54}B_3Cl_3F_{12}N_2P_2Ru_2$: C 51.08, H 3.73, N 1.92; found: C 51.31, H 4.05, N 1.91.

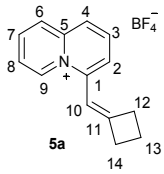
Preparation and characterization of complex 4



4: A mixture of **2** (100 mg, 0.10 mmol) and tetrafluoroboric acid (48 wt% solution in H_2O, 13 μL, 0.10 mmol) was sparged with carbon monoxide (CO) and stirred at RT for 2 h in DCM (10 mL) to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (15 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. The precipitate was purified by column chromatography (Bio-Beads™ S-X3 Support, 200-400 mesh, eluent: chloroform), and the second component was collected and evaporated under reduced pressure to obtain **4** as an orange solid. Yield: 40 mg, 64%.

Diagnostic peaks for **4** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2): δ = 9.18 (d, $^{3}J_{HH}$ = 6.4 Hz, 1H, C^{10}*H*), 8.08 (t, $^{3}J_{HH}$ = 7.8 Hz, 1H, C^{8}*H*), 7.87 (t, $^{3}J_{HH}$ = 6.4 Hz, 1H, C^{9}*H*), 7.86–7.68 (15H, Ph*H*), 6.88 (dd, $^{3}J_{HH}$ = 5.5 Hz, $^{3}J_{PH}$ = 17.3 Hz, 1H, C^{3}*H*), 6.72 (d, $^{3}J_{HH}$ = 5.5 Hz, 1H, C^{2}*H*,), 6.44 (d, $^{3}J_{HH}$ = 7.8 Hz, 1H, C^{7}*H*), 4.06 (dd, apparent t, $^{2}J_{HH}$ = 11.0 Hz, $^{3}J_{PH}$ = 11.0 Hz, 1H, C^{5}*H*), 3.92 (dd, apparent t, $^{2}J_{HH}$ = 11.0 Hz, $^{3}J_{PH}$ = 11.0 Hz, 1H, C^{5}*H*), 2.04 (m, 1H, C^{11}*H*), 1.38 (m, 1H, C^{13}*H*), 1.23 (m, 1H, C^{13}*H*), 1.11 (m, 1H, C^{12}*H*), and 1.03 ppm (m, 1H, C^{12}*H*). ^{31}P NMR (202.5 MHz, CD_2Cl_2): δ = 22.65 ppm (s, C*P*Ph$_3$). ^{13}C NMR plus ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 151.29 (s, C6), 150.46 (s, C1), 146.48 (s, C8), 145.84 (d, $^{2}J_{PC}$ = 10.5 Hz, C3), 141.48 (s, C10), 135.30 (d, J_{PC} = 3.0 Hz, Ph), 133.94 (d, J_{PC} = 10.8 Hz, Ph), 130.16 (d, J_{PC} = 12.9 Hz, Ph), 125.54 (s, C9), 125.39 (s, C7), 121.39 (d, $^{3}J_{PC}$ = 17.2 Hz, C2), 119.26 (d, $^{1}J_{PC}$ = 83.3 Hz, C4), 114.72 (d, J_{PC} = 89.8 Hz, Ph), 33.20 (d, $^{2}J_{PC}$ = 11.0 Hz, C5), 17.18 (s, C11), 12.86 (s, C13), and 6.38 ppm (s, C12). HRMS (ESI): *m/z* calcd for $[[C_{31}H_{28}NP]^{2+} + BF_4^-]^+$, 532.1988; found, 532.1988. IR (film): 3067, 2922, 2852, 1629, 1603, 1492, 1439, 1261, 1053, 956, 796, 725, 692, 521 cm^{-1}.

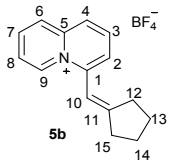
Preparation and characterization of complex 5a



5a: A mixture of **1** (200 mg, 0.22 mmol) and cyclobutylethyne (12.5 mL, 0.053 mmol/mL in DCM) was stirred at 60 °C for 1 h to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (20 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. Then, the precipitate was dissolved in 2 mL of DCM and extracted with water (3 × 3 mL). The aqueous phases were combined and evaporated under reduced pressure to obtain **5a** as a yellow oil. Yield: 27 mg, 43%.

Diagnostic peaks for **5a** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2): δ = 9.11 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, C^{9}*H*), 8.33 (d, $^{3}J_{HH}$ = 8.5 Hz, 1H, C^{6}*H*), 8.17-8.23 (m, 3H, C^{3}*H*, C^{4}*H*, C^{7}*H*), 8.00 (t, $^{3}J_{HH}$ = 7.1 Hz, 1H, C^{8}*H*), 7.73 (d, $^{3}J_{HH}$ = 6.9 Hz, 1H, C^{2}*H*), 6.57 (s, 1H, C^{10}*H*), 3.06 (t, $^{3}J_{HH}$ = 8.0 Hz, 2H, C^{14}*H*), 2.92 (t, $^{3}J_{HH}$ = 8.0 Hz, 2H, C^{12}*H*), and 2.14 (quint, $^{3}J_{HH}$ = 8.0 Hz, 2H, C^{13}*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 161.69 (s, C11), 142.68 (s, C1), 142.47 (s, C5), 135.78 and 135.59 (s, C3 and C7), 131.40 (s, C9), 127.56 (s, C6), 124.91 (s, C4), 123.61 (s, C2), 123.41 (s, C8), 109.99 (s, C10), 32.49 (s, C14), 31.55 (s, C12), and 16.79 ppm (s, C13). HRMS (ESI): *m/z* calcd for $[C_{14}H_{14}N]^{+}$, 196.1121; found, 196.1124; IR (film): 3116, 2960, 2917, 2849, 1653, 1635, 1457, 1405, 1346, 1286, 1261, 1053, 877, 808, 720, 705, 521 cm^{-1}.

Preparation and characterization of complex 5b

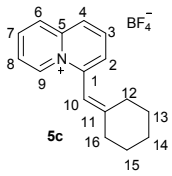


5b: A mixture of **1** (200 mg, 0.22 mmol) and cyclopentylethyne (62 mg, 0.66 mmol) in wet 1,2-dichloroethane (10 mL) was stirred at 60 °C for 1 h to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (20 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. Then, the precipitate was dissolved in 2 mL of DCM and extracted with water (3 × 3 mL). The

aqueous phases were combined and evaporated under reduced pressure to obtain **5b** as a yellow oil. Yield: 15 mg, 23%.

Diagnostic peaks for **5b** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2): δ = 9.22 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, C^{9}*H*), 8.47 (d, $^{3}J_{HH}$ = 8.6 Hz, 1H, C^{6}*H*), 8.31-8.37 (m, 3H, C^{3}*H*, C^{4}*H*, C^{7}*H*), 8.10 (t, $^{3}J_{HH}$ = 7.1 Hz, 1H, C^{8}*H*), 7.94 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, C^{2}*H*), 6.71 (s, 1H, C^{10}*H*), 2.81 (t, $^{3}J_{HH}$ = 7.2 Hz, 2H, C^{15}*H*), 2.49 (t, $^{3}J_{HH}$ = 7.0 Hz, 2H, C^{12}*H*), and 1.92-1.81 ppm (m, 4H, C^{13}*H*, C^{14}*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 163.40 (s, C11), 144.38 (s, C1), 143.33 (s, C5), 136.51 and 136.45 (s, C3 and C7), 132.39 (s, C9), 128.32 (s, C6), 125.85 (s, C4), 125.08 (s, C2), 124.37 (s, C8), 110.33 (s, C10), 35.23 (s, C12), 31.80 (s, C13), 26.36 (s, C14), and 25.52 ppm (s, C15). HRMS (ESI): *m/z* calcd for $[C_{15}H_{16}N]^{+}$, 210.1277; found, 210.1279; IR (film): 3116, 3070, 2959, 2921, 2851, 1646, 1623, 1456, 1404, 1054, 811, 791, 696, 521 cm^{-1}.

Preparation and characterization of complex 5c

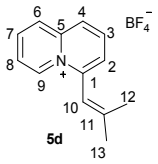


5c: A mixture of **1** (200 mg, 0.22 mmol) and cyclohexylethyne (71 mg, 0.66 mmol) in wet 1,2-dichloroethane (10 mL) was stirred at 60 °C for 1 h to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (20 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. Then, the precipitate was dissolved in 2 mL of DCM and extracted with water (3 × 3 mL). The aqueous phases were combined and evaporated under reduced pressure to obtain **5c** as a white solid. Yield: 46 mg, 67%.

Diagnostic peaks for **5c** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, CD_2Cl_2): δ = 9.22 (d, $^{3}J_{HH}$ = 7.2 Hz, 1H, C^{9}*H*), 8.50 (d, $^{3}J_{HH}$ = 8.7 Hz, 1H, C^{6}*H*), 8.31-8.41 (m, 3H, C^{3}*H*, C^{4}*H*, C^{7}*H*), 8.10 (t, $^{3}J_{HH}$ = 7.2 Hz, 1H, C^{8}*H*), 7.83 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, C^{2}*H*), 6.47 (s, 1H, C^{10}*H*), 2.59 (t, $^{3}J_{HH}$ = 6.0 Hz, 2H, C^{16}*H*), 2.30 (t, $^{3}J_{HH}$ = 6.2 Hz, 2H, C^{12}*H*), 1.86 (m, 2H, C^{15}*H*), 1.72 (m, 2H, C^{14}*H*), and 1.67 ppm (m, 2H, C^{13}*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 158.19 (s, C11), 143.55 (s, C1), 143.49 (s, C5), 136.60 and

136.43 (s, C3 and C7), 132.44 (s, C9), 128.37 (s, C6), 126.25 (s, C4), 126.05 (s, C2), 124.46 (s, C8), 111.64 (s, C10), 37.28 (s, C16), 30.86 (s, C12), 28.30 (s, C15), 27.92 (s, C13), and 25.91 ppm (s, C14). HRMS (ESI): *m/z* calcd for $[C_{16}H_{18}N]^+$, 224.1434; found, 224.1434. IR (KBr): 3052, 2963, 2937, 2853, 1641, 1622, 1450, 1403, 1345, 1262, 1084, 1031, 802 and 521 cm^{-1}.

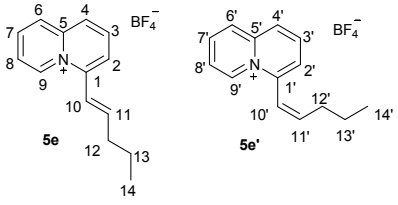
Preparation and characterization of complex 5d



5d: A mixture of **1** (200 mg, 0.22 mmol) and 3-methylbut-1-yne (45 mg, 0.66 mmol) in wet 1,2-dichloroethane (10 mL) was stirred at 60 °C for 1 h to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (20 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. Then, the precipitate was dissolved in 2 mL of dichloromethane (DCM) and extracted with water (3 × 3 mL). The aqueous phases were combined and evaporated under reduced pressure to obtain **5d** as a yellow oil. Yield: 35 mg, 59%.

Diagnostic peaks for **5d** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, $CDCl_3$): δ = 9.14 (d, $^3J_{HH}$ = 6.7 Hz, 1H, C^9*H*), 8.42 (d, $^3J_{HH}$ = 8.6 Hz, 1H, C^6*H*), 8.32 (d, $^3J_{HH}$ = 8.6 Hz, 1H, C^4*H*), 8.23-8.17 (m, 2H, C^3*H*, C^7*H*), 8.00 (t, $^3J_{HH}$ = 6.7 Hz, 1H, C^8*H*), 7.71 (d, $^3J_{HH}$ = 7.2 Hz, 1H, C^2*H*), 6.48 (s, 1H, C^{10}*H*), 2.11 (s, 3H, C^{13}*H*), and 1.79 ppm (s, 3H, C^{12}*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, $CDCl_3$): δ = 150.26 (s, C11), 143.55 (s, C1), 143.44 (s, C5), 136.83 and 136.52 (s, C3 and C7), 132.98 (s, C9), 128.72 (s, C6), 126.68 (s, C4), 126.13 (s, C2), 124.81 (s, C8), 115.42 (s, C10), 26.41 (s, C13), and 20.58 ppm (s, C12). HRMS (ESI): *m/z* calcd for $[C_{13}H_{14}N]^+$, 184.1121; found, 184.1120; IR (film): 3118, 2981, 2919, 2852, 1644, 1623, 1467, 1404, 1346, 1294, 1055, 885, 811, 787, 757, 521 cm^{-1}.

Preparation and characterization of complexes 5e/e′



5e/e′: A mixture of **1** (200 mg, 0.22 mmol) and hex-1-yne (54 mg, 0.66 mmol) in wet 1,2-dichloroethane (10 mL) was stirred at 60 °C for 1 h to give an orange solution. The solution was evaporated under vacuum to approximately 2 mL. The addition of diethyl ether (20 mL) to the residual gave an orange precipitate, and the precipitate was collected by filtration. Then, the precipitate was dissolved in 2 mL of DCM and extracted with water (3 × 3 mL). The aqueous phases were combined and evaporated under reduced pressure to obtain **5e/e′** as a yellow oil. Yield: 39 mg, 62%.

Diagnostic peaks for **5e** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, $CDCl_3$): δ = 9.23 (d, $^{3}J_{HH}$ = 5.3 Hz, 1H, C^{9}*H*), 8.51 (d, $^{3}J_{HH}$ = 7.5 Hz, 1H, C^{4}*H*), 8.43 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, C^{6}*H*), 8.26-8.32 (m, 2H, C^{7}*H*, C^{3}*H*), 8.10 (br, 1H, C^{8}*H*), 7.97 (d, $^{3}J_{HH}$ = 6.6 Hz, 1H, C^{2}*H*), 7.07 (d, $^{3}J_{HH}$ = 14.9 Hz, 1H, C^{10}*H*), 6.72 (m, 1H, C^{11}*H*), 2.46 (q, $^{3}J_{HH}$ = 7.1 Hz, 2H, C^{12}*H*), 1.62 (m, 2H, C^{13}*H*), and 1.00 ppm (t, $^{3}J_{HH}$ = 7.3 Hz, 3H, C^{14}*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, $CDCl_3$): δ = 147.61 (s, C11), 143.08 (s, C5), 142.43 (s, C1), 136.89 and 136.71 (s, C3 and C7), 132.52 (s, C9), 128.68 (s, C4), 126.87 (s, C6), 124.87 (s, C8), 123.80 (s, C2), 120.34 (s, C10), 35.44 (s, C12), 21.68 (s, C13), and 13.75 ppm (s, C14).

