

**Reductive Coupling of Diynes at Rhodium Gives Fluorescent
Rhodacyclopentadienes or Phosphorescent Rhodium 2,2'-Biphenyl
Complexes**

Electronic Supporting Information

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Experimental Section

General Information The compounds methyl 4-ethynylbenzoate and 4-ethynylthioanisole were prepared according to the literature.^{S1,S2} The compounds 1,8-dibromoocta-1,7-diyne and 1,7-dibromohepta-1,6-diyne were prepared *via* a modification of a bromination procedure employed for the synthesis of bromoacetylenes.^{S3} $[\text{Rh}(\mu\text{-Cl})(\text{COE})_2]_2$ (COE = cyclooctene) was synthesized according to a known procedure.^{S4,S5}

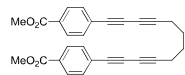
Synthesis

Bis(trimethylphosphine)- κ^2 -acetylacetonato rhodium(I) (**1**)^{S6}



A suspension of acetylacetonone (0.9 g, 9 mmol) and KOH (0.5 g, 9 mmol) in THF (150 mL) was added to a solution of $[\text{Rh}(\mu\text{-Cl})(\text{COE})_2]_2$ (COE = cyclooctene) (1.6 g, 2.2 mmol) in THF (10 mL) and the reaction was stirred for 1.5 h at room temperature. The solvent was removed *in vacuo* and the resulting residue was extracted with hexane (25 mL) to give $[(\kappa^2\text{-acac})\text{Rh}(\text{COE})_2]$.^{S7} The extract was added to a solution of PMe_3 (0.9 mL, 9 mmol) in toluene (20 mL). The reaction mixture was stirred and heated at reflux for 1 h, and then the solvent was removed *in vacuo*. Compound **1** was isolated as a yellow solid. Yield: 1.45 g (92%). ^1H NMR (500 MHz, C_6D_6 , r.t., ppm) δ : 5.41 (s, 1 H, CH), 1.89 (s, 6 H, CH_3), 1.19 (vt, $J = 3$ Hz, 18 H, 2 PMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, C_6D_6 , r.t., ppm) δ : 184.4, 99.9, 27.9, 18.7 (vt, $J_{\text{C-P}} = 14$ Hz). $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, C_6D_6 , r.t., ppm) δ : 7.41 (d, $J_{\text{Rh-P}} = 186$ Hz, 2 P). Elem. Anal. Calcd. (%) for $\text{C}_{11}\text{H}_{25}\text{P}_2\text{O}_2\text{Rh}$: C, 37.30; H, 7.11. Found: C, 37.10; H, 7.38. MS (ES^+) $m/z = 354$ [M^+].

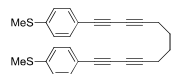
1,12-Bis(*p*-carbomethoxyphenyl)dodeca-1,3,9,11-tetrayne (2a)



The compounds CuCl (4.9 mg, 0.05 mmol) and NH₂OH·HCl (5 mg, 0.07 mmol) were added to a degassed solution of *n*-BuNH₂ (20 mL) and MeOH (70 mL). One equivalent of 1,8-dibromoocta-1,7-diyne (0.44 g, 1.7 mmol) was added and the mixture was cooled to 0 °C. Two equivalents of methyl 4-ethynylbenzoate (0.50 g, 3.2 mmol) were added and the reaction mixture was stirred for 30 min. at 0 °C. Then, the reaction was allowed to warm to room temperature and was stirred for another 12 h, after which the volatiles were removed *in vacuo*. The resulting residue was dissolved in CH₂Cl₂ (5 mL) and purified by column chromatography (silica gel), eluted with hexane and CH₂Cl₂ (2:1).

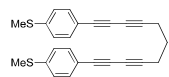
The solvent of the combined fractions was removed *in vacuo* and the product was recrystallized from MeOH to give **2a** as a white solid. Yield: 0.26 g (37%). ¹H NMR (500 MHz, CDCl₃, r.t., ppm) δ: 7.97 (d, *J* = 8 Hz, 4 H, CH_{arom}), 7.52 (d, *J* = 8 Hz, 4 H, CH_{arom}), 3.91 (s, 6 H, CH₃), 2.44 (m, 4 H, CH₂), 1.74 (m, 4 H, CH₂). ¹³C {¹H} NMR (126 MHz, CDCl₃, r.t., ppm) δ: 166.6, 132.6, 130.2, 129.7, 126.9, 85.7, 77.3, 74.3, 65.6, 52.5, 27.3, 19.4. Elem. Anal. Calcd. (%) for C₂₈H₂₂O₄: C, 79.60; H, 5.25. Found: C, 79.25; H, 5.36. MS (MALDI-TOF) *m/z*: 422 [M⁺].

1,12-Bis(*p*-methylthiophenyl)dodeca-1,3,9,11-tetrayne (2b)



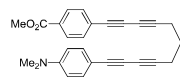
The compounds CuCl (4.9 mg, 0.05 mmol) and NH₂OH·HCl (5.0 mg, 0.07 mmol) were added to a degassed solution of *n*-BuNH₂ (30 mL) and MeOH (80 mL). One equivalent of 1,8-dibromoocta-1,7-diyne (2.00 g, 7.6 mmol) was added and the mixture was cooled to 0 °C. Two equivalents of 4-ethynylthioanisole (2.36 g, 15.9 mmol) were added and the reaction mixture was stirred for 30 min. at 0 °C. Then, the reaction was allowed to warm to room temperature and was stirred for 12 h. The volatiles were removed *in vacuo*, and the resulting residue was dissolved in CH₂Cl₂ (10 mL) and purified by column chromatography (silica gel), eluting with hexane and CH₂Cl₂ (2:1). The solvent

1,11-Bis(*p*-methylthiophenyl)undeca-1,3,9,11-tetrayne (**5b**)



The compounds CuCl (4.9 mg, 0.1 mmol) and NH₂OH·HCl (5.1 mg, 0.1 mmol) were added to a degassed solution of *n*-BuNH₂ (30 mL) and MeOH (80 mL). One equivalent of 1,7-dibromohepta-1,6-diyne (1.12 g, 4.5 mmol) was added and the mixture was cooled to 0 °C. Two equivalents of 4-ethynylthioanisole (1.30 g, 9.1 mmol) were added and the reaction mixture was stirred for 30 min. at 0 °C. Then, the reaction was allowed to warm to room temperature and stirred for another 12 h, after which the volatiles were removed *in vacuo*. The resulting residue was dissolved in CH₂Cl₂ (5 mL) and purified by column chromatography (silica gel), eluting with hexane and CH₂Cl₂ (2:1). The solvent of the combined fractions was removed *in vacuo* and the product was recrystallized from MeOH to give **5b** as a white solid. Yield: 0.4 g (22.3%). ¹H NMR (500 MHz, CD₂Cl₂, r.t., ppm) δ: 7.38 (d, *J* = 8 Hz, 4 H, CH_{arom}), 7.16 (d, *J* = 8 Hz, 4 H, CH_{arom}), 2.54 (m, 4 H, CH₂), 2.48 (s, 6 H, CH₃), 1.84 (m, 2 H, CH₂). ¹³C{¹H} NMR (126 MHz, CD₂Cl₂, r.t., ppm) δ: 141.3, 133.1, 125.9, 118.0, 83.7, 75.3, 74.4, 66.2, 27.3, 19.1, 15.3. Elem. Anal. Calcd. (%) for C₂₅H₂₀S₂: C, 78.08; H, 5.24; S, 16.68. Found: C, 78.15; H, 5.23; S, 16.68. MS (MALDI-TOF) *m/z*: 769 [2M + H]⁺, 384 [M]⁺.

D/A-substituted α,ω -bis(phenylbutadiynyl)alkane (**8**)



CuCl (5 mg, 0.1 mmol) followed by NH₂OH·HCl (2 mg, 0.1 mmol) were added to a mixture of *n*-BuNH₂ (30 mL) and MeOH (70 mL). The mixture was stirred and heated to 75 °C. 4-Ethynyl-*N,N*-dimethylaniline (1.1 g, 8.0 mmol), methyl 4-ethynylbenzoate (1.2 g, 8.0 mmol), and 1,7-dibromohepta-1,6-diyne (2.0 g, 8.0 mmol) were added, and the reaction mixture was rapidly stirred at 75 °C for 1 h. As soon as the reaction was complete, the volatiles were removed *in vacuo* and the resulting residue was dissolved in CH₂Cl₂ and recrystallized by addition of MeOH. Purification *via* column chromatography (silica gel) with CH₂Cl₂ as eluent and concentration *in vacuo* gave **8** as a

yellow solid. Yield: 0.58 g (10%). ^1H NMR (500 MHz, CD_2Cl_2 , r.t., ppm) δ : 7.94 (d, $J = 8$ Hz, 2 H, CH_{arom}), 7.53 (d, $J = 8$ Hz, 2 H, CH_{arom}), 7.32 (d, $J = 8$ Hz, 2 H, CH_{arom}), 6.60 (d, $J = 8$ Hz, 2 H, CH_{arom}), 3.89 (s, 3 H, CH_3), 2.97 (s, 6 H, CH_3), 2.54 (m, 4 H, CH_2), 1.83 (m, 2 H, CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CD_2Cl_2 , r.t., ppm) δ : 166.5, 151.1, 134.1, 132.8, 130.7, 129.8, 12.8, 112.0, 107.9, 85.5, 82.3, 77.1, 74.3, 72.4, 66.8, 65.8, 52.6, 40.3, 27.4, 19.2, 19.1. Elem. Anal. Calcd. (%) for $\text{C}_{27}\text{H}_{23}\text{NO}_2$: C, 82.42; H, 5.89; N, 3.56. Found: C, 82.25; H, 6.12; N, 3.49. MS (MALDI-TOF) m/z : 393 $[\text{M}]^+$.