Diagnostic peaks for **5e′** are as follows: ^{1}H NMR with ^{1}H-^{13}C HSQC (500.2 MHz, $CDCl_3$): δ = 9.19 (d, $^{3}J_{HH}$ = 5.3 Hz, 1H, C$^{9'}$*H*), 8.59 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, C$^{6'}$*H*), 8.51 (d, $^{3}J_{HH}$ = 7.5 Hz, 1H, C$^{4'}$*H*), 8.26-8.32 (m, 2H, C$^{7'}$*H*, C$^{3'}$*H*), 8.10 (br, 1H, C$^{8'}$*H*), 7.81 (d, $^{3}J_{HH}$ = 6.6 Hz, 1H, C$^{2'}$*H*), 6.82 (d, $^{3}J_{HH}$ = 11.2 Hz, 1H, C$^{10'}$*H*), 6.53 (m, 1H, C$^{11'}$*H*), 2.17 (q, $^{3}J_{HH}$ = 6.8 Hz, 2H, C$^{12'}$*H*), 1.49 (m, 2H, C$^{13'}$*H*), and 0.88 ppm (t, $^{3}J_{HH}$ = 7.3 Hz, 3H, C$^{14'}$*H*). ^{13}C NMR with ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, $CDCl_3$): δ = 145.13 (s, C1′), 144.83 (s, C11′), 143.52 (s, C5′), 137.07 and 136.41 (s, C3′ and C7′), 132.82 (s, C9′), 128.89 (s, C6′), 127.31 (s, C4′), 125.63 (s, C2′), 124.98 (s, C8′), 119.32 (s, C10′), 31.28 (s, C12′), 22.13 (s, C13′), and 13.69 ppm (s, C14′). HRMS (ESI): *m/z* calcd for $[C_{14}H_{16}N]^{+}$, 198.1277; found, 198.1277; IR (film): 3053, 2960, 2918, 2849, 1643, 1622, 1457, 1399, 1345, 1266, 1053, 813, 733 and 699 cm^{-1}.

8. NMR Spectra

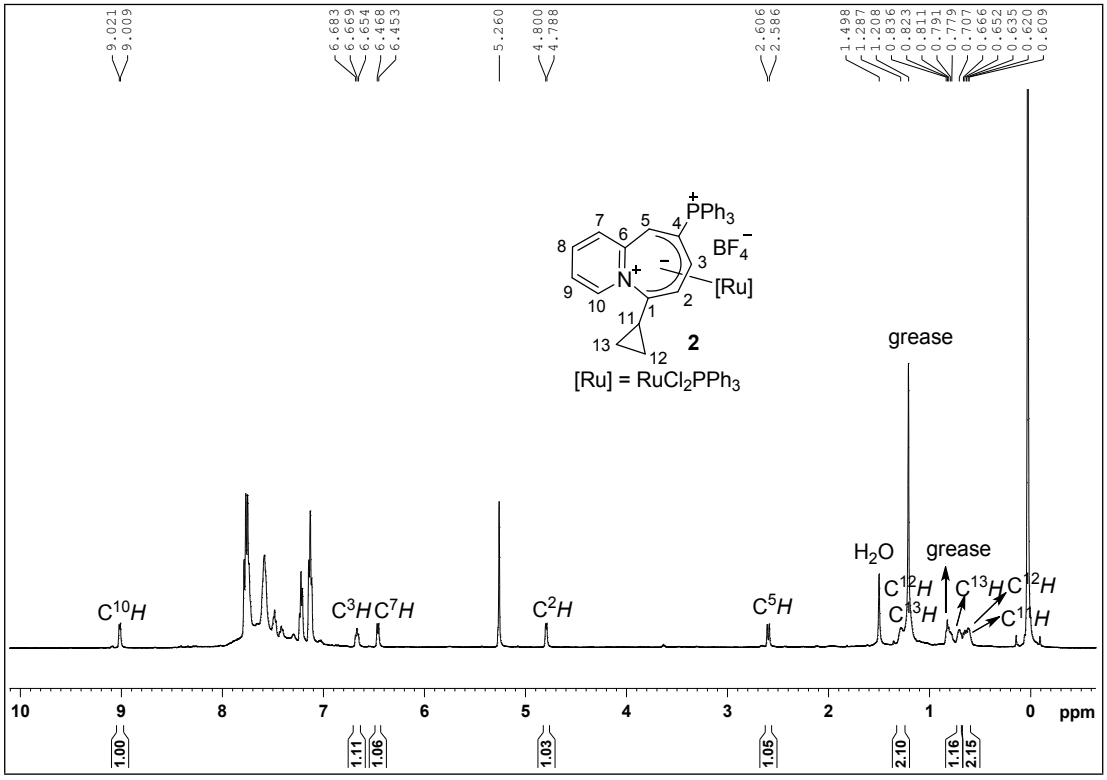


Figure S9 The ^{1}H NMR (500.2 MHz, CD_2Cl_2) spectrum of complex **2**.

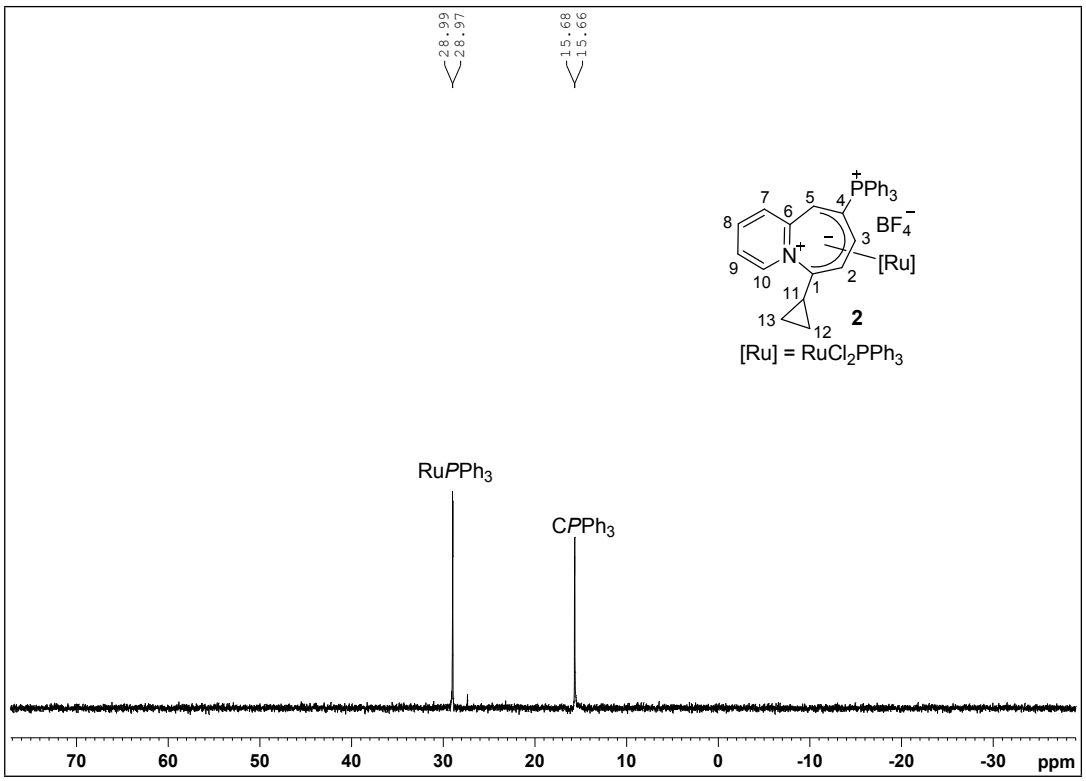


Figure S10 The $^{31}P\{^{1}H\}$ NMR (202.5 MHz, CD_2Cl_2) spectrum of complex **2**.

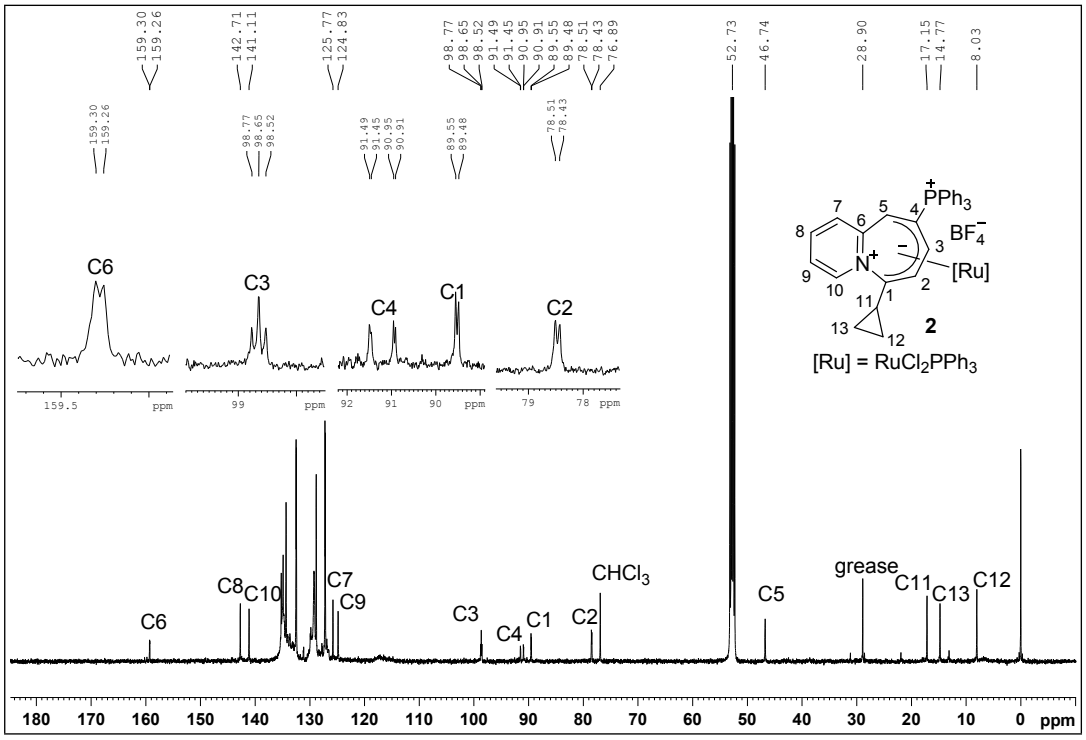


Figure S11 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum of complex **2**.

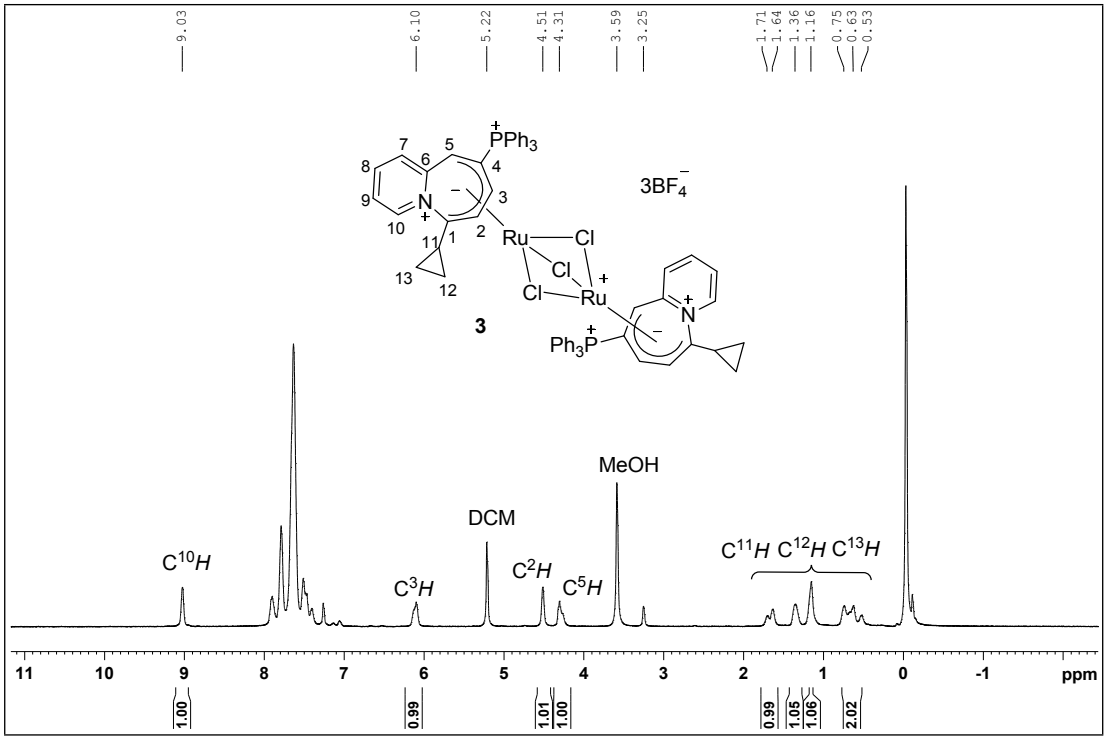


Figure S12 The ^{1}H NMR (500.2 MHz, CD_2Cl_2/CD_3OH) spectrum of complex **3**.

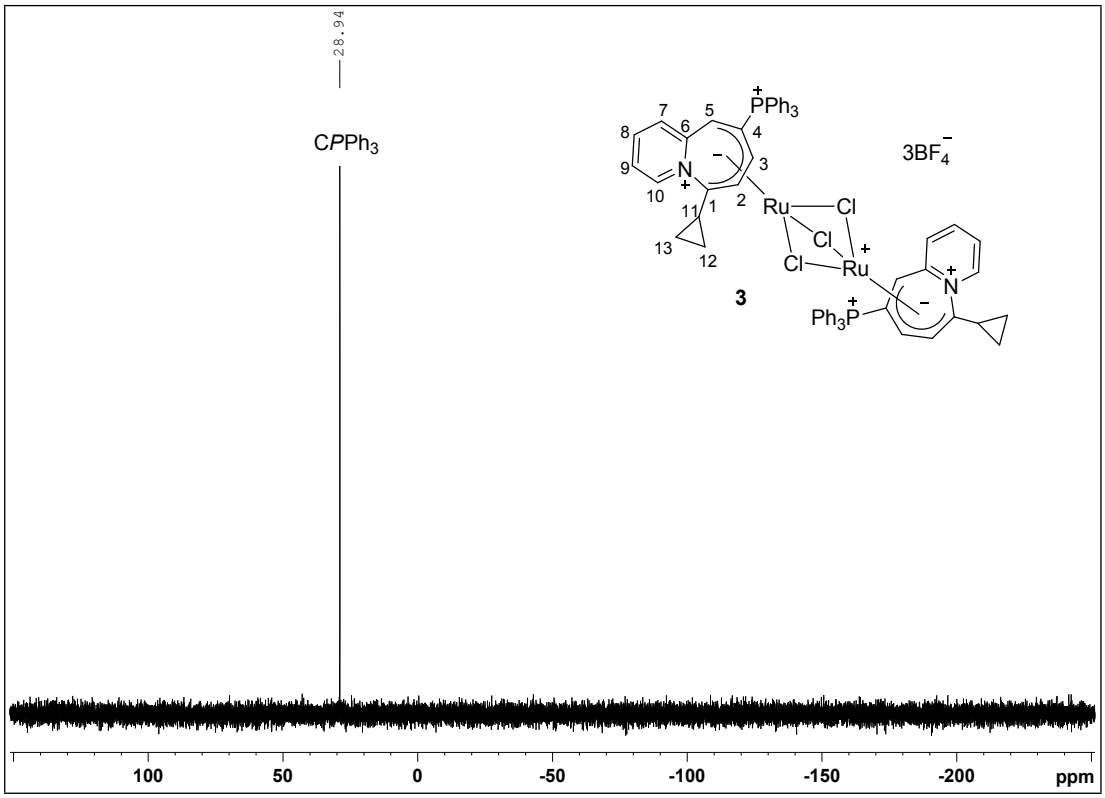


Figure S13 The $^{31}P\{^{1}H\}$ NMR (202.5 MHz, CD_2Cl_2/CD_3OH) spectrum of complex **3**.