Single-Crystal X-ray Diffraction



Figure S1. Molecular structure of **2b** in the solid state at 100 K. Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

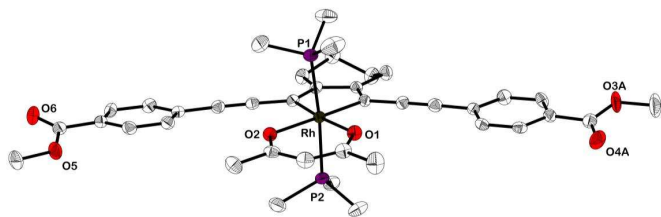


Figure S2. Molecular structure of **3a** in the solid state at 120 K. One phenylene ring with attached methoxycarbonyl group is disordered between two positions with occupancies of 70% (A) and 30% (B); position B and all hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

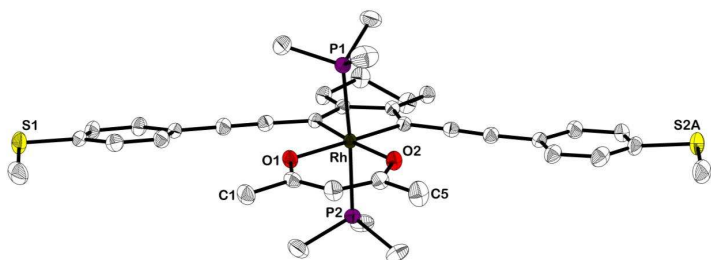


Figure S3. Molecular structure of **3b** in the solid state at 120 K. The S(2)Me group is disordered between two positions with occupancies of 64% (A) and 36% (B). Acac methyl groups C(1)H₃ and C(5)H₃ were treated as rotationally disordered over two sites with equal occupancies. Position B and all hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

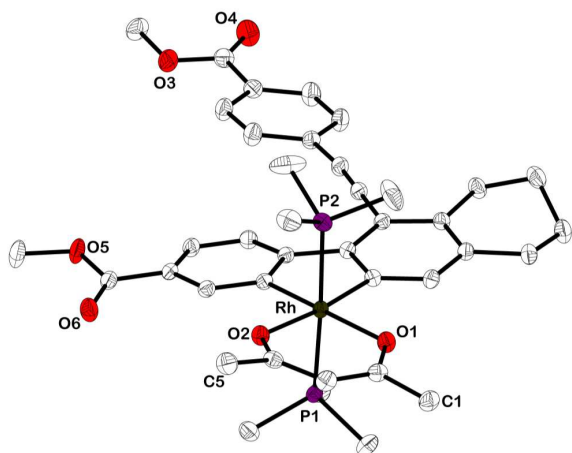


Figure S4. Molecular structure of **4a** in the solid state at 120 K. Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

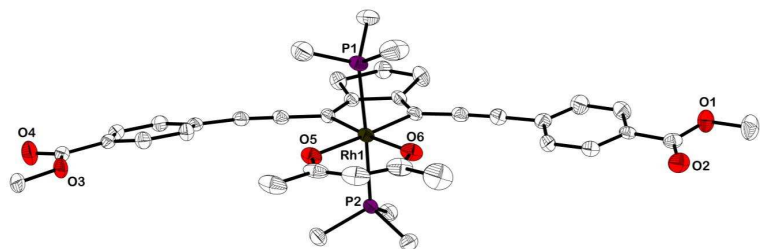


Figure S5. Molecular structure of **6a** in the solid state at 100 K. Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

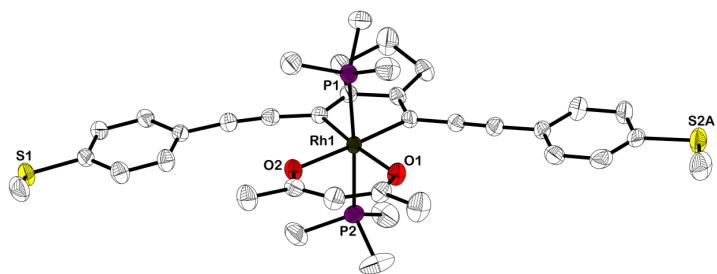


Figure S6. Molecular structure of **6b** in the solid state at 168 K. The S(2)Me group is disordered between two positions with occupancies of 67% (A) and 33% (B). Position B and all hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

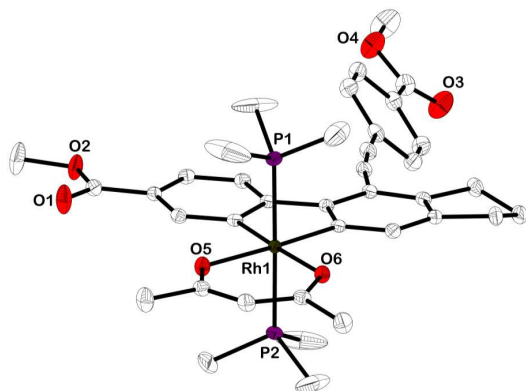


Figure S7. Molecular structure of **7a** in the solid state at 100 K. Hydrogen atoms and an *n*-hexane molecule of crystallization (located on a crystallographic inversion center) are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

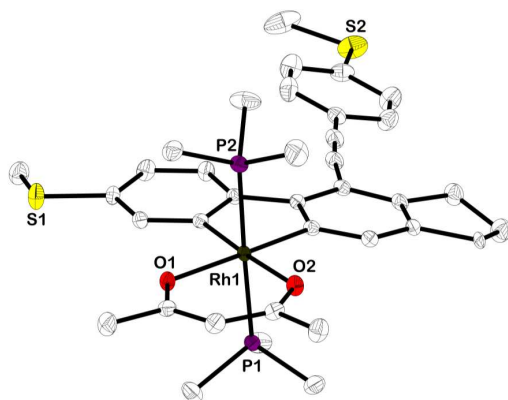


Figure S8. Molecular structure of **7b** in the solid state at 100 K. Hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

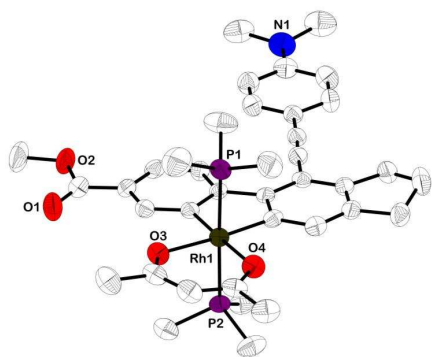


Figure S9. Molecular structure of **9** in the solid state at 168 K. The methyl groups at P1 are disordered between two positions with occupancies of 60% (A) and 40% (B). Positions B, the half molecule of THF (disordered around an inversion center) and all hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

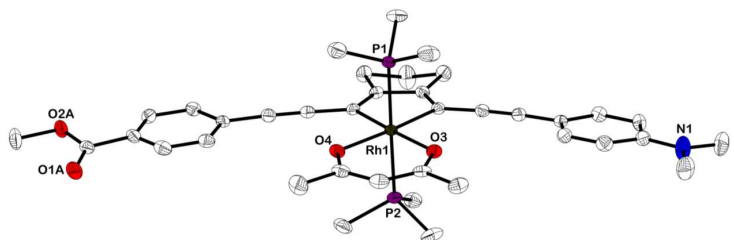


Figure S10. Molecular structure of **11** in the solid state at 100 K. The methoxycarbonyl group is disordered between two positions with occupancies of 90% (A) and 10% (B). Position B and all hydrogen atoms are omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

Table S1. Crystal data and X-ray experimental details.

Compound	2b	3a	3b	4a	4a	6a
CCDC	1419146	1419147	1419148	1419150	1419149	1419151
Formula	C ₂₆ H ₂₂ S ₂	C ₃₉ H ₄₇ O ₆ P ₂ Rh	C ₃₇ H ₄₇ O ₂ P ₂ S ₂ Rh	C ₃₉ H ₄₇ O ₆ P ₂ Rh		C ₃₈ H ₄₅ O ₆ P ₂ Rh
$\rho/\text{g cm}^{-3}$	1.263	1.377	1.380	1.429	1.441	1.373
μ/mm^{-1}	0.26	0.59	0.71	0.61	0.61	0.59
M_r	398.60	776.62	752.72	776.62		762.59
T/K	100	120	120	120	100	100
Crystal system	triclinic	triclinic	triclinic	monoclinic		triclinic
Space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>		<i>P</i> -1
<i>a</i> /Å	5.589(3)	9.8978(8)	9.7099(8)	14.276(2)	14.2261(6)	9.7677(6)
<i>b</i> /Å	10.297(5)	10.0553(8)	9.7832(8)	24.309(3)	24.1982(11)	10.7334(6)
<i>c</i> /Å	19.390(9)	19.9344(16)	20.008(2)	10.5470(14)	10.5338(4)	17.8794(11)
α°	77.395(13)	102.462(6)	97.636(7)	90	90	94.3812(17)
β°	87.061(14)	99.966(6)	103.479(7)	99.423(8)	99.075(2)	94.8291(17)
γ°	74.316(14)	98.427(6)	96.458(7)	90	90	97.3760(16)
<i>V</i> /Å ³	1048.4(9)	1872.8(3)	1811.5(3)	3610.6(8)	3580.8(3)	1845.15(19)
<i>Z</i>	2	2	2	4	4	2
$2\theta_{\text{max}}^\circ$	52	60	60	60	53.7	52
Unique refls.	3942	10253	10123	10309	7668	7887
Parameters	254	469	431	453	443	493
wR_2 (all data)	0.200	0.101	0.076	0.071	0.088	0.078
R_1 [$I > 2\sigma(I)$]	0.069	0.046	0.034	0.031	0.035	0.032

Compound	6b	7a	7b	9	11
CCDC	1419152	1419153	1419154	1419155	1419156
Formula	C ₃₆ H ₄₅ O ₂ P ₂ S ₂ Rh	C ₃₈ H ₄₅ O ₆ P ₂ Rh ·½C ₈ H ₁₄	C ₃₆ H ₄₅ O ₂ P ₂ S ₂ Rh	C ₃₈ H ₄₈ NO ₄ P ₂ Rh ·½C ₄ H ₈ O	C ₃₈ H ₄₈ NO ₄ P ₂ Rh
$\rho/\text{g cm}^{-3}$	1.370	1.363	1.411	1.351	1.335
μ/mm^{-1}	0.71	0.56	0.73	0.57	0.58
M_r	738.69	805.72	738.74	783.68	747.62
T/K	168	100	100	168	100
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P-1$	$P-1$
$a/\text{\AA}$	10.087(3)	16.788(3)	12.4163(9)	10.881(2)	9.5111(5)
$b/\text{\AA}$	36.862(11)	16.669(3)	10.6623(7)	13.483(2)	9.5174(5)
$c/\text{\AA}$	9.693(3)	14.073(3)	26.669(2)	13.895(3)	21.0321(11)
$\alpha/^\circ$	90	90	90	87.453(2)	82.662(2)
$\beta/^\circ$	96.398(4)	94.562(6)	100.025(4)	73.294(2)	80.516(2)
$\gamma/^\circ$	90	90	90	80.672(2)	85.479(2)
$V/\text{\AA}^3$	3581.9(19)	3925.6(12)	3476.7(4)	1926.8(6)	1859.19(17)
Z	4	4	4	2	2
$2\theta_{\text{max}}/^\circ$	50	52	52	50	52
Unique refls.	6245	7706	6834	6762	7286
Parameters	418	446	397	494	440
wR_2 (all data)	0.089	0.091	0.092	0.106	0.060
$R_1 [I > 2\sigma(I)]$	0.036	0.031	0.034	0.049	0.025

Photoluminescence Spectra

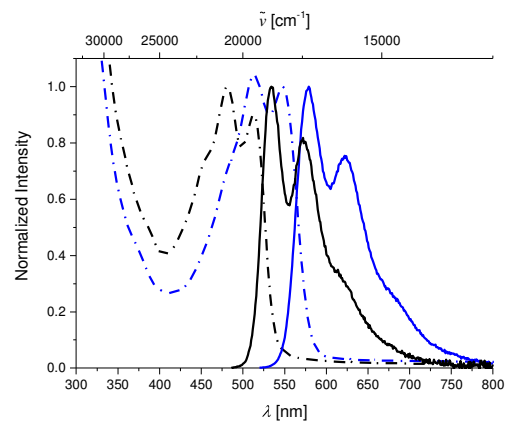


Figure S11. Excitation (dashed) and emission (solid) spectra of **3a** (blue), **3b** (black) in degassed toluene solution at 298 K.

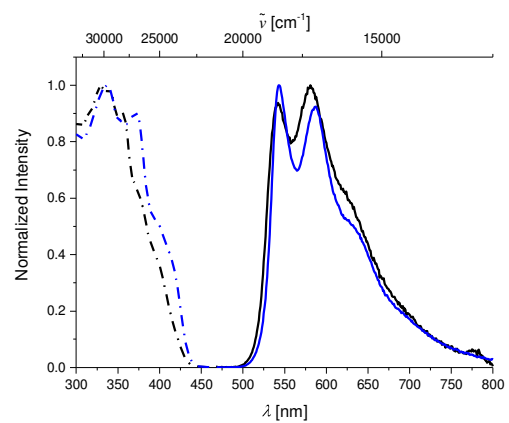


Figure S12. Excitation (dashed) and emission (solid) spectra of **4a** (blue), **4b** (black) in degassed toluene solution at 298 K.

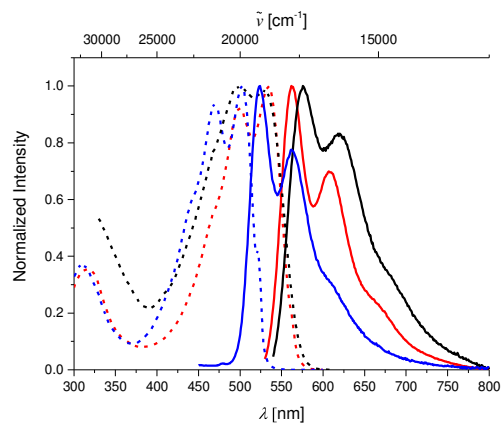


Figure S13. Excitation (dashed) and emission (solid) spectra of **6a** (red), **6b** (blue) and **11** (black) in degassed toluene solution at 298 K.

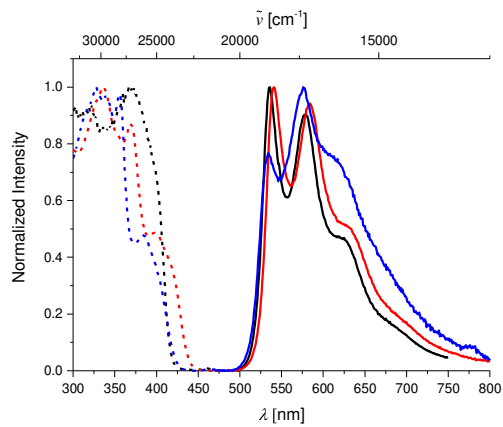


Figure S14. Excitation (dashed) and emission (solid) spectra of **7a** (red), **7b** (black) and **9** (blue) in degassed toluene solution at 298 K.

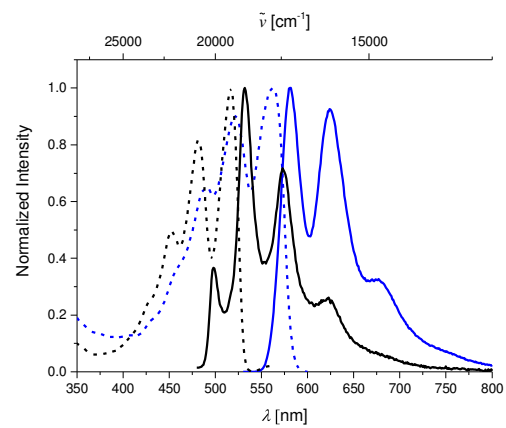


Figure S15. Excitation (dashed) and emission (solid) spectra of **3a** (blue), **3b** (black) in degassed 2-MeTHF at 77 K.

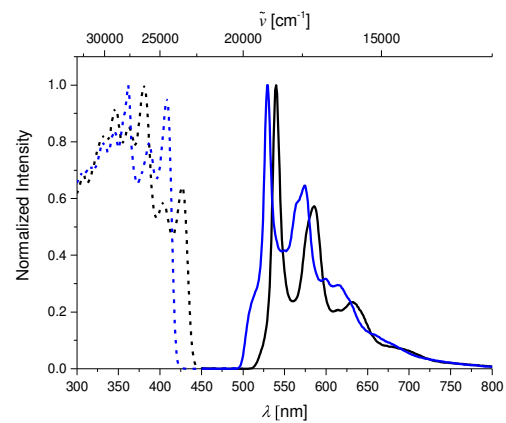


Figure S16. Excitation (dashed) and emission (solid) spectra of **4a** (black), **4b** (blue) in degassed 2-MeTHF at 77 K.

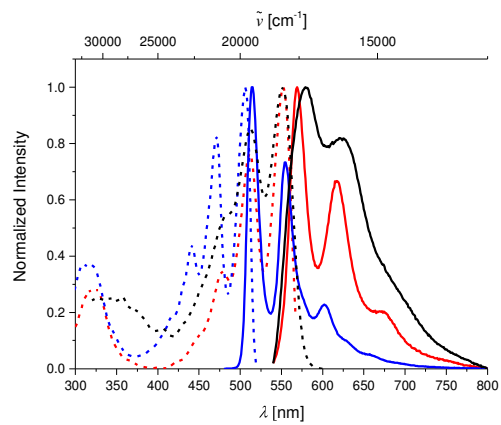


Figure S17. Excitation (dashed) and emission (solid) spectra of **6a** (red), **6b** (blue) and **11** (black) in degassed 2-MeTHF at 77 K.