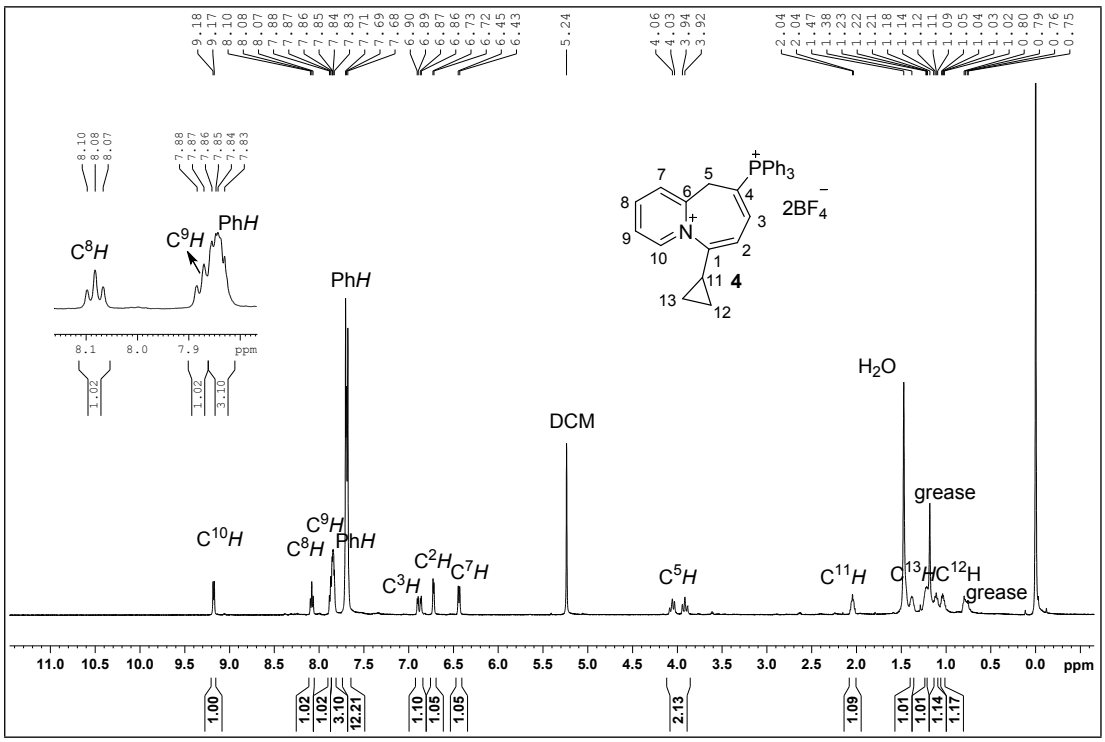


Figure S14 The ^{1}H NMR (500.2 MHz, CD_2Cl_2) spectrum of complex **4**.

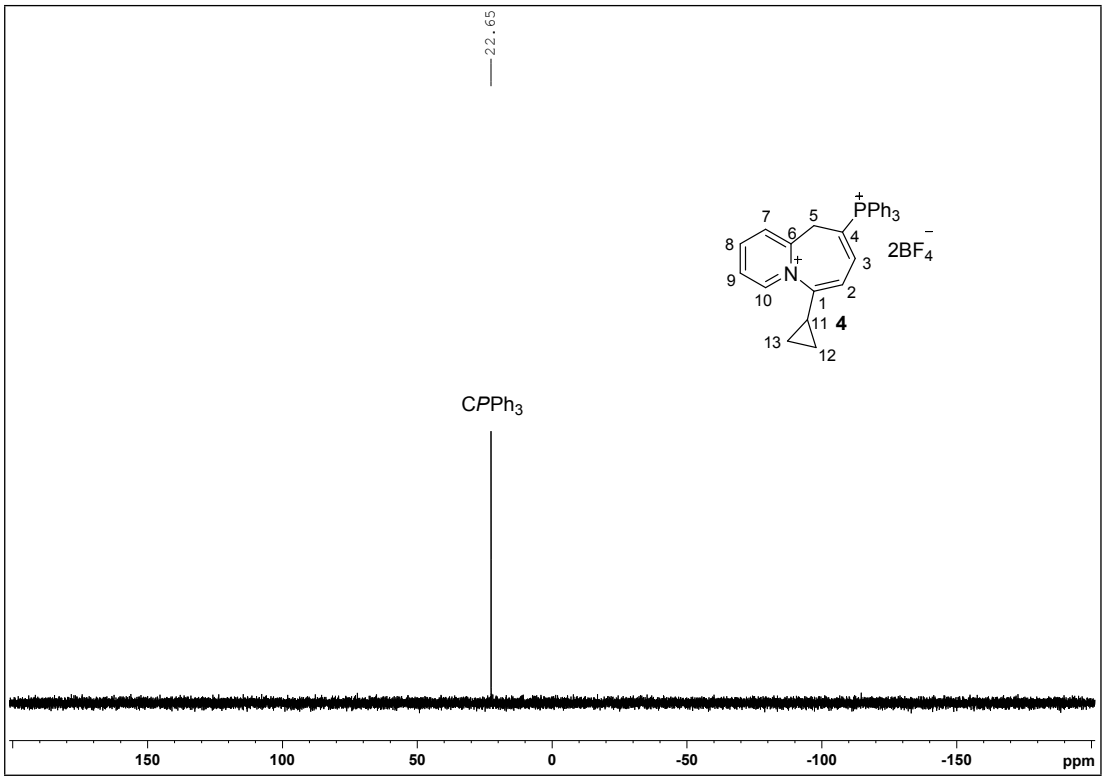


Figure S15 The $^{31}P\{^{1}H\}$ NMR (202.5 MHz, CD_2Cl_2) spectrum of complex **4**.

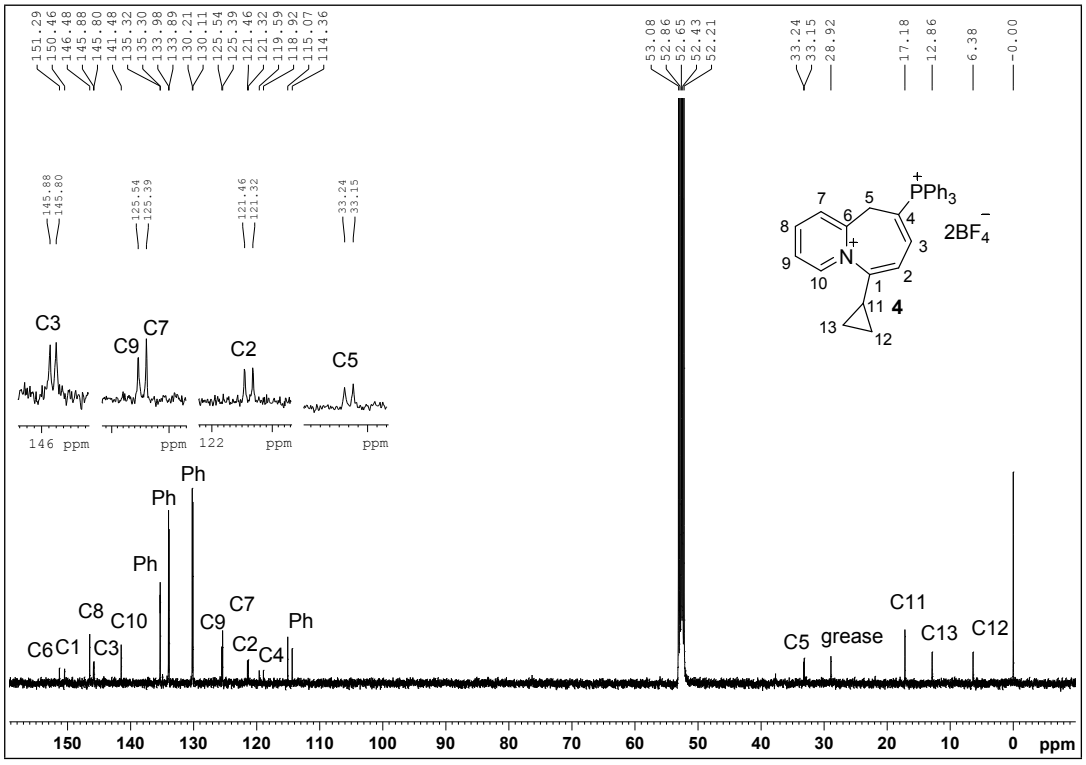


Figure S16 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum of complex **4**.

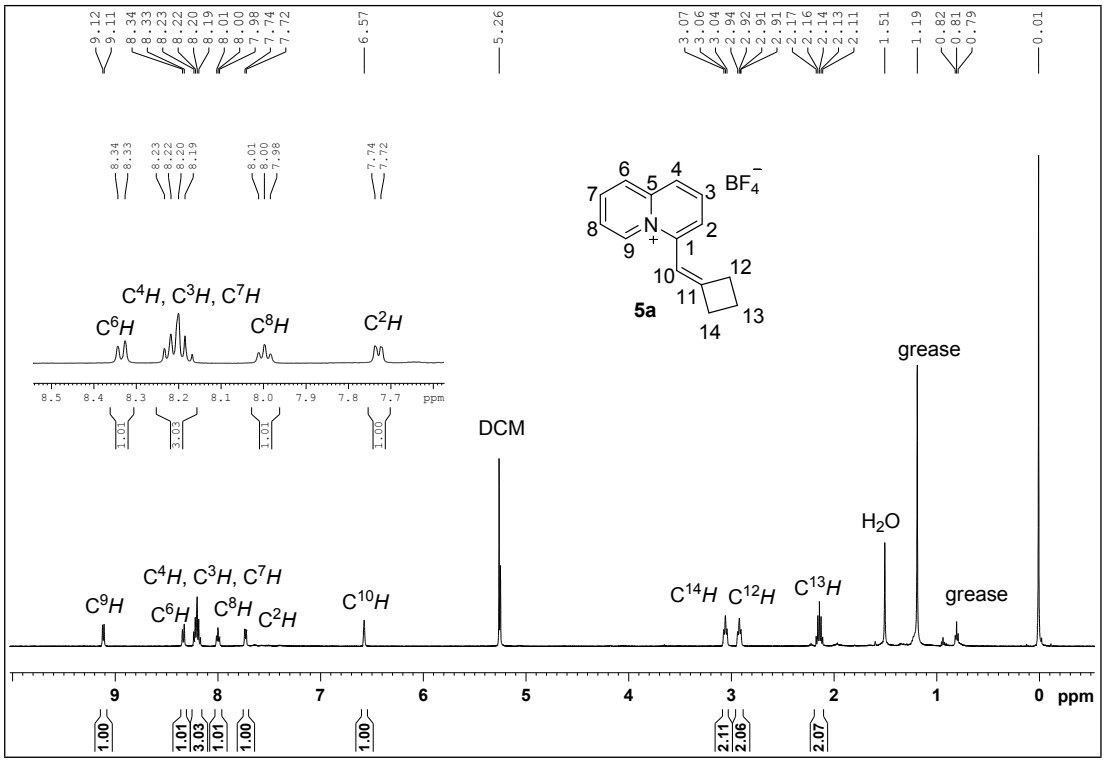


Figure S17 The ^{1}H NMR (500.2 MHz, CD_2Cl_2) spectrum of complex **5a**.

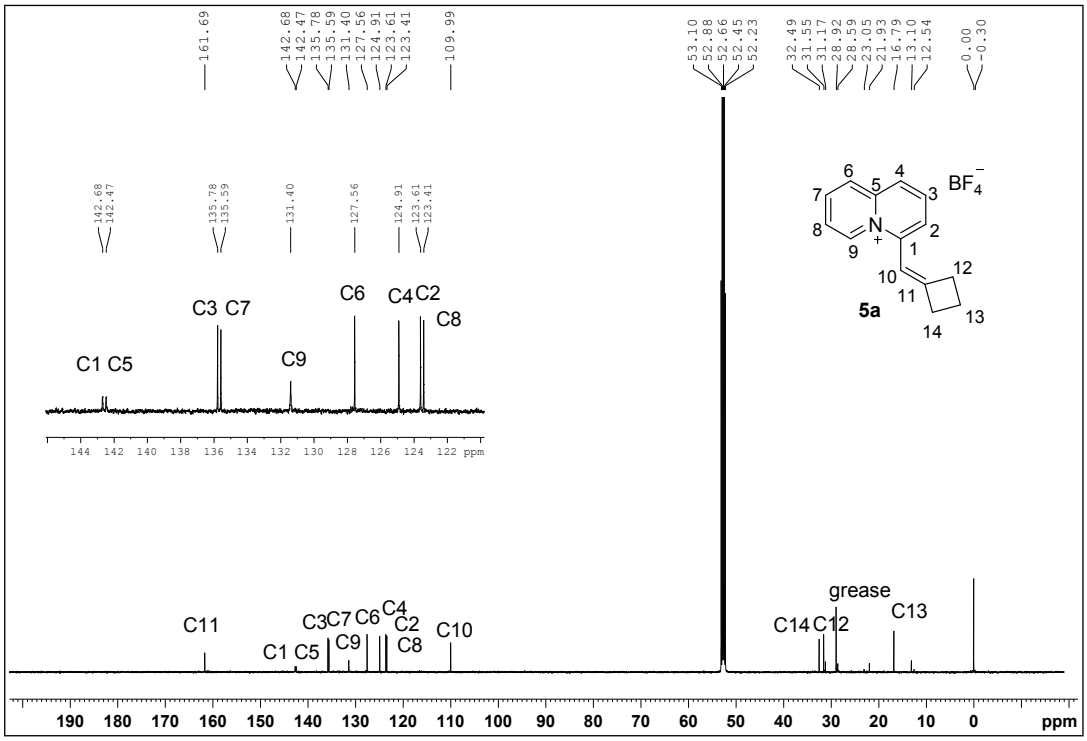


Figure S18 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum of complex **5a**.