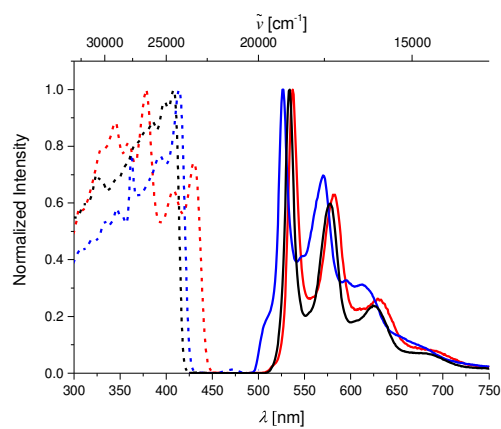


Figure S18. Excitation (dashed) and emission (solid) spectra of **7a** (red), **7b** (blue) and **9** (black) in degassed 2-MeTHF at 77 K.

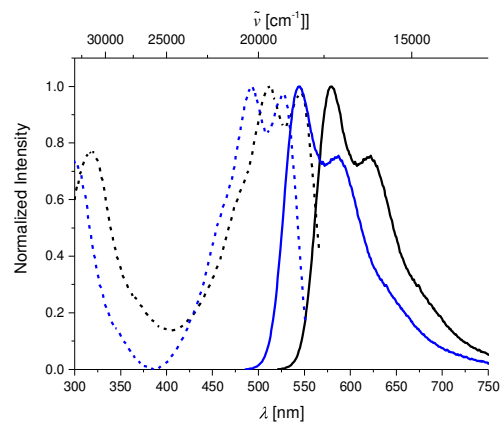


Figure S19. Excitation (dashed) and emission (solid) spectra of **3a** (black), **3b** (blue) in degassed 2-MeTHF at 298 K.

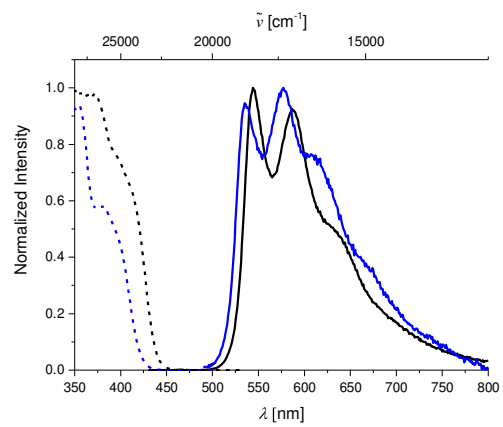


Figure S20. Excitation (dashed) and emission (solid) spectra of **4a** (black), **4b** (blue) in degassed 2-MeTHF at 298 K.

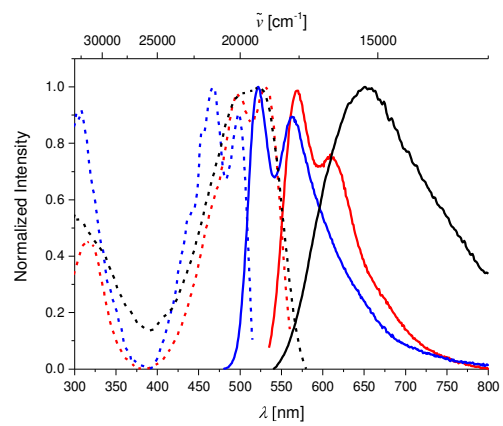


Figure S21. Excitation (dashed) and emission (solid) spectra of **6a** (red), **6b** (blue) and **11** (black) in degassed 2-MeTHF at 298 K.

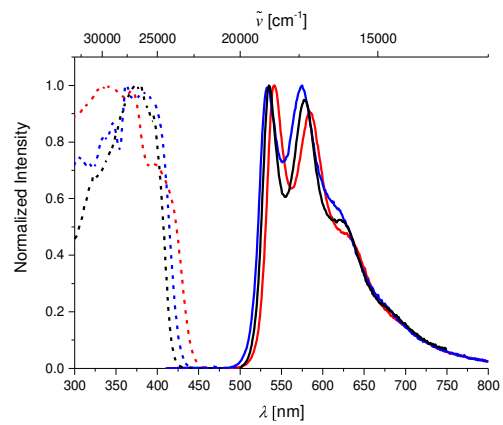


Figure S22. Excitation (dashed) and emission (solid) spectra of **7a** (red), **7b** (blue) and **9** (black) in degassed 2-MeTHF at 298 K.

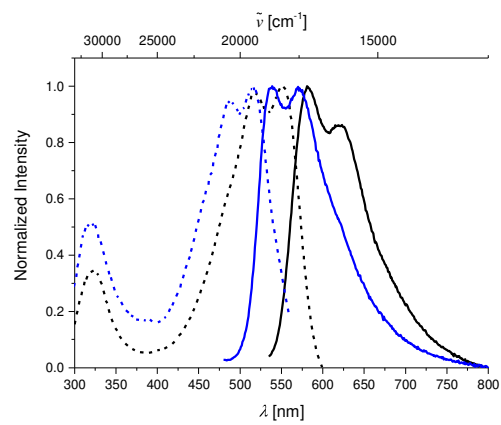


Figure S23. Excitation (dashed) and emission (solid) spectra of **3a** (black), **3b** (blue) in PMMA films at 298 K.

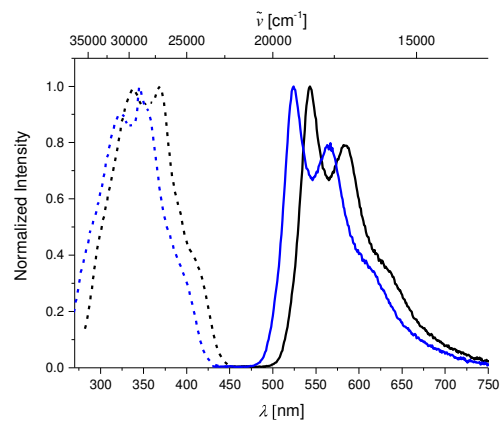


Figure S24. Excitation (dashed) and emission (solid) spectra of **4a** (black), **4b** (blue) in PMMA films at 298 K.

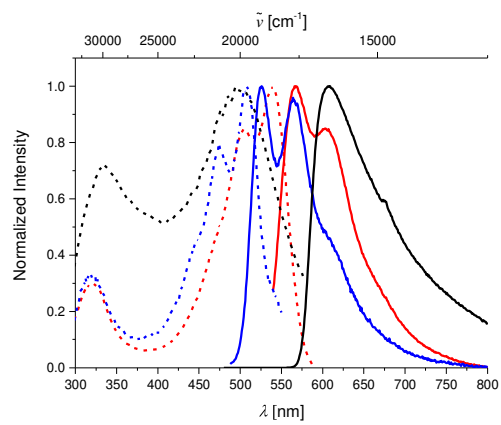


Figure S25. Excitation (dashed) and emission (solid) spectra of **6a** (red), **6b** (blue) and **11** (black) in PMMA films at 298 K.

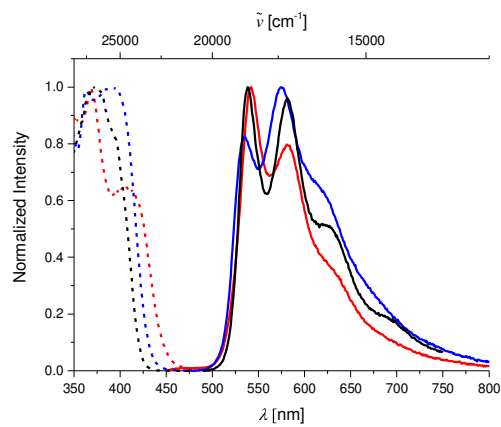


Figure S26. Excitation (dashed) and emission (solid) spectra of **7a** (red), **7b** (black) and **9** (blue) in PMMA films at 298 K.

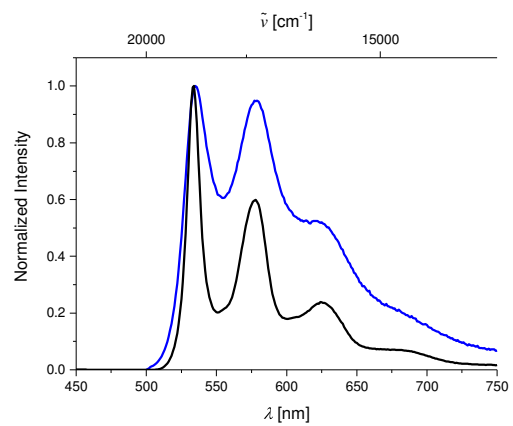


Figure S27. Emission spectra of **9** at 298 K (blue) and 77 K (black) in degassed 2-MeTHF.

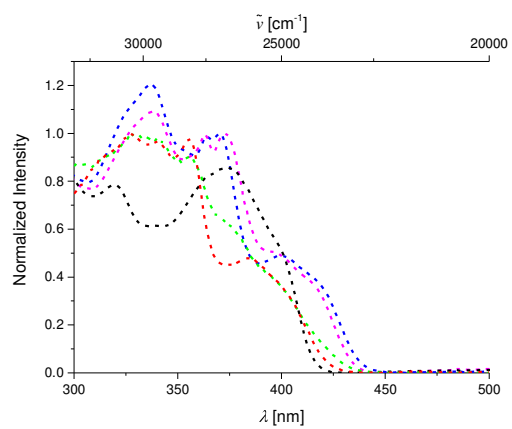


Figure S28. Absorption spectra of **4a** (magenta), **4b** (green), **7a** (blue), **7b** (red), and **9** (black) in degassed toluene solution at 298 K.