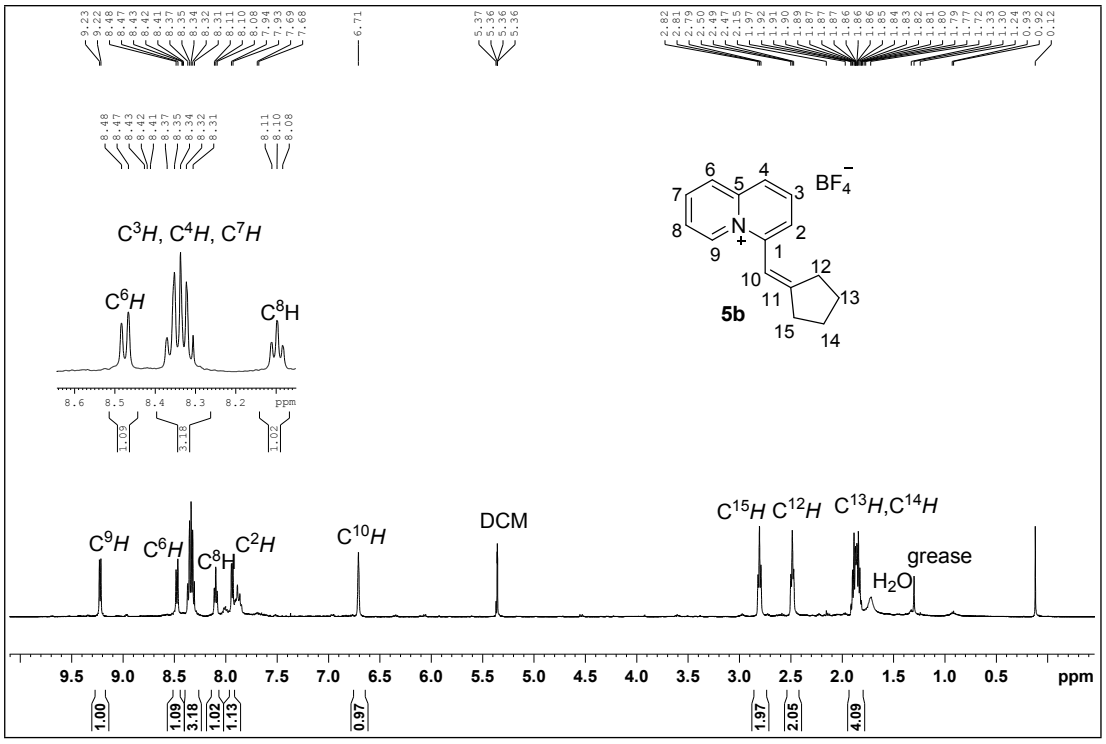


Figure S19 The ^{1}H NMR (500.2 MHz, CD_2Cl_2) spectrum of complex **5b**.

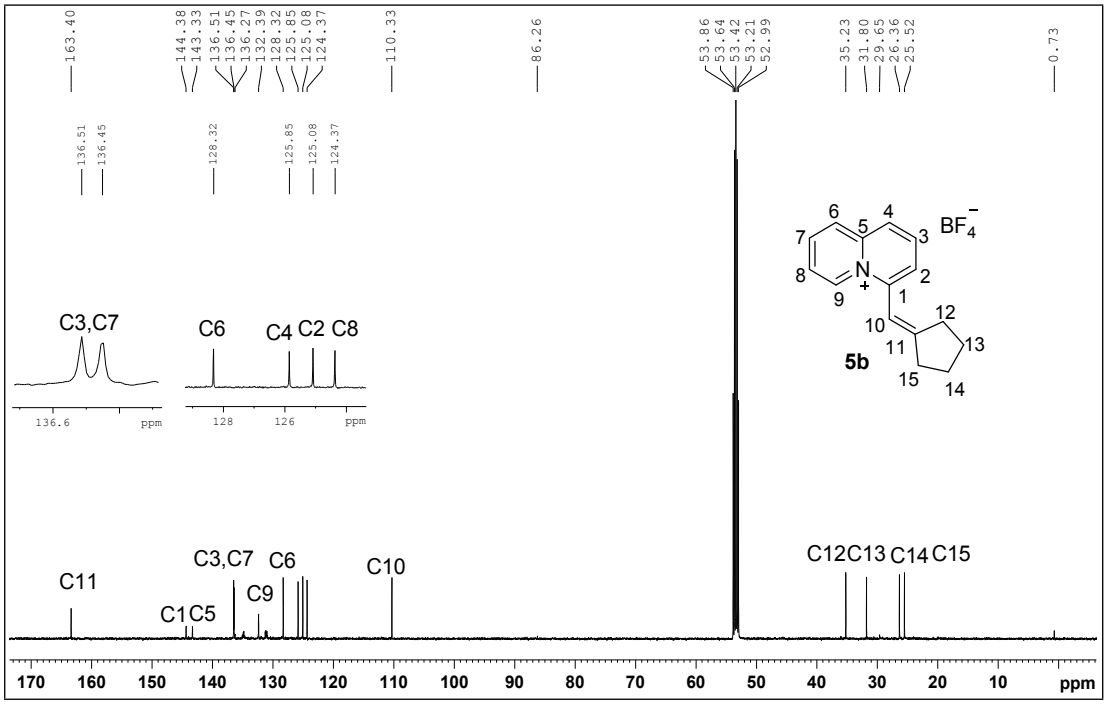


Figure S20 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum of complex **5b**.

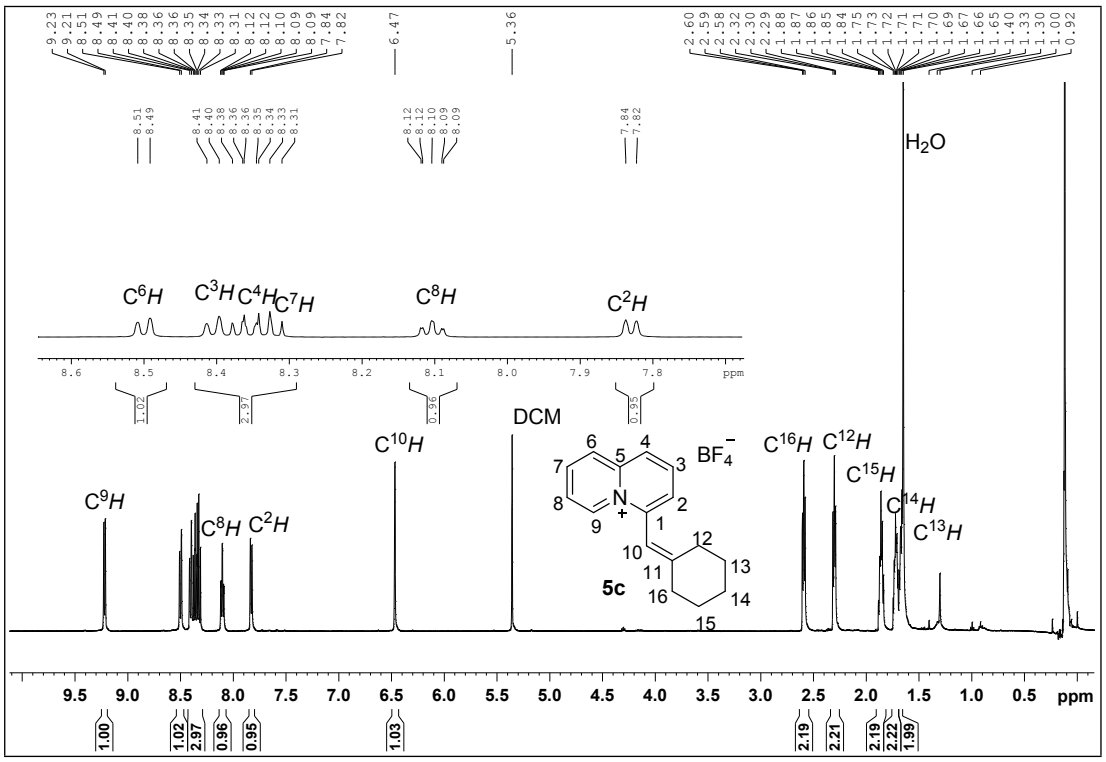


Figure S21 The ^{1}H NMR (500.2 MHz, CD_2Cl_2) spectrum of complex **5c**.

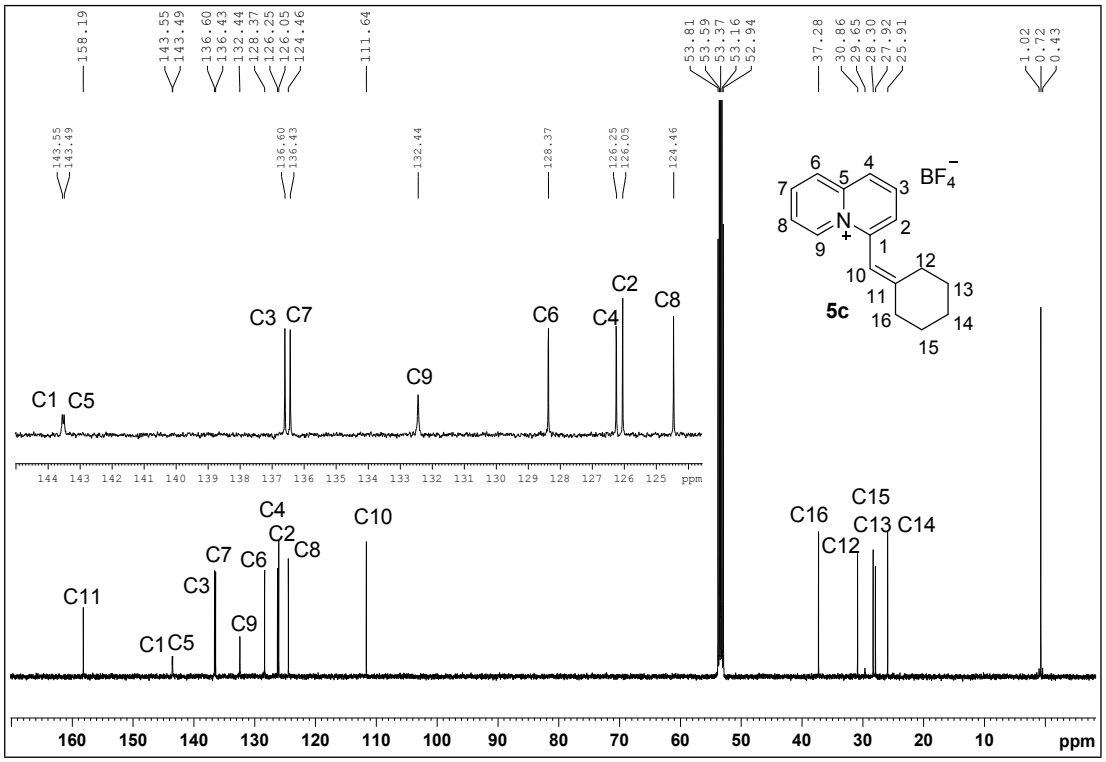


Figure S22 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2) spectrum of complex **5c**.

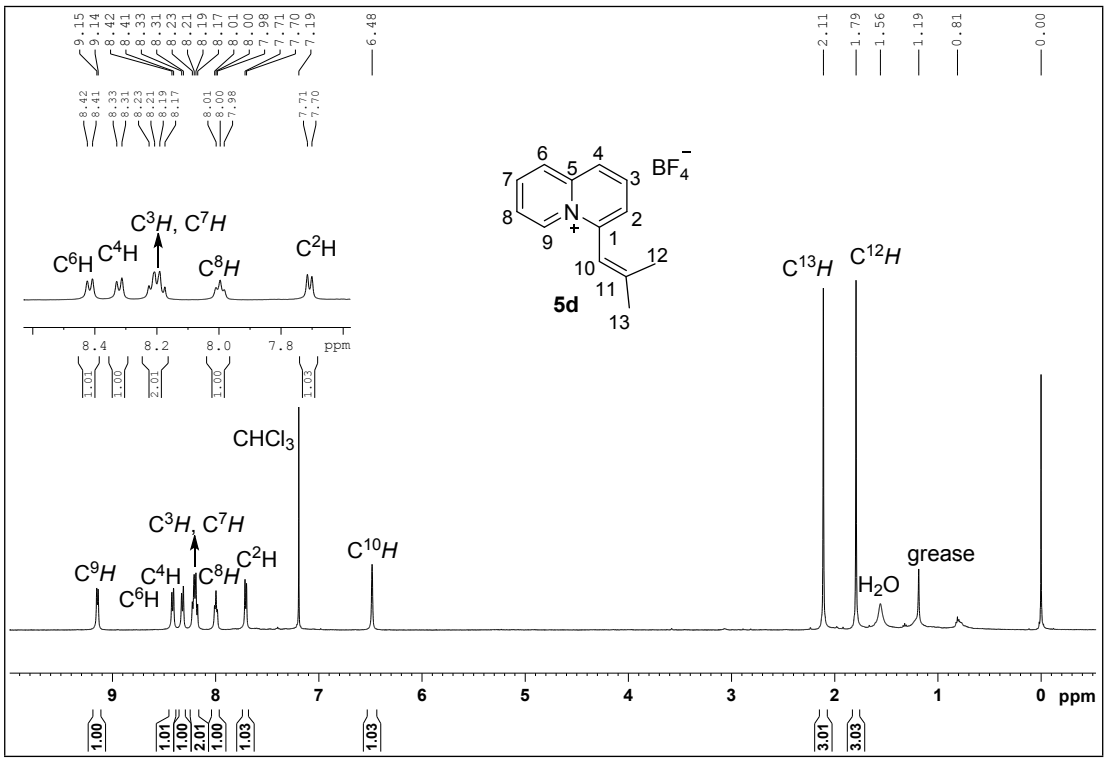


Figure S23 The ^{1}H NMR (500.2 MHz, $CDCl_3$) spectrum of complex **5d**.

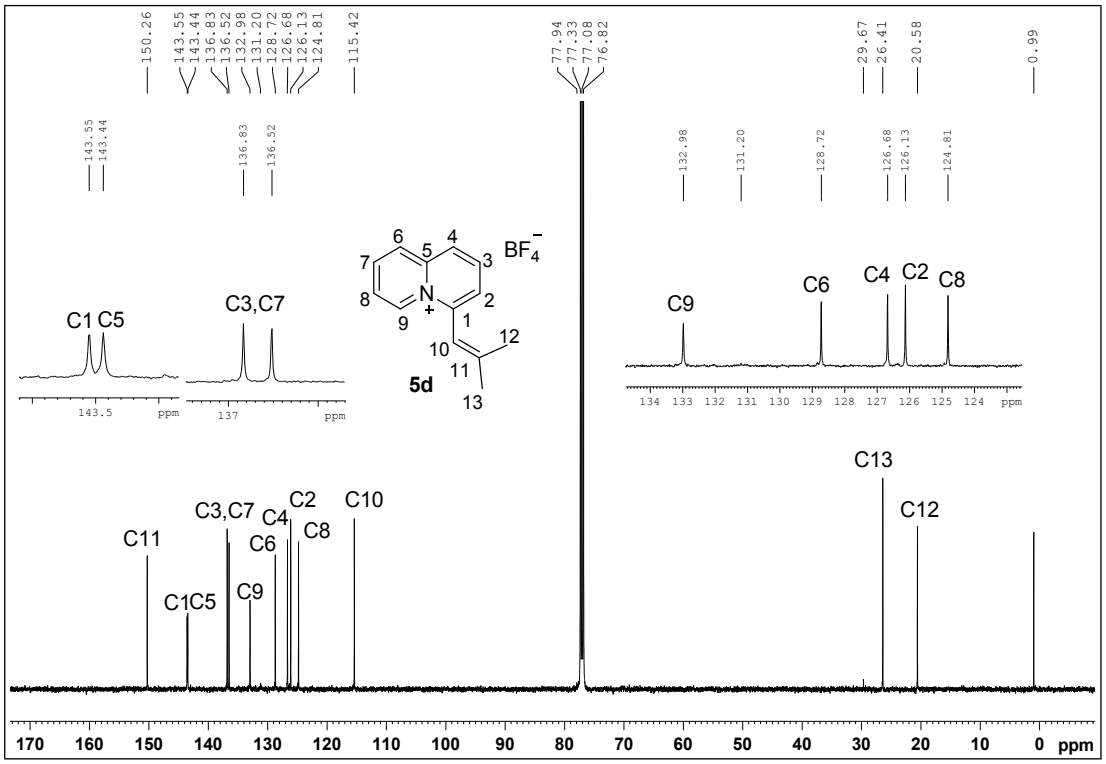


Figure S24 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$) spectrum of complex **5d**.

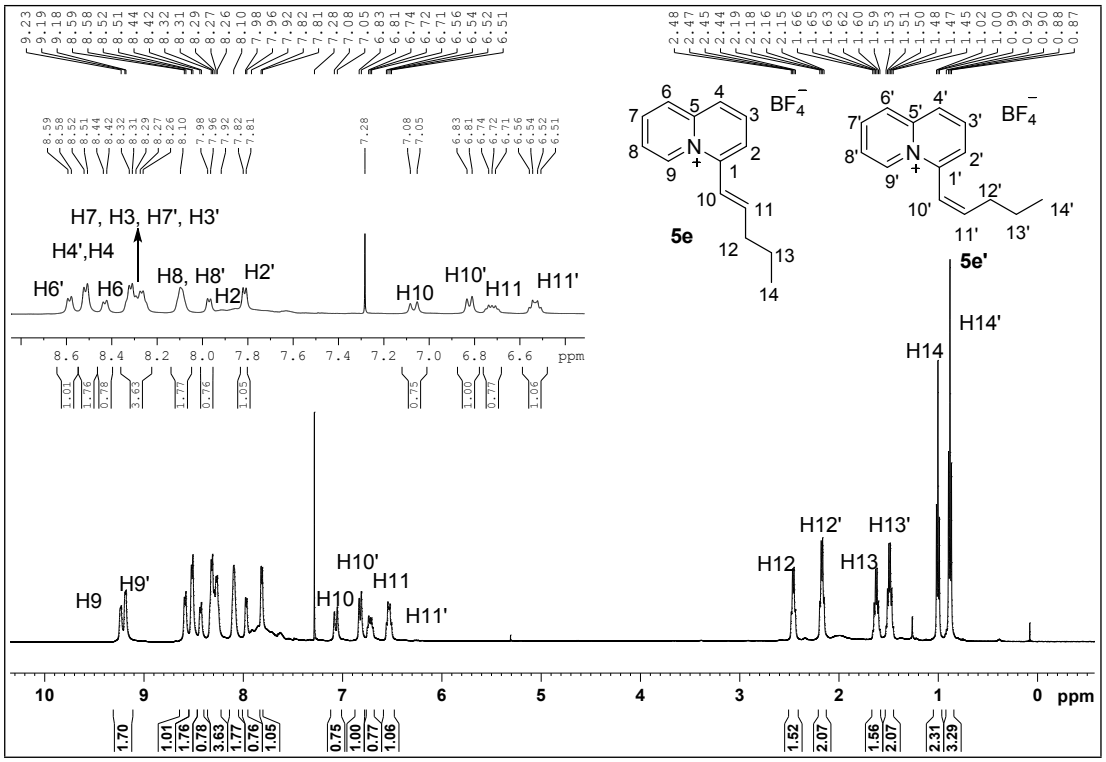


Figure S25 The ^{1}H NMR (500.2 MHz, $CDCl_3$) spectrum of complex **5e/e′**.

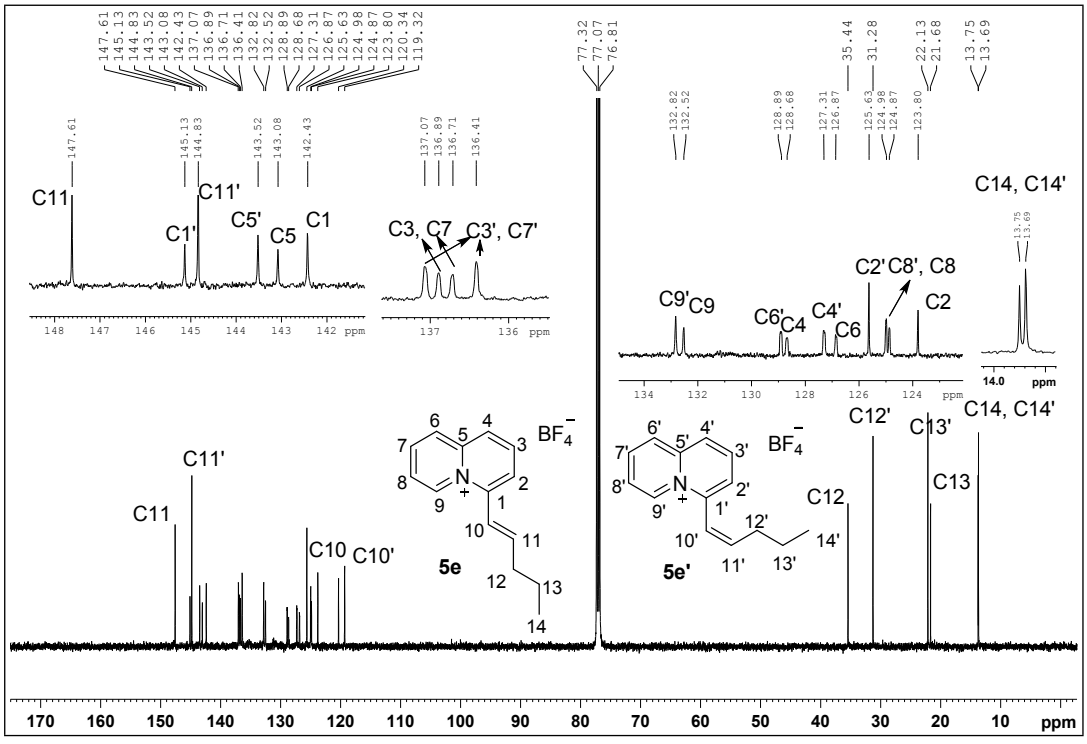
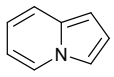


Figure S26 The $^{13}C\{^{1}H\}$ NMR (125.8 MHz, $CDCl_3$) spectrum of complex **5e/e′**.

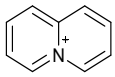
9. Cartesian coordinates together with the symmetry and electronic energies for all the complexes calculated in this study.



I

Symmetry = C_1 E = -363.7914065 a.u.

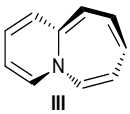
N	0.27871900	-0.66451000	-0.00009200
C	2.41198100	-0.00495600	0.00013300
C	1.57858200	-1.11239400	-0.00010800
C	1.61487000	1.15913300	0.00047200
H	1.95617100	2.18507200	0.00055300
C	-0.97209000	1.41526000	-0.00034400
H	-0.97826200	2.50105000	-0.00028400
C	0.28102200	0.75271000	-0.00053500
C	-0.89744600	-1.38219000	0.00014900
H	-0.79329000	-2.46135100	0.00019600
C	-2.14042300	0.69596900	-0.00000100
H	-3.09975700	1.20365100	0.00042100
C	-2.09593000	-0.73170100	0.00029500
H	-3.01085300	-1.31421500	0.00036000
H	3.49356300	-0.04347700	0.00060500
H	1.79799400	-2.17015400	-0.00157300



II

Symmetry = C_1 E = -402.2924033 a.u.

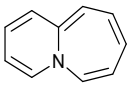
N	0.00001900	-0.66515100	0.00011300
C	1.19602700	-1.36422500	-0.00033400
C	2.39443200	-0.71254000	-0.00028400
H	3.30860300	-1.29539300	-0.00084400
C	0.00003800	0.72844100	0.00001000
C	-1.19624400	-1.36436000	0.00035900
H	-1.10268900	-2.44309700	0.00041700
C	-2.39438700	-0.71254800	0.00021000
H	-3.30871800	-1.29517800	0.00076900
C	-1.24556300	1.40158200	-0.00026300
H	-1.22926500	2.48602100	-0.00038200
C	2.42822600	0.70336800	0.00025600
H	3.37859000	1.22637800	0.00102700
C	1.24553500	1.40146300	0.00021800
H	1.22945200	2.48590300	0.00036900
C	-2.42811700	0.70350200	-0.00031400
H	-3.37859400	1.22630400	-0.00066800
H	1.10280300	-2.44297800	-0.00061800



III

Symmetry = C_1 E = -441.145942 a.u.

N	0.23633200	-0.63539700	-0.05198700
C	-2.17317200	1.18912900	-0.35975100
C	-0.84964400	1.56193300	0.07661700
H	-0.67496700	2.62251900	0.23665600
C	0.27025500	0.77218100	0.15539700
C	1.59395900	1.32428700	0.36566000
H	1.65707400	2.35173900	0.71101000
C	-0.84590300	-1.42439300	0.50106800
C	2.71427900	0.61010100	0.07448900
H	3.69476300	1.06145400	0.20118500
C	-2.74808500	-0.04005100	-0.35263800
H	-3.76317900	-0.15048600	-0.72513500
C	1.38090200	-1.32411700	-0.37783200
H	1.22263500	-2.37627000	-0.59414600
C	2.61234300	-0.74600800	-0.38660200
H	3.48596700	-1.31881500	-0.67223600
C	-2.14857700	-1.19450400	0.30565400
H	-2.82951600	-1.90414400	0.77657500
H	-2.77532300	2.01565300	-0.73814600
H	-0.50991000	-2.22521100	1.15578400

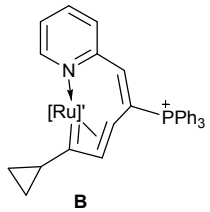


III-constr

Symmetry = C_s E = -441.142129 a.u.

N	0.00000000	0.74177300	0.00000000
C	-0.14765200	-1.76241000	0.00000000
H	0.50056800	-2.63353700	0.00000000
C	0.54486000	-0.57769900	0.00000000
C	1.99673800	-0.61715700	0.00000000
H	2.44302300	-1.60609700	0.00000000

C	2.78033100	0.49146700	0.00000000
H	3.86226300	0.39171900	0.00000000
C	0.82110500	1.84794200	0.00000000
H	0.29586000	2.79585300	0.00000000
C	2.17850900	1.79099200	0.00000000
H	2.76408600	2.70149000	0.00000000
C	-1.41580800	1.03898200	0.00000000
C	-2.48966500	0.24249600	0.00000000
H	-3.42929900	0.79133200	0.00000000
C	-2.61113900	-1.21883000	0.00000000
H	-3.62121500	-1.61695400	0.00000000
C	-1.56532100	-2.06798600	0.00000000
H	-1.78969300	-3.13367700	0.00000000
H	-1.57734400	2.11067700	0.00000000

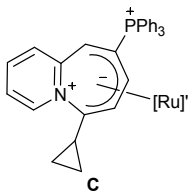


B

[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1382.3942135 a.u.

Ru	2.41670764	-0.59298638	0.63988472
Cl	3.06219886	0.22320112	2.74371132
Cl	2.51564334	-2.81793238	1.33569085
P	-2.12846457	-0.00424963	-0.09213435
N	2.39822905	1.57798804	0.17497890
C	0.52783364	-0.82340519	-0.18965271
H	-0.00315642	-1.67894185	0.23166694
C	1.34303291	2.28803467	-0.29536883
C	-0.33040612	0.38378538	-0.27144888
C	0.01476601	1.68618301	-0.37943006
H	-0.77905329	2.41831468	-0.49672255
C	3.57901584	2.20154029	0.32105825
H	4.37863560	1.60559663	0.74340800
C	1.47702419	3.64438787	-0.63243519
H	0.60958886	4.18698249	-0.99454767
C	3.78094618	3.54087818	-0.00905325
H	4.76047480	3.98387529	0.13405459
C	2.70786031	4.27886289	-0.50048620
H	2.82148177	5.32579520	-0.76390394
C	2.74775794	-0.69397676	-1.22695903
C	1.48583281	-1.29365324	-1.19683772
C	3.84588509	-0.62109872	-2.14465141
C	3.85984767	-1.54778236	-3.38072556
C	3.60593868	-0.10355169	-3.57931404
H	4.81396136	-0.39392532	-1.70864120
H	3.03474588	-2.24422270	-3.48575404
H	4.83413010	-1.95609366	-3.62995887
H	4.39455703	0.52275092	-3.98511357
H	2.59616000	0.21640439	-3.81718991
C	-2.50213073	-1.35927723	-1.26028180
C	-3.22963400	-2.48986260	-0.86201629
C	-2.03605110	-1.25143867	-2.58313225
C	-3.49988011	-3.49884024	-1.78781059
H	-3.57212001	-2.59482772	0.16160464
C	-2.31594285	-2.26251718	-3.50063368
H	-1.44886101	-0.39094174	-2.89240481
C	-3.04898177	-3.38482524	-3.10385235
H	-4.05843319	-4.37586678	-1.47578713
H	-1.95671550	-2.17780801	-4.52181219
H	-3.26113319	-4.17334983	-3.81964729
C	-2.45331481	-0.50325100	1.63357374
C	-3.79048485	-0.69814562	2.03060298
C	-1.41057404	-0.67368319	2.55842764
C	-4.07242010	-1.08473703	3.33884753
H	-4.60606144	-0.53696783	1.33102216
C	-1.70837821	-1.05871768	3.86701973
H	-0.37424044	-0.50710241	2.28500657
C	-3.03205224	-1.26892458	4.25522389
H	-5.10349439	-1.23559570	3.64380846
H	-0.89778998	-1.19132088	4.57662511
H	-3.25661915	-1.56930962	5.27431964
C	-3.17507283	1.45074741	-0.45232641
C	-3.83714260	1.58543982	-1.68249329
C	-3.30153200	2.45128273	0.52906162
C	-4.61466630	2.71749915	-1.92860972
H	-3.76298190	0.81055793	-2.43789284
C	-4.07667258	3.58044075	0.26986528
H	-2.81139109	2.34295262	1.49203769
C	-4.73260908	3.71390551	-0.95727924
H	-5.13368366	2.81542965	-2.87718946
H	-4.17640829	4.34932755	1.02995668
H	-5.34251397	4.59101955	-1.15220613
H	1.43506392	-2.35486920	-1.46563355

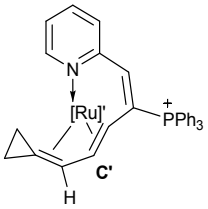


C

[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1382.4112795 a.u.