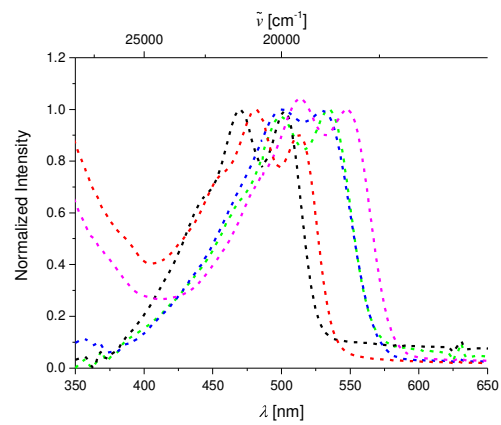


Figure S29. Absorption spectra of **3a** (magenta), **3b** (red), **6a** (green), **6b** (black), and **11** (blue) in degassed toluene solution at 298 K.

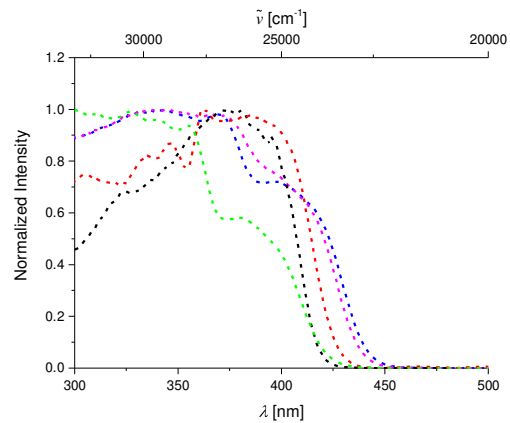


Figure S30. Absorption spectra of **4a** (magenta), **4b** (green), **7a** (blue), **7b** (red), and **9** (black) in degassed 2-MeTHF solution at 298 K.

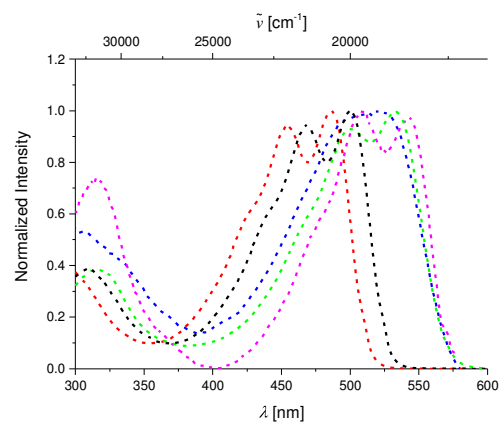


Figure S31. Absorption spectra of **3a** (magenta), **3b** (red), **6a** (green), **6b** (black), and **11** (blue) in degassed 2-MeTHF solution at 298 K.

Table S2. Selected photophysical properties of rhodacyclopentadienes and rhodium biphenyl complexes measured in degassed solvents at 298 K, 77 K and in PMMA films at 298 K. The longest-wavelength absorption maximum was chosen as the excitation wavelength for the emission spectra.

c	Temp. (K)	Solvent	λ_{maxAbs} (nm) (ϵ (mol ⁻¹ cm ⁻¹ dm ³))	λ_{maxEm} (nm)	Φ_{PL}	τ
3a	298	Toluene	514 (34000)	579	0.50	$\tau = 2.5$ ns (100%)
	77	2-MeTHF		581		$\tau = 2.8$ ns (100%)
	298	2-MeTHF	514	579	0.24	$\tau = 0.5$ ns (100%)
	298	PMMA film		581	0.43	$\tau = 2.5$ ns (100%)
3b	298	Toluene	481 (23000)	534	0.13	$\tau_1 = 2.0$ ns (25%) $\tau_2 = 0.5$ ns (75%)
	77	2-MeTHF		532		$\tau_1 = 0.9$ ns (57%) $\tau_2 = 2.4$ ns (43%)
	298	2-MeTHF	494	544	0.09	$\tau = 0.4$ ns (100%)
	298	PMMA film		539	0.06	$\tau_1 = 1.1$ ns (72%) $\tau_2 = 2.6$ ns (28%)
	298	Toluene	535 (37600)	563	0.54	$\tau = 1.7$ ns (100%)
	77	2-MeTHF		569		$\tau_1 = 2.1$ ns (90%) $\tau_2 = 3.1$ ns (10%)
6a	298	2-MeTHF	531	570	0.57	$\tau = 1.7$ ns (100%)
	298	PMMA film		567	0.49	$\tau = 2.1$ ns (100%)
6b	298	Toluene	503 (33500)	522	0.07	$\tau_1 = 0.3$ ns (77%) $\tau_2 = 0.1$ ns (23%)
	77	2-MeTHF		515		$\tau = 2.2$ ns (100%)
	298	2-MeTHF	466	522	0.08	$\tau = 0.2$ ns (100%)
	298	PMMA film		526	0.11	$\tau_1 = 0.6$ ns (56%) $\tau_2 = 1.6$ ns (44%)
4a	298	Toluene	410 (8430)	545	0.12	$\tau = 162$ μ s (100%)
	77	2-MeTHF		540		$\tau = 537$ μ s (100%)
	298	2-MeTHF	372	544	0.33	$\tau = 372$ μ s (100%)
	298	PMMA film		543	0.03	$\tau_1 = 20$ μ s (69%) $\tau_2 = 70$ μ s (31%)
4b	298	Toluene	390 (11400)	542	0.01	$\tau_1 = 43$ μ s (40%) $\tau_2 = 119$ μ s (60%)
	77	2-MeTHF		530		$\tau_1 = 2747$ μ s (80%) $\tau_2 = 3944$ μ s (20%)
	298	2-MeTHF	356	577	0.02	$\tau = 81$ μ s (100%)
	298	PMMA film		524	0.04	$\tau_1 = 19$ μ s (71%) $\tau_2 = 71$ μ s (29%)

Table S3. Selected photophysical properties of rhodacyclopentadienes and rhodium biphenyl complexes measured in degassed solvents at 298 K, 77 K and in PMMA films at 298 K. The longest-wavelength absorption maximum was chosen as the excitation wavelength for the emission spectra.

Entry	Temp. (K)	Solvent	λ_{maxAbs} (nm) (ϵ ($\text{mol}^{-1} \text{cm}^{-1} \text{dm}^3$))	λ_{maxEm} (nm)	Φ_{PL}	τ	
7a	298	Toluene	377 (9600)	540	0.14	$\tau = 181 \mu\text{s}$ (100%)	
	77	2-MeTHF		537		$\tau_1 = 374 \mu\text{s}$ (97%) $\tau_2 = 1335 \mu\text{s}$ (3%)	
	298	2-MeTHF	368	541	0.16	$\tau = 338 \mu\text{s}$ (100%)	
	298	PMMA film		542	0.02	$\tau_1 = 12 \mu\text{s}$ (76%) $\tau_2 = 41 \mu\text{s}$ (24%)	
	7b	298	Toluene	382 (12000)	535	0.02	$\tau_1 = 61 \mu\text{s}$ (98%) $\tau_2 = 163 \mu\text{s}$ (2%)
		77	2-MeTHF		527		$\tau_1 = 1922 \mu\text{s}$ (73%) $\tau_2 = 2774 \mu\text{s}$ (27%)
298		2-MeTHF	383	534	0.10	$\tau = 646 \mu\text{s}$ (100%)	
298		PMMA film		542	0.05	$\tau_1 = 1.6 \mu\text{s}$ (20%) $\tau_2 = 20 \mu\text{s}$ (80%)	
9		298	Toluene	371 (16300)	536	0.29	$\tau_1 = 164 \mu\text{s}$ (12%) $\tau_2 = 496 \mu\text{s}$ (88%)
		77	2-MeTHF		534		$\tau_1 = 680 \mu\text{s}$ (66%) $\tau_2 = 1100 \mu\text{s}$ (34%)
	298	2-MeTHF	380	535	0.21	$\tau_1 = 45 \mu\text{s}$ (34%) $\tau_2 = 210 \mu\text{s}$ (66%)	
	298	PMMA film		538	0.09	$\tau_1 = 3.5 \mu\text{s}$ (27%) $\tau_2 = 14 \mu\text{s}$ (73%)	
	11	298	Toluene	498 (31000)	576	0.22	$\tau = 0.8 \text{ ns}$ (100%)
		77	2-MeTHF		582		$\tau_1 = 2.2 \text{ ns}$ (98%) $\tau_2 = 4.5 \text{ ns}$ (2%)
298		2-MeTHF	522	651	0.13	$\tau = 0.5 \text{ ns}$ (100%)	
298		PMMA film		600	0.15	$\tau_1 = 1.1 \text{ ns}$ (67%) $\tau_2 = 2.8 \text{ ns}$ (33%)	

Computational Details

Table S4. Cartesian coordinates of the optimized ground state S_0 of **3a**.