Ru	-1.42698408	1.01764437	0.32055822
Cl	-0.98043000	1.72340580	2.50985914
Cl	-2.02053822	3.25163723	-0.29894500
P	1.80799866	-0.18391664	-0.21284504
N	-2.90961925	-1.59850807	-0.02859290
C	-0.70982549	0.02682926	-1.49534230
H	-0.10679650	0.45620102	-2.29143548
C	-1.81378286	-1.98011820	0.67674498
C	-0.04119413	-0.40456457	-0.28050944
C	-0.76180822	-0.97913992	0.84005854
H	-0.19167322	-1.10470263	1.75408632
C	-3.93097107	-2.45539445	-0.27784746
H	-4.75024045	-2.05763499	-0.85955146
C	-1.77756818	-3.26730904	1.22480384
H	-0.91279122	-3.55454272	1.81260330
C	-3.91676014	-3.74126890	0.22737358
H	-4.75320386	-4.40053291	0.02639196
C	-2.83058382	-4.14820737	1.01134961
H	-2.80716609	-5.14426032	1.44246963
C	-2.97351013	-0.15506763	-0.48193993
C	-2.10743695	0.18967384	-1.59278588
C	-4.38068092	0.35231424	-0.40080139
C	-4.84340282	1.60297559	-1.09797826
C	-5.35187634	0.28399625	-1.59179755
H	-4.82285703	0.17210229	0.57726384
H	-4.12351822	2.15373846	-1.69260305
H	-5.51420453	2.24259733	-0.53320999
H	-6.38220090	0.00271172	-1.38859455
H	-4.96572403	-0.08423748	-2.53995570
C	2.44190135	-1.06558020	-1.68530741
C	3.42564760	-0.48416947	-2.49887424
C	1.93304802	-2.33923930	-1.99875965
C	3.89867320	-1.17695749	-3.61477197
H	3.81792516	0.50092190	-2.26984472
C	2.41453179	-3.02347286	-3.11296063
H	1.16439408	-2.79423080	-1.38010126
C	3.39669469	-2.44262898	-3.92121251
H	4.65790788	-0.72316277	-4.24427540
H	2.02139573	-4.00670665	-3.35317931
H	3.76679072	-2.97674074	-4.79122777
C	2.37619306	1.55097942	-0.23468380
C	3.68750803	1.79554778	0.21850392
C	1.58349363	2.61042328	-0.70075099
C	4.19453886	3.09284199	0.19653011
H	4.30417567	0.98622763	0.59711074
C	2.09910636	3.90719938	-0.70070800
H	0.55787546	2.46567703	-1.01937986
C	3.40009739	4.14906601	-0.25948033
H	5.20421275	3.27922688	0.54957440
H	1.46636370	4.72419150	-1.03225151
H	3.79372586	5.16115770	-0.25898615
C	2.44926559	-0.95620903	1.31200509
C	3.21990820	-2.12762189	1.26177092
C	2.17660277	-0.33344920	2.54514778
C	3.71295726	-2.67817612	2.44609428
H	3.44683817	-2.60200059	0.31279288
C	2.67037863	-0.89970703	3.71949957
H	1.57357663	0.57011186	2.59401177
C	3.43838795	-2.06719371	3.67121875
H	4.31693380	-3.57972311	2.40757808
H	2.45678389	-0.42279714	4.67114514
H	3.82678548	-2.49757835	4.58965188
H	-2.47139470	0.81197795	-2.40489511

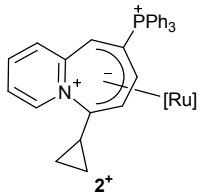


[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1382.3878622 a.u.

Ru	2.64538074	-0.60233103	0.25997941
Cl	3.07604626	0.05788583	2.49691235
Cl	3.72882106	-2.63340924	0.78338980
P	-2.10995196	-0.06455759	0.01018716
N	2.43558465	1.54358892	0.02450272
C	0.57558360	-0.77144445	0.33460359
H	0.26252966	-1.16985407	1.30278555
C	1.32499356	2.26990832	-0.23844028
C	-0.30831865	0.35008881	-0.09031976

C	0.01360179	1.63483003	-0.33791719
H	-0.78190980	2.32872166	-0.59514952
C	3.61022207	2.18642683	0.15214516
H	4.47069366	1.56965692	0.38657194
C	1.39180651	3.66463322	-0.39004796
H	0.48169820	4.21678087	-0.60162551
C	3.74427015	3.56538445	0.01235082
H	4.72199619	4.02022071	0.12662529
C	2.60958276	4.32382273	-0.26566004
H	2.67052518	5.40138304	-0.38065304
C	1.99694560	-1.69339234	-1.57479187
C	1.08645813	-1.84864360	-0.49491239
C	2.52009575	-0.45077669	-1.96543894
C	3.47935532	-0.11612516	-3.04329193
C	2.16699757	0.65183942	-2.90557163
C	-2.34606340	-1.69026189	-0.78761917
C	-2.99459246	-2.74461351	-0.12893715
C	-1.84216577	-1.87725324	-2.08810064
C	-3.15218522	-3.97156995	-0.77600023
H	-3.36427743	-2.62158679	0.88291505
C	-2.00947963	-3.10456889	-2.72665570
H	-1.30875726	-1.07721182	-2.59398574
C	-2.66625148	-4.15079435	-2.07194925
H	-3.65067166	-4.78737297	-0.26174148
H	-1.62018856	-3.24682514	-3.73016024
H	-2.79033590	-5.10754692	-2.57020393
C	-2.59530626	-0.10578386	1.77273349
C	-3.94735278	-0.34112707	2.08715200
C	-1.66629779	0.13483143	2.79779999
C	-4.35413520	-0.36381972	3.41944982
H	-4.68057987	-0.49373882	1.30010058
C	-2.08780810	0.11142150	4.12880831
H	-0.62508294	0.34998186	2.58133001
C	-3.42420119	-0.14270623	4.44004064
H	-5.39682724	-0.54793490	3.65954192
H	-1.36552602	0.29392465	4.91830232
H	-3.74493241	-0.16120949	5.47728880
C	-3.15014006	1.20470809	-0.80145499
C	-3.67766967	1.00982940	-2.08741282
C	-3.41583165	2.40001954	-0.10765281
C	-4.45493319	2.00833335	-2.67520471
H	-3.50480813	0.08303367	-2.62318011
C	-4.18914055	3.39297540	-0.70709632
H	-3.03885761	2.54791845	0.90001346
C	-4.70770780	3.19860643	-1.99020477
H	-4.86900446	1.85020982	-3.66630628
H	-4.39636833	4.31167008	-0.16675392
H	-5.31675415	3.97049544	-2.45107787
H	1.02698747	-2.85318778	-0.08509903
H	2.55717393	-2.59265505	-1.82144740
H	2.23778783	1.69042049	-2.59957502
H	1.36911001	0.45574852	-3.61924978
H	4.38163496	0.43112532	-2.77876186
H	3.61344266	-0.82113102	-3.86148081



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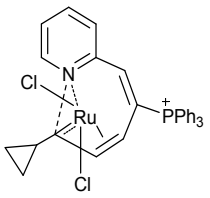
[Ru] = $RuCl_2(PPh_3)$

Symmetry = C_1 E = -2083.8777023 a.u.

Ru	0.41713400	0.12530800	-0.94311600
Cl	-0.33468800	-2.22450700	-0.61486000
Cl	1.39588200	-0.50796000	-3.10974100
P	-3.12324100	-0.24966400	-0.05993900
N	0.52826300	2.96171300	0.21625200
C	-1.38961300	1.31628800	-1.57879600
H	-2.11904400	1.10872900	-2.35410200
C	-0.14015700	2.24031400	1.16281100
C	-1.52897800	0.69530100	-0.29993200
C	-0.60722900	0.89874200	0.80429300
H	-0.76969100	0.26261500	1.66887300
C	0.92916900	4.23404600	0.46627800
H	1.42725500	4.73552300	-0.35049700
C	-0.33018500	2.80181900	2.43047900
H	-0.83046100	2.20242100	3.18322800
C	0.73734600	4.82501900	1.70179000
H	1.08816200	5.83756000	1.86459900
C	0.11686000	4.08745900	2.71325000
H	-0.02231600	4.51210400	3.70266500
C	0.89496900	2.29702400	-1.08881000
C	-0.18233600	1.94820800	-1.96373600
C	2.13507200	2.90755700	-1.67282800
C	2.55117800	2.72547600	-3.10666500
C	2.07743500	4.07885100	-2.66479200
H	2.95940400	2.94304800	-0.96836900
H	1.92980000	2.12564200	-3.76122100

H	3.61382100	2.58136800	-3.27341700
H	2.80259700	4.88249900	-2.55819400
H	1.09607800	4.40480300	-3.00367200
C	-4.36216700	1.11552900	-0.15926300
C	-5.54733200	0.96426300	-0.89340900
C	-4.11224200	2.32964200	0.50665800
C	-6.47265700	2.00873200	-0.94986400
H	-5.75041900	0.04361100	-1.42831900
C	-5.04289400	3.36539600	0.44872600
H	-3.19324800	2.47304100	1.06690900
C	-6.22540600	3.20631600	-0.27898600
H	-7.38528400	1.88254400	-1.52444000
H	-4.84261300	4.29839100	0.96730900
H	-6.94724200	4.01623200	-0.32639000
C	-3.56828200	-1.49245300	-1.32482600
C	-4.68833100	-2.29645600	-1.04516600
C	-2.88650800	-1.63293300	-2.54286100
C	-5.13072600	-3.22199300	-1.98980300
H	-5.20836400	-2.21290600	-0.09539300
C	-3.34243200	-2.56075800	-3.47907000
H	-1.98148600	-1.07668400	-2.75047200
C	-4.46118600	-3.35069300	-3.20850500
H	-5.99177000	-3.84498200	-1.76737300
H	-2.80261800	-2.67694200	-4.41364400
H	-4.80383400	-4.07557900	-3.94102600
C	-3.26100400	-1.00914500	1.60499200
C	-3.94972900	-0.34417100	2.63366000
C	-2.72829800	-2.29061600	1.83087600
C	-4.08883900	-0.95117100	3.88212600
H	-4.39606500	0.62915900	2.46383600
C	-2.88291300	-2.88965300	3.08111100
H	-2.18778000	-2.80197100	1.04206100
C	-3.55790500	-2.22282700	4.10691100
H	-4.62656100	-0.43490400	4.67180800
H	-2.47823000	-3.88358900	3.24777200
H	-3.67878600	-2.69759600	5.07641600
H	-0.01879200	2.02696400	-3.03431000
P	2.47263800	-0.69216000	0.20864400
C	3.25761200	-2.31333700	-0.27405300
C	2.84173700	-3.04262800	-1.39477100
C	4.31498000	-2.80213500	0.51358500
C	3.48063400	-4.24276400	-1.72010400
H	2.03410400	-2.67432100	-2.01217400
C	4.94593200	-3.99937400	0.18259800
H	4.64898900	-2.25743800	1.39067100
C	4.52853800	-4.72408500	-0.93692500
H	3.14969100	-4.79918300	-2.59250400
H	5.76082400	-4.36594300	0.80073500
H	5.01923300	-5.65890800	-1.19408300
C	3.89349500	0.49910500	0.05378000
C	4.00339700	1.62919600	0.88138300
C	4.84546300	0.30927400	-0.95917400
C	5.06174500	2.52708400	0.72521800
H	3.26931800	1.80407300	1.66268000
C	5.89302000	1.21809200	-1.12519400
H	4.77162400	-0.54987000	-1.61715700
C	6.01044400	2.32323900	-0.28008700
H	5.14704000	3.38191400	1.39124500
H	6.62431300	1.05265900	-1.91133900
H	6.83684800	3.01807800	-0.40022600
C	2.26466400	-0.91326400	2.05917100
C	1.09683700	-1.53904800	2.52691400
C	3.26071200	-0.57535400	2.99059500
C	0.91953700	-1.78891400	3.88850700
H	0.34318800	-1.85963200	1.81530400
C	3.07906800	-0.82699200	4.35317200
H	4.18875400	-0.12010200	2.66483400
C	1.90585500	-1.42782600	4.80852000
H	0.00871400	-2.27566000	4.22683300
H	3.86397900	-0.55795900	5.05482100
H	1.76777500	-1.62533900	5.86801500

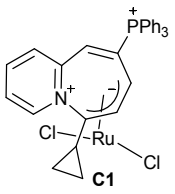


B-C1-TS

Symmetry = C_1 E = -1382.3631702 a.u.

Ru	-2.19432400	-1.15945800	-0.81927300
Cl	-1.81917900	0.17544100	-2.70393000
Cl	-2.62797700	-3.35159000	-0.19229400
P	2.05081000	-0.01527000	0.20546800
N	-2.51695200	1.95102300	0.28744500
C	-0.61378100	-0.73962200	0.51844500
H	-0.04496600	-1.64149000	0.74685200
C	-1.29547300	2.48919600	0.04327700
C	0.24745700	0.42660400	0.24939000

C	-0.04096400	1.74260600	0.09011400
H	0.80491800	2.40056500	-0.07824800
C	-3.59867400	2.73089600	0.18456000
H	-4.54838100	2.25532500	0.38933300
C	-1.17981500	3.85408300	-0.28889100
H	-0.19394400	4.26893400	-0.47142400
C	-3.55087400	4.08161500	-0.15296900
H	-4.47018400	4.65320100	-0.21970100
C	-2.30737600	4.65799400	-0.39380100
H	-2.21583400	5.70666800	-0.65865900
C	-2.97581200	-0.07954700	0.55921400
C	-1.89456200	-0.73976600	1.20049800
C	-4.38350200	-0.02158900	0.95952900
C	-4.89088200	-0.99496700	2.02705500
C	-4.81729300	0.46055400	2.34243300
H	-5.07718300	0.14637400	0.13965300
H	-4.18079400	-1.67276100	2.48746800
H	-5.85884100	-1.44206900	1.82441800
H	-5.73931600	1.03195200	2.40642600
H	-4.02910400	0.79845800	3.00992500
C	2.37772900	-0.90015000	1.77529200
C	3.00759000	-2.15267800	1.80232100
C	1.94848300	-0.30381100	2.97564600
C	3.22313000	-2.79240100	3.02444400
H	3.31683400	-2.63689800	0.88291700
C	2.17352200	-0.94867300	4.19023900
H	1.42968700	0.65098600	2.96225000
C	2.81307600	-2.19165300	4.21532600
H	3.70680600	-3.76418600	3.04101900
H	1.84272300	-0.48535500	5.11482800
H	2.98242800	-2.69435600	5.16281500
C	2.45954200	-1.05035700	-1.23848400
C	3.79532500	-1.46699800	-1.40322300
C	1.49494800	-1.37231200	-2.20294900
C	4.14563200	-2.23398900	-2.51125000
H	4.55792400	-1.18543100	-0.68243600
C	1.86235900	-2.13634700	-3.31326900
H	0.47510100	-1.01395500	-2.11951200
C	3.17813100	-2.57382100	-3.46318400
H	5.17410900	-2.55870100	-2.63644600
H	1.11286100	-2.37941400	-4.06004800
H	3.45684500	-3.16984800	-4.32712900
C	3.10523300	1.47686600	0.09297100
C	3.78565600	1.98726900	1.20874600
C	3.23150400	2.10860600	-1.15832000
C	4.58036200	3.12641500	1.07260000
H	3.71380900	1.49579900	2.17270200
C	4.02200800	3.24989800	-1.28074800
H	2.72605900	1.70684200	-2.03174800
C	4.69621300	3.75870500	-0.16677700
H	5.11348900	3.51388300	1.93542300
H	4.11992600	3.73382500	-2.24777300
H	5.31851200	4.64292600	-0.26802500
H	-2.07842500	-1.49444200	1.96540600

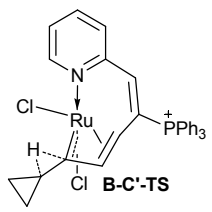


C1

Symmetry = C_1 E = -1382.3790929 a.u.

Ru	-2.11694000	-1.14920700	-0.83570100
Cl	-1.92332600	0.52708800	-2.51424000
Cl	-2.38195400	-3.41019000	-0.30824300
P	2.07937200	0.01598800	0.19013500
N	-2.68108600	1.57191200	0.39993000
C	-0.56451400	-0.83218900	0.57593600
H	-0.03702200	-1.75946700	0.79176500
C	-1.46111200	2.23131200	0.39923000
C	0.26564500	0.34166400	0.39288700
C	-0.14024400	1.63965300	0.41997500
H	0.62869100	2.39916000	0.34444400
C	-3.80373200	2.29319300	0.09956500
H	-4.71630800	1.72829000	0.03461700
C	-1.46567300	3.63681600	0.26280300
H	-0.50776400	4.14168500	0.31097000
C	-3.81288300	3.65626700	-0.09157000
H	-4.75234600	4.14518400	-0.32184700
C	-2.61597400	4.36377000	0.03065200
H	-2.58057800	5.44229300	-0.08040600
C	-2.90269400	0.10747500	0.62490400
C	-1.88418600	-0.77252400	1.15340300
C	-4.33725000	-0.22372700	0.98525400
C	-4.71854600	-1.12773200	2.13446700
C	-5.03036700	0.33779100	2.22329600
H	-4.98380100	-0.34366500	0.11656500
H	-3.94916700	-1.51668800	2.79230600
H	-5.52803500	-1.82672500	1.94969900

H	-6.06060400	0.67110200	2.13029300
H	-4.42953200	0.93100700	2.90842200
C	2.53036800	-1.14506000	1.52925800
C	3.21451200	-2.33989500	1.26437100
C	2.14894500	-0.82945000	2.84680500
C	3.53249800	-3.20148900	2.31595600
H	3.48620500	-2.60869700	0.24979400
C	2.47539600	-1.69456600	3.88889200
H	1.58808400	0.07721300	3.05763200
C	3.16994300	-2.87881400	3.62422900
H	4.05761700	-4.12839200	2.10727900
H	2.18020000	-1.44923000	4.90452800
H	3.41807400	-3.55378000	4.43780400
C	2.45276900	-0.67953300	-1.45210200
C	3.80084000	-0.94504100	-1.76481000
C	1.44768800	-0.89604800	-2.40449500
C	4.12710100	-1.45994900	-3.01646500
H	4.58921700	-0.74279300	-1.04510000
C	1.79201000	-1.40546800	-3.65899400
H	0.41206800	-0.64745700	-2.19893400
C	3.12222600	-1.69530400	-3.96156500
H	5.16484900	-1.66972400	-3.25720300
H	1.01138900	-1.56559500	-4.39617000
H	3.38234200	-2.09410400	-4.93761100
C	3.04014100	1.56760400	0.33934200
C	3.74099400	1.89484600	1.50980600
C	3.07162700	2.43714600	-0.76687900
C	4.46001600	3.08929000	1.57412700
H	3.74450800	1.22085100	2.35935400
C	3.78770000	3.63056600	-0.68862800
H	2.55445000	2.17835000	-1.68633400
C	4.48130400	3.95686100	0.48040200
H	5.00947200	3.33569900	2.47755100
H	3.81422300	4.29780500	-1.54482300
H	5.04624600	4.88277700	0.53408300
H	-2.17763800	-1.55524800	1.84254800

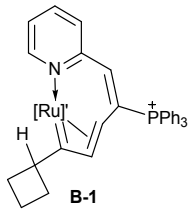


B-C'-TS

Symmetry = C_1 E = -1382.312837 a.u.

Ru	-2.48016300	-0.56719600	-0.62836400
Cl	-2.45182000	0.07831300	-2.91428600
Cl	-3.20397000	-2.76169100	-1.17355200
P	2.12489100	-0.03585900	0.10224200
N	-2.36095500	1.53515400	-0.22329200
C	-0.52590300	-0.86426300	0.01683000
H	-0.01487000	-1.61104500	-0.59308900
C	-1.34735900	2.21821000	0.36769400
C	0.32286700	0.31806300	0.29704300
C	-0.03621200	1.60062500	0.53222000
H	0.74335800	2.31245100	0.78922200
C	-3.49132900	2.20146500	-0.52452700
H	-4.25421500	1.62905300	-1.04064700
C	-1.49517700	3.57109000	0.71940100
H	-0.66783200	4.08403400	1.19984200
C	-3.69296500	3.54383100	-0.21691100
H	-4.62754300	4.02011800	-0.49240600
C	-2.67881400	4.24198500	0.43735900
H	-2.80071600	5.28691700	0.70484100
C	-2.60614300	-0.80160600	1.38893700
C	-1.44845300	-1.51950000	0.92549400
C	-3.24462800	-0.57430500	2.57980500
C	-3.26606500	-0.64479400	4.04902100
C	-4.43032300	-0.02815800	3.25516000
H	-3.56835100	-1.54495200	1.53969700
H	-2.58329100	0.00822500	4.59153100
H	-3.43781800	-1.60804800	4.52476800
H	-5.36621500	-0.58316200	3.22787000
H	-4.55235900	1.05367900	3.24850000
C	2.47803700	-1.59506500	0.98852800
C	3.21071200	-2.62764300	0.38622700
C	1.98729400	-1.75085200	2.29725700
C	3.46209300	-3.80242700	1.09686600
H	3.57099900	-2.52817800	-0.63186300
C	2.24793100	-2.92600700	2.99971800
H	1.39515800	-0.96602000	2.76011800
C	2.98626800	-3.95077800	2.40057100
H	4.02445500	-4.60289100	0.62619800
H	1.86903000	-3.04532600	4.01028500
H	3.18258100	-4.86768100	2.94819900
C	2.47754600	-0.19032200	-1.68289800
C	3.81985400	-0.30759400	-2.09342700
C	1.44508000	-0.17705400	-2.63514200
C	4.11811600	-0.43349000	-3.44824000

H	4.62633700	-0.28762800	-1.36563200
C	1.76058600	-0.30301700	-3.98965900
H	0.40174600	-0.06360600	-2.35798900
C	3.08881200	-0.43555100	-4.39560800
H	5.15303000	-0.52394300	-3.76407600
H	0.95570700	-0.29447500	-4.71790000
H	3.32634000	-0.53355000	-5.45076000
C	3.16575900	1.31551100	0.76245600
C	3.77621500	1.21371800	2.02221500
C	3.34231600	2.47597000	-0.01350200
C	4.55151500	2.26942500	2.50245300
H	3.66531700	0.31456600	2.61865200
C	4.11529200	3.52661900	0.47880700
H	2.89490300	2.55149500	-1.00007100
C	4.71913900	3.42411800	1.73509300
H	5.03106600	2.18436000	3.47283400
H	4.25472700	4.41897600	-0.12383400
H	5.32794400	4.24094000	2.11125000
H	-1.49293100	-2.60766000	0.89970300



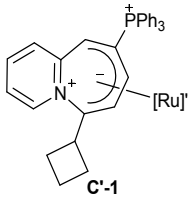
B-1

[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1421.7048116a.u.

Ru	2.17960500	-0.85566300	0.54895000
Cl	2.76518600	-0.66817600	2.80953700
Cl	2.18177600	-3.18208400	0.60373500
P	-2.31984500	0.05827700	-0.18192800
N	2.21171300	1.37129400	0.72067000
C	0.32985100	-0.76837100	-0.38087000
H	-0.23688300	-1.69313500	-0.25459900
C	1.19196900	2.21548900	0.42667800
C	-0.51003300	0.43263100	-0.15370700
C	-0.14089200	1.70260300	0.12109400
H	-0.91541000	2.46179000	0.17912000
C	3.38986900	1.89639500	1.09709000
H	4.15785800	1.18432800	1.37099100
C	1.36203500	3.60773700	0.49545400
H	0.52180000	4.25415300	0.26307400
C	3.62702400	3.26808300	1.17257600
H	4.60284000	3.62457300	1.48389500
C	2.59214900	4.14493800	0.85941600
H	2.73346000	5.22003900	0.90965900
C	2.60462900	-0.46700900	-1.26036200
C	1.31494400	-0.94561400	-1.46092500
H	1.21949400	-1.85000900	-2.07487100
C	-2.64058400	-0.90607000	-1.70035000
C	-3.39179600	-2.08973200	-1.67133300
C	-2.10375500	-0.44060900	-2.91462000
C	-3.61474600	-2.79470900	-2.85523200
H	-3.78896800	-2.46996900	-0.73653600
C	-2.33706700	-1.14988800	-4.09137100
H	-1.49711700	0.46068600	-2.94066800
C	-3.09323100	-2.32543300	-4.06200400
H	-4.19168800	-3.71395600	-2.83026200
H	-1.92249600	-0.78993300	-5.02811900
H	-3.26817800	-2.87906000	-4.97962500
C	-2.74969100	-0.89225300	1.31634900
C	-4.11057800	-1.14073300	1.57978200
C	-1.76356400	-1.35705600	2.20109900
C	-4.47265300	-1.87009800	2.71008400
H	-4.88245000	-0.75764000	0.91811100
C	-2.14115800	-2.08413500	3.33156500
H	-0.71054100	-1.15940000	2.03321000
C	-3.48870300	-2.34486200	3.58319800
H	-5.52212700	-2.06177800	2.91190500
H	-1.37423400	-2.44253400	4.01097300
H	-3.77566500	-2.91206500	4.46361100
C	-3.32628300	1.58425200	-0.17309400
C	-3.93875800	2.05977600	-1.34286500
C	-3.47635700	2.28715500	1.03691300
C	-4.69033000	3.23468900	-1.30081500
H	-3.84619100	1.51409400	-2.27570200
C	-4.22515800	3.46241200	1.06554100
H	-3.02547700	1.91287400	1.95137000
C	-4.83148400	3.93605300	-0.10162500
H	-5.17089500	3.59612500	-2.20478300
H	-4.34357000	4.00120800	2.00071600
H	-5.42109600	4.84757000	-0.07332800
C	3.78229900	-0.32419400	-2.12436800
C	4.17464200	1.11845100	-2.62475100
C	5.22208500	-0.46266300	-1.55328900
H	3.64001900	-0.97652400	-2.99842300
C	5.66345100	0.71118900	-2.46671600

H	6.33782300	1.45671000	-2.03761900
H	6.09005200	0.35814700	-3.41033100
H	3.88035400	1.88689800	-1.90395100
H	3.81064600	1.40096000	-3.61605000
H	5.70552200	-1.43338700	-1.68704100
H	5.25908700	-0.20090300	-0.49113100

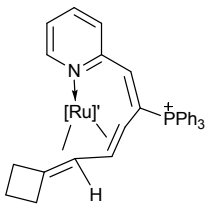


C'-1

[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1421.7237987 a.u.

Ru	-1.24274600	1.05115200	0.21627800
Cl	-0.72333300	1.87429600	2.34963300
Cl	-2.00395300	3.22148200	-0.44989000
P	1.99456000	-0.18946300	-0.19150300
N	-2.73401700	-1.56390000	-0.08387900
C	-0.48778000	-0.00377100	-1.53618800
H	0.14087900	0.39822500	-2.32697000
C	-1.66888800	-1.91090000	0.68697700
C	0.14770100	-0.40654900	-0.29367700
C	-0.60976300	-0.91398200	0.83482800
H	-0.06422200	-1.00444600	1.76803500
C	-3.72329300	-2.45131100	-0.35325500
H	-4.50421800	-2.11037800	-1.01380500
C	-1.65114400	-3.17033100	1.29566300
H	-0.81086400	-3.42277800	1.93289800
C	-3.72656100	-3.71310100	0.21028100
H	-4.54200200	-4.39129800	-0.01277500
C	-2.68475000	-4.07133900	1.07274600
H	-2.67553100	-5.04642000	1.54976000
C	-2.78740700	-0.14472700	-0.59131100
C	-1.88308800	0.16237000	-1.67894700
C	2.65510900	-1.09829000	-1.63563800
C	3.66027500	-0.53573400	-2.43613500
C	2.14603100	-2.37409000	-1.93976100
C	4.15402200	-1.24906800	-3.52987200
H	4.05305300	0.45086200	-2.21444000
C	2.64823200	-3.07895200	-3.03174600
H	1.36089800	-2.81454900	-1.33134900
C	3.65148300	-2.51671600	-3.82709800
H	4.92968400	-0.80970600	-4.14950100
H	2.25467800	-4.06372100	-3.26490100
H	4.03755800	-3.06686300	-4.68001100
C	2.56136800	1.54578000	-0.23806500
C	3.86012900	1.80571600	0.24060600
C	1.77766400	2.59207300	-0.74817900
C	4.36400100	3.10407800	0.20029300
H	4.46993400	1.00786400	0.65311700
C	2.28947900	3.88988500	-0.76798600
H	0.76195900	2.43318100	-1.09135300
C	3.57865000	4.14641000	-0.30039200
H	5.36426800	3.30197500	0.57327600
H	1.66429800	4.69693000	-1.13628700
H	3.96958400	5.15941500	-0.31508900
C	2.60801200	-0.93550300	1.35808800
C	3.36339500	-2.11783900	1.34127700
C	2.32876000	-0.28425000	2.57487700
C	3.83349700	-2.65133400	2.54253400
H	3.59654600	-2.61353400	0.40485900
C	2.80044100	-0.83317200	3.76647300
H	1.73838300	0.62872100	2.59719400
C	3.55217300	-2.01206300	3.75159900
H	4.42551700	-3.56150200	2.52971900
H	2.58262200	-0.33371600	4.70554600
H	3.92309700	-2.42902700	4.68336200
H	-2.22623800	0.77523600	-2.50797500
C	-4.16354700	0.50683300	-0.60252100
H	-3.94616800	1.57584500	-0.65969000
C	-5.20598100	0.30535100	0.53022100
H	-5.13963800	0.99497300	1.37573400
H	-5.23817200	-0.71783200	0.92170600
C	-6.31813400	0.54625800	-0.52885400
H	-7.20261300	-0.09374600	-0.47646900
H	-6.64302000	1.59002000	-0.54707400
C	-5.29518700	0.24400000	-1.66022200
H	-5.37324000	-0.78439700	-2.02902300
H	-5.29200800	0.90657200	-2.53039300



C-1

[Ru]' = $RuCl_2$

Symmetry = C_1 E = -1421.7301295 a.u.