C	1.281856	-1.173915	-3.209005	C	1.59276	3.823762	0.057448	H	-7.42886	-1.968668	0.051349
C	-1.6375	-0.921595	-3.094388	C	1.101662	-1.503797	3.161721	H	-4.988527	-1.461165	0.054946
C	2.447115	-3.958141	-0.111437	C	0.787062	5.058143	-0.359813	H	5.981683	2.462221	-0.045261
C	11.656201	-0.041549	0.010271	C	-1.425608	3.896169	-0.034615	H	0.611029	5.041662	-1.445631
C	9.417675	-0.72379	0.018765	C	-1.677335	-0.573282	3.133591	H	2.496502	3.715646	-0.55523
C	-0.051506	-3.691596	-0.057794	C	-0.55923	5.095021	0.366415	H	0.767106	-2.50005	2.855953
C	-2.55393	-3.906171	0.031132	C	0.516616	1.350484	3.244811	H	-8.314296	2.234745	-0.043616
C	0.040227	1.460262	-3.233759	H	1.217298	-1.074679	-4.299244	H	-1.784997	4.054194	-1.064316
C	7.004274	-1.285523	0.021357	H	1.182434	-2.226853	-2.929751	H	-5.868814	2.755141	-0.041226
C	1.218954	-3.068255	-0.06834	H	-1.644917	-0.828212	-4.186921	H	2.124857	-1.351565	2.80579
C	7.997436	-0.292041	0.007053	H	11.906607	-0.647058	-0.867196	H	-2.037428	-1.533719	2.754949
C	-1.306126	-3.04226	0.00742	H	3.074146	-3.669207	-0.963166	H	1.365169	5.966497	-0.145998
C	5.65902	-0.937897	0.011068	H	2.250728	-0.807379	-2.856657	H	1.947953	3.970716	1.090251
C	-11.191629	-1.739482	0.029461	H	-1.697583	-1.977189	-2.815041	H	-2.380146	0.202956	2.816759
C	7.61988	1.061106	-0.017377	H	2.201327	-5.020961	-0.189529	H	1.071952	-1.425258	4.255018
C	5.267748	0.421835	-0.012926	H	-0.030123	1.32897	-4.319798	H	-2.327294	3.834589	0.587457
C	6.274371	1.414503	-0.027076	H	-0.06384	-4.777008	-0.089026	H	-1.093809	6.027239	0.142524
C	3.891093	0.769572	-0.021991	H	-2.332477	-4.976322	-0.013379	H	-1.614161	-0.600229	4.227896
C	-7.083159	-0.938182	0.030689	H	-3.196068	-3.636641	-0.816239	H	1.560092	1.565356	2.996456
C	-9.487283	-0.136412	0.000743	H	7.313043	-2.328621	0.040329	H	-0.108517	2.174159	2.888405
C	2.690497	1.042415	-0.023114	H	11.903464	-0.609868	0.913108	H	-0.382757	5.083991	1.452341
C	-5.72098	-0.657214	0.032572	H	-11.268662	-2.829047	0.053059	H	0.407223	1.242714	4.330352
C	-8.022816	0.106502	0.003123	H	12.207777	0.901423	-0.008405	O	9.78649	-1.882599	0.041846
C	1.308149	1.281867	-0.019167	H	-2.497924	-0.398518	-2.666222	O	10.275388	0.317181	0.000443
C	-5.260013	0.680014	0.00702	H	3.040094	-3.796441	0.797138	O	1.457154	-1.826023	-0.039085
C	-1.26177	1.341202	0.027192	H	4.88634	-1.703128	0.021355	O	-9.794708	-1.44971	0.028391
C	-3.867159	0.956432	0.009057	H	-0.77423	2.100677	-2.884526	O	-1.517979	-1.794445	0.050054
C	-2.654678	1.171132	0.018184	H	0.993557	1.930458	-2.977814	O	-10.331814	0.738485	-0.022354
C	-7.574495	1.437304	-0.022443	H	-11.671592	-1.342904	-0.871355	P	-0.074086	-0.193644	-2.384134
C	0.774627	2.55549	0.002559	H	-3.122312	-3.696306	0.945557	P	-0.00673	-0.217906	2.387168
C	-6.214355	1.723706	-0.020633	H	8.387106	1.831038	-0.028332	Rh	-0.007802	-0.232335	0.002616
C	-0.668159	2.589487	0.01835	H	-11.678046	-1.304024	0.908569				

Table S5. TD-DFT results of the first 5 singlet and triplet excitations of **3a**.

State	Transition (%) ^{a)}	Energy		f	State	Transition (%) ^{a)}	Energy	
		[eV]	[nm]				[eV]	[nm]
S ₁	H → L (98)	2.23	556	1.10	T ₁	H → L (94)	0.99	1252
S ₂	H → L+1 (93)	3.00	413	0.01	T ₂	H-2 → L (23) H → L+1 (66)	2.25	550
S ₃	H → L+3 (19) H → L+4 (73)	3.13	396	0.00	T ₃	H-6 → L (23) H-2 → L+1 (12) H → L+3 (39)	2.85	435
S ₄	H → L+2 (92)	3.27	380	0.01	T ₄	H-6 → L+4 (10) H → L+3 (12) H → L+4 (70)	2.90	428
S ₅	H-1 → L (92)	3.29	376	0.01	T ₅	H-1 → L+2 (94)	2.96	419

a) Only contributions > 10% are given.

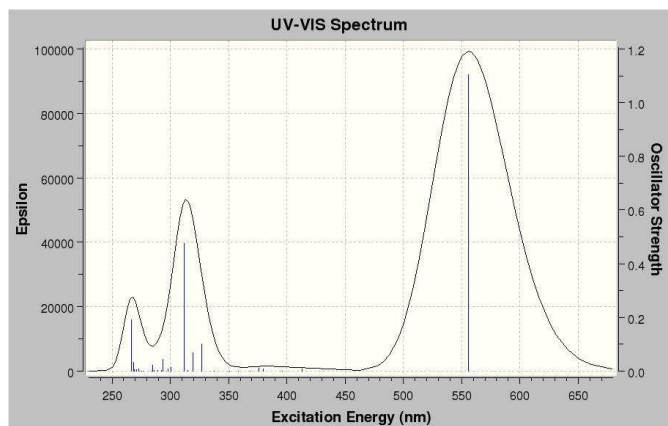
**Figure S32.** Calculated absorption spectrum of **3a**.

Table S6. Cartesian coordinates of the optimized ground state S_0 of **4a**.

Rh	-2.696456	-0.055526	0.001543	H	-3.714866	-2.16261	-2.877368	C	5.578181	0.633767	0.098363
P	-2.646533	-0.008597	-2.386342	C	-1.069697	0.345267	3.240762	H	4.83319	1.421556	0.186957
P	-2.671478	-0.082558	2.390298	H	-0.288884	-0.340759	2.89931	C	6.933166	0.951867	0.087374
O	-4.309438	-1.527081	0.014717	H	-1.184568	0.264003	4.328182	H	7.251666	1.988009	0.166874
O	-4.256453	1.45784	-0.027448	H	-0.778267	1.36505	2.973313	C	7.897232	-0.062564	-0.023505
O	9.628567	1.536442	0.068217	C	-3.892945	1.080975	3.189783	C	7.485383	-1.400623	-0.123112
O	10.220482	-0.629311	-0.132706	H	-3.693135	2.100249	2.846236	H	8.245083	-2.174492	-0.208276
O	0.784101	5.593764	0.020199	H	-3.805672	1.034706	4.281805	C	6.1329	-1.722774	-0.112536
O	-1.46254	5.444636	-0.003246	H	-4.908019	0.801499	2.890615	H	5.813493	-2.759677	-0.191097
C	-6.453307	-2.496794	-0.00587	C	-3.105484	-1.736879	3.133648	C	-0.375253	4.89791	0.008572
H	-6.278284	-3.068022	-0.926037	H	-4.072743	-2.061828	2.740766	C	0.633101	7.010818	0.017236
H	-7.515335	-2.243485	0.057614	H	-3.146448	-1.671688	4.227193	H	1.647341	7.41799	0.027094
H	-6.186286	-3.150931	0.832427	H	-2.345438	-2.464077	2.833287	H	0.080232	7.346571	0.901253
C	-5.550989	-1.276436	-0.000426	C	-1.161687	1.204471	0.001685	H	0.098251	7.34484	-0.87847
C	-6.161587	-0.000588	-0.022897	C	-1.293777	2.59472	0.000735	C	9.356539	0.220914	-0.03768
H	-7.247444	0.01905	-0.031908	H	-2.281159	3.053151	-0.005976	C	11.017374	1.866139	0.061221
C	-5.505428	1.254691	-0.032772	C	-0.16151	3.428634	0.009758	H	11.064888	2.95378	0.152072
C	-6.361434	2.506858	-0.035741	C	1.121398	2.858693	0.016492	H	11.488111	1.540271	-0.871976
H	-6.205816	3.048468	0.905663	H	1.997126	3.502583	0.020269	H	11.532852	1.390472	0.901985
H	-7.428277	2.294541	-0.150793	C	1.267326	1.472422	0.017606	C	-0.597663	-5.137262	0.004696
H	-6.031427	3.172223	-0.841797	H	2.263124	1.043251	0.022721	H	-1.466977	-5.331933	-0.637121
C	-1.046333	-0.466152	-3.223883	C	0.141298	0.62778	0.013537	H	-0.89719	-5.443667	1.019223
H	-0.780887	-1.494529	-2.961888	C	0.120903	-0.844659	0.02388	C	0.597367	-5.981462	-0.432673
H	-0.254518	0.199295	-2.867701	C	-1.199717	-1.36678	0.016853	H	0.385801	-7.046008	-0.268954
H	-1.147117	-0.372223	-4.311593	C	-1.38518	-2.748933	0.003344	H	0.775088	-5.849533	-1.509645
C	-3.036577	1.662148	-3.116562	H	-2.402634	-3.142673	-0.014623	C	1.838006	-5.547261	0.344403
H	-2.272081	2.376056	-2.796096	C	-0.306035	-3.650089	0.009624	H	2.694094	-6.192344	0.108551
H	-4.004952	1.998236	-2.733868	C	1.005006	-3.156598	0.034156	H	1.643076	-5.66037	1.420718
H	-3.057533	1.609944	-4.211934	C	1.217073	-1.748741	0.030321	C	2.19597	-4.09315	0.033242
C	-3.888921	-1.134663	-3.208834	C	2.575999	-1.312666	0.022851	H	2.945637	-3.73315	0.748216
H	-3.794404	-1.077059	-4.299743	C	3.770033	-1.042638	0.01129	H	2.682873	-4.040634	-0.952772
H	-4.898865	-0.835514	-2.911632	C	5.155967	-0.709178	-0.00123				

Table S7. TD-DFT results of the first 5 singlet and triplet excitations of **4a**.