Ru	-2.38217658	-0.05578585	0.76751598
Cl	-1.78729561	-1.07984854	2.78286685
Cl	-3.34159480	1.73896944	1.98947587
P	2.26615198	0.21842912	-0.14683152
N	-2.05440607	-1.91128370	-0.19811806
C	-0.44872871	0.60478276	0.33436372
H	-0.03280524	1.13206791	1.19282421
C	-0.94790092	-2.33541466	-0.86230778
C	0.50798309	-0.33820893	-0.29221175
C	0.28020441	-1.54588776	-0.85639114
H	1.11866061	-2.06049304	-1.31751706
C	-3.11325514	-2.74049044	-0.12242412
H	-3.96295344	-2.37489160	0.44709760
C	-0.93038092	-3.58337151	-1.50840692
H	-0.03681492	-3.88600995	-2.04513513
C	-3.14963038	-3.99494476	-0.72165349
H	-4.03457268	-4.61299999	-0.61756647
C	-2.03681707	-4.42148863	-1.44608211
H	-2.02803655	-5.38780864	-1.94014457
C	-2.23571933	0.84257307	-1.41928238
C	-1.43276918	1.40182257	-0.35849467
H	-1.64621531	2.40303157	0.00614227
C	2.31218640	1.98577954	-0.60801323
C	2.95373771	2.93351063	0.20202211
C	1.67738050	2.39013153	-1.79652388
C	2.97037862	4.27487144	-0.18389405
H	3.42507797	2.63653227	1.13237183
C	1.70375805	3.73116735	-2.17471081
H	1.15541071	1.66720891	-2.41756638
C	2.35120180	4.67305840	-1.36965616
H	3.46271481	5.00752706	0.44804350
H	1.21321838	4.04164543	-3.09226275
H	2.36494615	5.71820363	-1.66397842
C	2.81897274	-0.03140864	1.57510864
C	4.17606323	0.19025825	1.88124453
C	1.92621429	-0.44739884	2.57553779
C	4.62477533	0.01742023	3.18846860
H	4.87928315	0.48255901	1.10624116
C	2.39223505	-0.61777770	3.88101992
H	0.87978829	-0.65101328	2.36876081
C	3.73239650	-0.38220231	4.18893215
H	5.67060053	0.18914169	3.42447952
H	1.69612345	-0.93611530	4.65067748
H	4.08687442	-0.51562096	5.20673045
C	3.37630656	-0.75200575	-1.22991124
C	3.81726662	-0.24776491	-2.46329257
C	3.78125697	-2.03197405	-0.80829895
C	4.65073829	-1.02343552	-3.26959161
H	3.53161465	0.74678076	-2.78842059
C	4.61056489	-2.79995255	-1.62447751
H	3.46662138	-2.41929083	0.15626542
C	5.04480789	-2.29709270	-2.85401601
H	4.99795742	-0.62698308	-4.21884274
H	4.92595971	-3.78502209	-1.29419046
H	5.69772933	-2.89453458	-3.48333754
C	-3.53208879	1.24581028	-1.63713766
C	-4.40069867	2.39753556	-1.18317337
C	-4.61366345	0.69774423	-2.54687854
C	-5.59094481	1.76465623	-1.96475644
H	-4.05394307	3.35684571	-1.59042414
H	-4.50274582	2.51205776	-0.09773693
H	-1.84995149	0.01610824	-2.01131599
H	-6.07797145	2.40837123	-2.69996534
H	-6.35252014	1.33794760	-1.30782442
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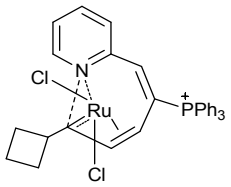
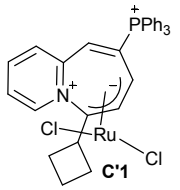


B-1-C'1-TS

Symmetry = C_1 E = -1421.6771258 a.u.

Ru	-2.04331100	-1.05726700	-1.02423700
Cl	-1.59167200	0.34523700	-2.83722800
Cl	-2.46463700	-3.28388800	-0.52610900
P	2.18448500	-0.05399800	0.26546100
N	-2.34719700	2.01596700	0.14334300
C	-0.50782300	-0.73089300	0.38793600
H	0.02782400	-1.65845900	0.59103300
C	-1.09603500	2.53598600	0.05343200
C	0.39045100	0.42791000	0.23964000
C	0.13659100	1.75808400	0.15842100
H	1.00498900	2.40595800	0.10154100
C	-3.39394600	2.82434100	-0.06024900
H	-4.37218300	2.36774200	-0.00412400

C	-0.91967500	3.91203100	-0.19743500
H	0.08796700	4.31087200	-0.25109800
C	-3.28426800	4.18601800	-0.33284700
H	-4.17983400	4.77746500	-0.48891700
C	-2.01228200	4.74629300	-0.39247300
H	-1.87203300	5.80365000	-0.59379400
C	-2.85413200	-0.01918300	0.36553800
C	-1.81212100	-0.71999600	1.02416500
C	-4.28065000	0.06594000	0.78432400
C	-4.95790100	-1.27315700	1.26207000
C	-4.67140600	0.68707900	2.16410100
H	-4.89059700	0.47604200	-0.02604400
H	-4.23940300	-1.97302800	1.69336100
H	-5.54306500	-1.80289600	0.50769800
H	-5.03644500	1.71845900	2.16931500
H	-3.84385600	0.60619700	2.87674100
C	2.39691600	-1.09812300	1.75460200
C	3.00919200	-2.35806200	1.69312100
C	1.90055300	-0.61743800	2.98061000
C	3.14035200	-3.12082800	2.85514100
H	3.36862200	-2.75337000	0.74978100
C	2.04138200	-1.38479500	4.13518100
H	1.39436200	0.34275700	3.03285500
C	2.66363000	-2.63525500	4.07339900
H	3.61024400	-4.09808600	2.80277000
H	1.65847500	-1.01072300	5.07984900
H	2.76720900	-3.23354100	4.97363300
C	2.65411400	-0.95076800	-1.25042500
C	3.98931500	-1.37807800	-1.38987100
C	1.73206200	-1.16284400	-2.28455900
C	4.38054600	-2.04645300	-2.54700900
H	4.72038000	-1.18075400	-0.61080600
C	2.14059200	-1.82877200	-3.44268300
H	0.71406800	-0.79571200	-2.21566900
C	3.45502200	-2.27724600	-3.57078500
H	5.40843900	-2.37958800	-2.65350500
H	1.42393400	-1.98705800	-4.24260100
H	3.76576300	-2.79697500	-4.47226000
C	3.27593300	1.41220800	0.36626900
C	3.88038200	1.80401300	1.57044500
C	3.51046600	2.14765800	-0.81055600
C	4.70714300	2.92803500	1.59537400
H	3.72612800	1.23236800	2.47897900
C	4.33235800	3.27264900	-0.77218000
H	3.06574700	1.83723000	-1.75166300
C	4.93082400	3.66280200	0.42936200
H	5.18142600	3.22332600	2.52632800
H	4.51411900	3.83604600	-1.68238600
H	5.57837300	4.53425400	0.45380400
H	-2.04504400	-1.48233800	1.76911600
C	-5.70662000	-0.45170000	2.34160500
H	-5.79151500	-0.89866000	3.33530900
H	-6.70383800	-0.15088200	2.00662200

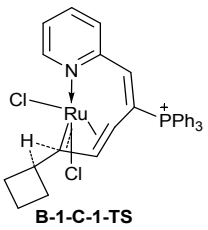


C'1

Symmetry = C_1 E = -1421.6942702 a.u.

Ru	-1.97117100	-1.03769900	-1.02751100
Cl	-1.67401800	0.67451800	-2.65448500
Cl	-2.32827500	-3.30614600	-0.58998300
P	2.22147900	-0.02825100	0.24495100
N	-2.49206300	1.64862400	0.25535200
C	-0.46544000	-0.80987100	0.45334800
H	0.02371200	-1.76168000	0.65139000
C	-1.26190500	2.27642100	0.39254000
C	0.40945800	0.34260300	0.37797800
C	0.03946500	1.64864300	0.46899300
H	0.83065900	2.38875200	0.49193800
C	-3.55585400	2.40909400	-0.14747200
H	-4.46042300	1.86984700	-0.36300300
C	-1.22447200	3.68671000	0.32698000
H	-0.26544000	4.16402500	0.49261200
C	-3.51739100	3.77830500	-0.27860200
H	-4.41317000	4.29818300	-0.59789500
C	-2.33021500	4.45178100	0.01507100
H	-2.26387000	5.53332100	-0.03575300
C	-2.77797200	0.19436100	0.44390900
C	-1.80467900	-0.72715400	0.98187500
C	-4.24661600	-0.07646300	0.80217600
C	-4.70434800	-1.41902900	1.45278500
C	-4.94113100	0.66621000	1.99361600
H	-4.86550100	0.03988100	-0.09635600
H	-3.97165500	-1.83054100	2.15014800
H	-5.01391500	-2.21214000	0.77007200
H	-5.47059800	1.60223800	1.78890300

H	-4.23474100	0.83461600	2.81460800
C	2.56491000	-1.32816400	1.48451200
C	3.25363400	-2.50026300	1.14146400
C	2.10074400	-1.14376300	2.80035700
C	3.49165500	-3.47177400	2.11540900
H	3.59029200	-2.66673500	0.12440400
C	2.34739200	-2.11822900	3.76499800
H	1.53674800	-0.25415900	3.06806000
C	3.04507400	-3.28084200	3.42351000
H	4.01994100	-4.38091600	1.84553700
H	1.98752300	-1.97469000	4.77924400
H	3.23024400	-4.04136700	4.17608100
C	2.66050600	-0.57649000	-1.43611100
C	4.01846800	-0.82551400	-1.71843700
C	1.69095600	-0.70953400	-2.43930800
C	4.38957300	-1.23887700	-2.99508700
H	4.77959800	-0.68860200	-0.95525400
C	2.08038000	-1.11667900	-3.71762400
H	0.64849200	-0.47485400	-2.25303000
C	3.42017600	-1.38899600	-3.99318300
H	5.43481000	-1.43561100	-3.21341800
H	1.32710700	-1.21080800	-4.49360200
H	3.71561600	-1.70794000	-4.98836700
C	3.21901800	1.46512900	0.59999400
C	3.83620000	1.65962000	1.84500700
C	3.36182600	2.42956800	-0.41492300
C	4.58369100	2.81566500	2.07317400
H	3.75330400	0.91229800	2.62649600
C	4.10532800	3.58378800	-0.17317700
H	2.91026000	2.27359700	-1.39038300
C	4.71595400	3.77711200	1.06926100
H	5.06850900	2.95907900	3.03400400
H	4.21813300	4.32413400	-0.95939400
H	5.30278500	4.67269700	1.25064000
H	-2.14072700	-1.51427100	1.64565400
C	-5.78294000	-0.61337600	2.22153200
H	-5.98155700	-0.90441500	3.25579600
H	-6.73206100	-0.57408500	1.67818300



B-1-C-1-TS

Symmetry = C_1 E = -1421.6532926 a.u.

Ru	-2.26305800	-0.19669800	0.87539700
Cl	-2.31312200	-2.00650800	2.41013500
Cl	-2.93750800	1.30589400	2.57598300
P	2.26872700	0.22126900	-0.11453900
N	-2.02141000	-1.75304100	-0.61427000
C	-0.43360900	0.64410000	0.37402100
H	0.06637100	1.06745000	1.24715100
C	-1.00951500	-1.89108300	-1.51166500
C	0.49376200	-0.13795700	-0.47667000
C	0.23222600	-1.14392400	-1.34260200
H	1.05315300	-1.53788200	-1.93518300
C	-3.06791700	-2.59743600	-0.70103300
H	-3.82243600	-2.48850400	0.06878300
C	-1.07676900	-2.84631500	-2.54127800
H	-0.25194400	-2.92344800	-3.24282900
C	-3.18821900	-3.56914900	-1.69064100
H	-4.05825500	-4.21670700	-1.69893200
C	-2.17821300	-3.68686600	-2.64449500
H	-2.23887200	-4.42612300	-3.43707700
C	-2.67351100	1.04340800	-0.65925900
C	-1.48968700	1.54982800	-0.05574700
C	-3.67931700	1.60561500	-1.44192300
C	-5.14924200	1.26969300	-1.56759600
C	-3.81862300	2.92482000	-2.17352700
H	-2.73998100	0.54741000	-1.78457700
H	-5.61589000	0.84813000	-0.67416400
H	-5.38289000	0.64427700	-2.43589800
H	-3.59988000	2.84794600	-3.24403100
H	-3.26584900	3.76752300	-1.75011200
C	2.47395000	2.03686500	-0.07110200
C	3.14070300	2.67121400	0.98658500
C	1.94002000	2.79999500	-1.12499900
C	3.28338800	4.05971800	0.98041100
H	3.53433000	2.09467900	1.81650400
C	2.09270800	4.18527800	-1.12410600
H	1.39947600	2.31816800	-1.93531900
C	2.76537400	4.81495200	-0.07280400

H	3.79488000	4.54893700	1.80356300
H	1.68133100	4.77328100	-1.93904500
H	2.87793000	5.89500200	-0.07206400
C	2.67012300	-0.53125900	1.50096100
C	4.01378700	-0.53556600	1.92338000
C	1.67397800	-1.10715000	2.30662500
C	4.34752600	-1.09303600	3.15560500
H	4.79498900	-0.12078600	1.29235200
C	2.02446500	-1.66332400	3.53856600
H	0.63336500	-1.14170800	2.00082800
C	3.35298300	-1.65225700	3.96478200
H	5.38355000	-1.09583400	3.48065500
H	1.24744100	-2.10364100	4.15548900
H	3.61822200	-2.08571300	4.92453300
C	3.38737600	-0.50973300	-1.36341800
C	3.95186300	0.27287900	-2.38259600
C	3.66922200	-1.88673400	-1.29623900
C	4.78545300	-0.32162800	-3.33028600
H	3.75995900	1.33936100	-2.43065000
C	4.49976600	-2.47095400	-2.25153600
H	3.25725200	-2.49394100	-0.49570500
C	5.05700400	-1.69002800	-3.26785000
H	5.22843900	0.28782400	-4.11206400
H	4.71966100	-3.53271600	-2.19464300
H	5.71024100	-2.14700600	-4.00528400
H	-1.60692600	2.47337700	0.51148500
C	-5.35046300	2.78979700	-1.88349500
H	-6.01683900	3.02233300	-2.71543700
H	-5.65013500	3.35310900	-0.99826600

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