State	Transition (%) ^{a)}	Energy		f	State	Transition (%) ^{a)}	Energy	
		[eV]	[nm]				[eV]	[nm]
S ₁	H → L (97)	3.03	409	0.22	T ₁	H-1 → L (35) H → L (29) H-2 → L (10)	2.17	572
S ₂	H-1 → L (96)	3.33	373	0.59	T ₂	H → L (30) H-1 → L+1 (30) H → L+1 (22)	2.53	490
S ₃	H-2 → L (87)	3.60	345	0.13	T ₃	H-2 → L+2 (65) H-1 → L+2 (20)	2.95	421
S ₄	H → L+1 (78) H-3 → L (12)	3.77	329	0.10	T ₄	H → L+1 (27) H → L (22) H-6 → L (11)	2.99	415
S ₅	H-2 → L (74) H → L+1 (12)	3.84	323	0.05	T ₅	H-2 → L (32) H-2 → L+1 (20) H-1 → L (19)	2.96	419

a) Only contributions > 10% are given.

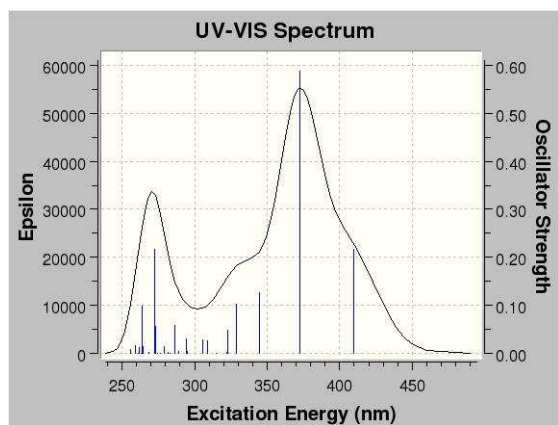
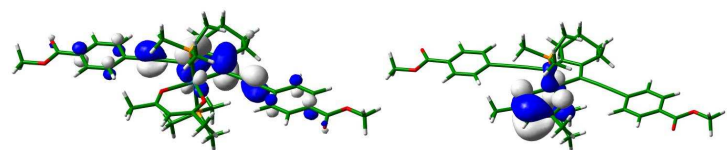
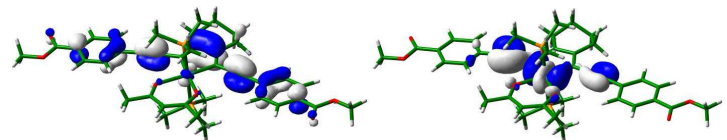


Figure S33. Calculated absorption spectrum of **4a**.



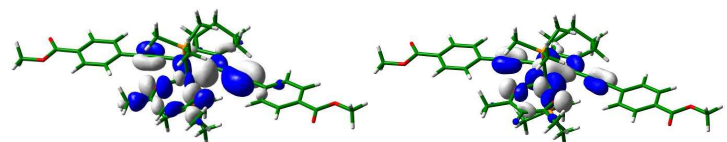
HOMO (178)

HOMO-1 (177)



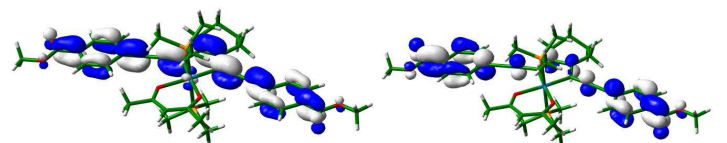
HOMO-2 (176)

HOMO-3 (175)



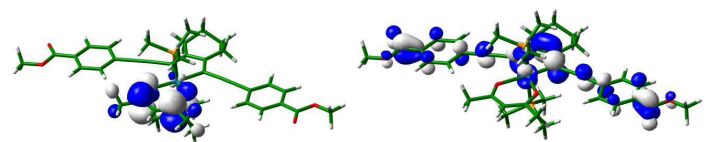
HOMO-4 (174)

HOMO-5 (173)



LUMO (179)

LUMO+1 (180)



LUMO+2 (181)

LUMO+3 (182)

Figure S34. Selected molecular orbitals of **3a**. Contour values: ± 0.035 [e/bohr^3] $^{1/2}$.

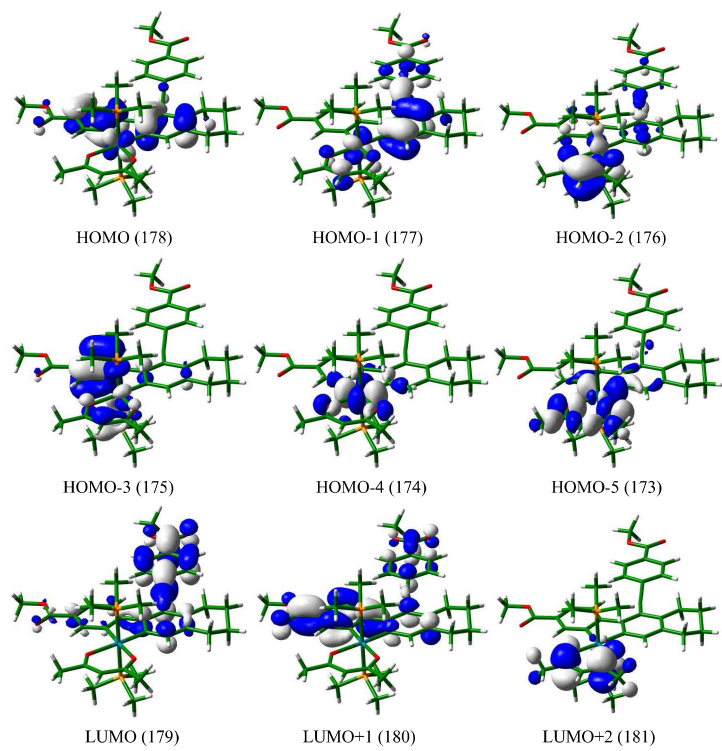


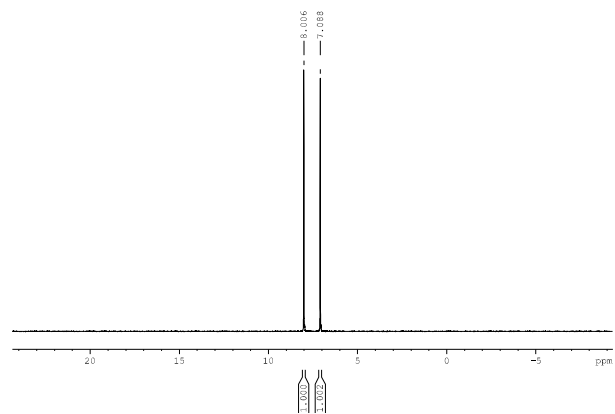
Figure S35. Selected molecular orbitals of **4a**. Contour values: ± 0.035 [e/bohr^3] $^{1/2}$.

References

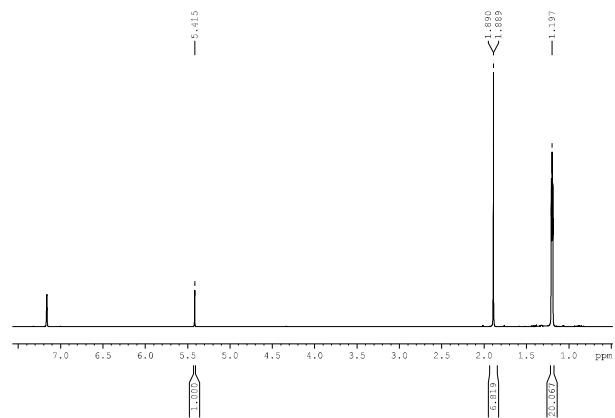
- (S1) A. S. Batsanov, J. C. Collings, I. J. S. Fairlamb, J. P. Holland J. A. K. Howard, Z. Lin, T. B. Marder, A. C. Parsons, R. W. Ward, J. Zhu, *J. Org. Chem.* **2005**, *70*, 703.
- (S2) P. Nguyen, Z. Yuan, L. Agocs, G. Lesley, T. B. Marder, *Inorg. Chim. Acta* **1994**, *220*, 289.
- (S3) G. Eglinton, W. McCrae, *J. Chem. Soc.* **1963**, 2295.
- (S4) A. van der Ent, A. L. Onderdelinden, R. A. Schunn, *Inorg. Synth.* **1973**, *14*, 92-95.
- (S5) G. Giordano, R. H. Crabtree, *Inorg. Synth.* **1979**, *19*, 218-220.
- (S6) M.-H. Thibault, M. G. Tay, A. S. Batsanov, J. A. K. Howard, T. M. Marder, *J. Organomet. Chem.* **2013**, *730*, 104-107.
- (S7) C. Dai, E. G. Robins, A. J. Scott, W. Clegg, D. S. Yufit, J. A. K. Howard, T. B. Marder, *Chem. Commun.* **1998**, *18*, 1983-1984.

NMR-spectra

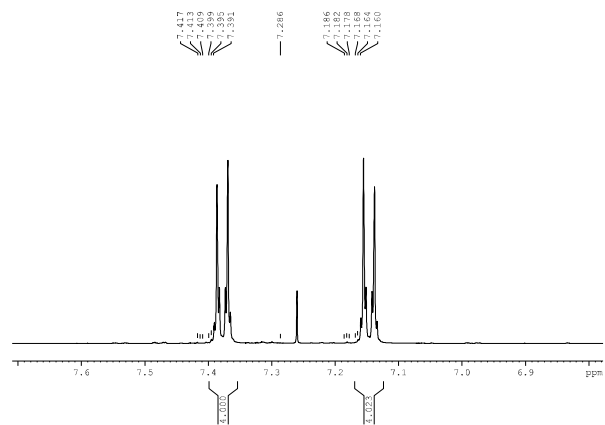
Bis(trimethylphosphine)- κ^2 -acetylacetonato rhodium(I) (1)^{S6}



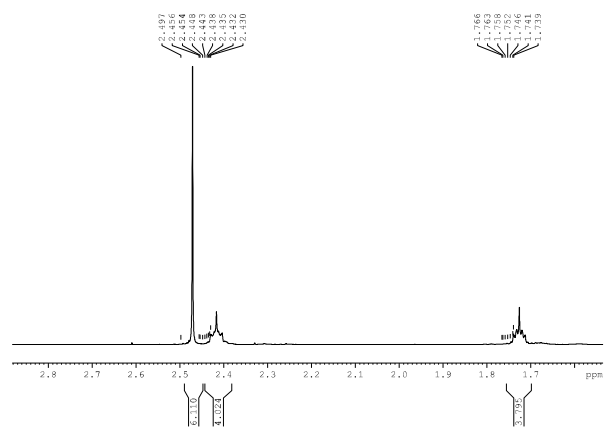
³¹P{¹H} NMR, 202 MHz, (C₆D₆).



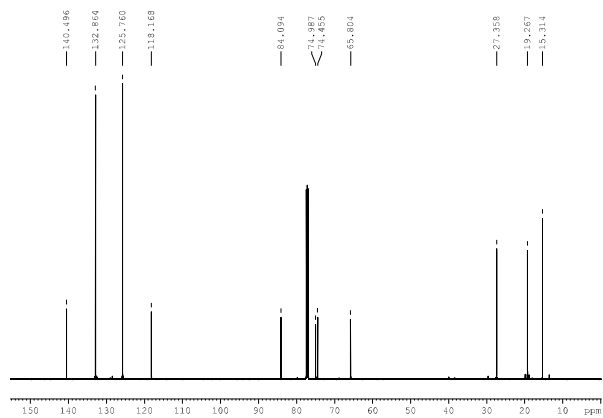
¹H NMR, 500 MHz, (C₆D₆).



^1H NMR, 500 MHz, (CDCl_3).

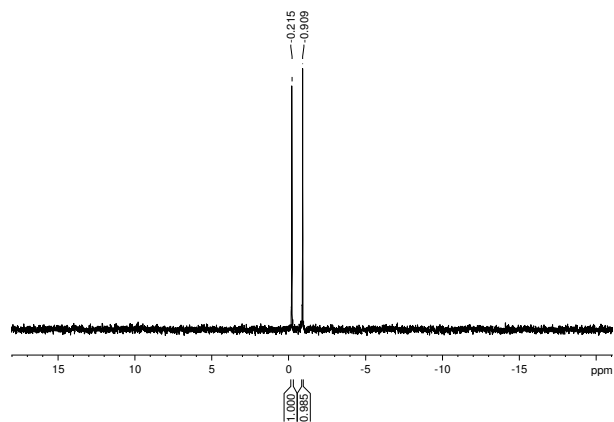
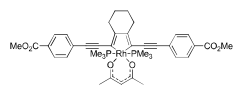


^1H NMR, 500 MHz, (CDCl_3).

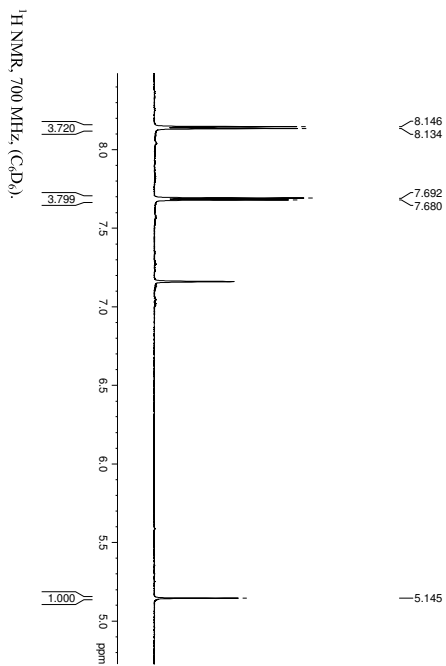
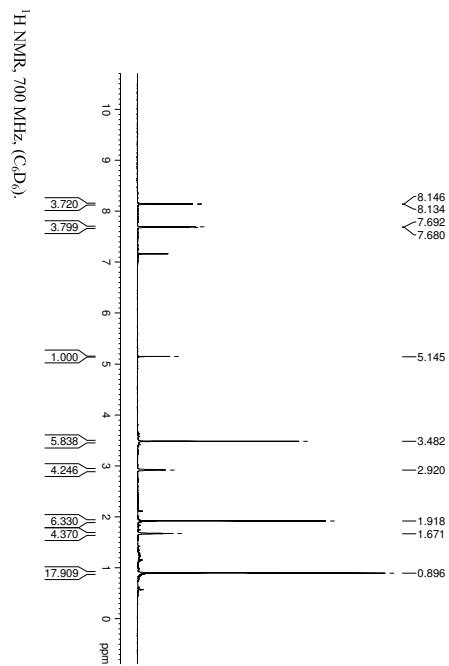


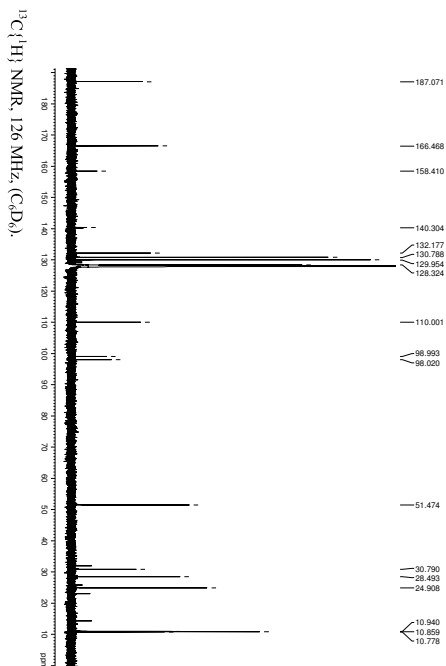
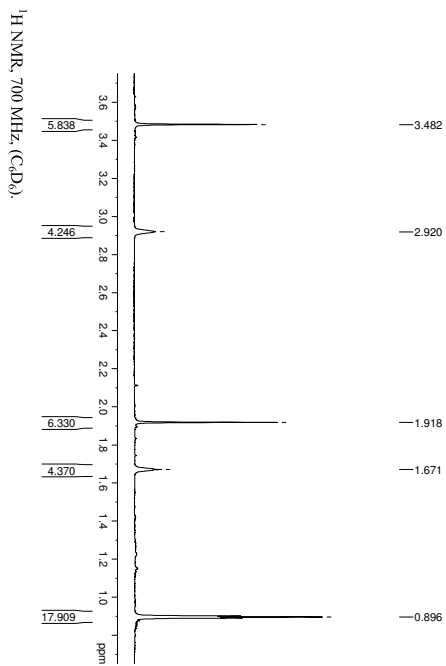
$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (CDCl_3).

2,5-Bis(*p*-carbomethoxyphenylethynyl)rhodacyclopenta-2,4-diene (3a)

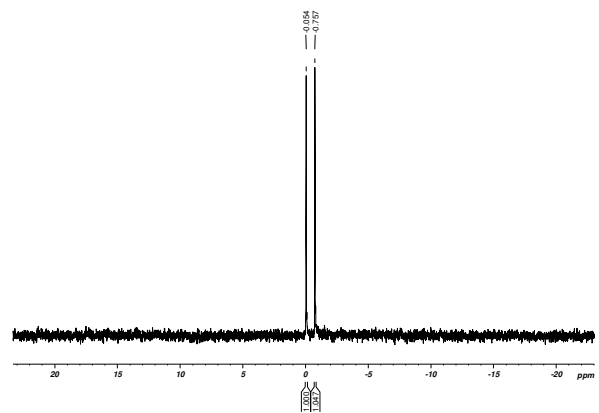
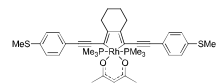


$^{31}\text{P}\{^1\text{H}\}$ NMR, 161 MHz, (C_6D_6).

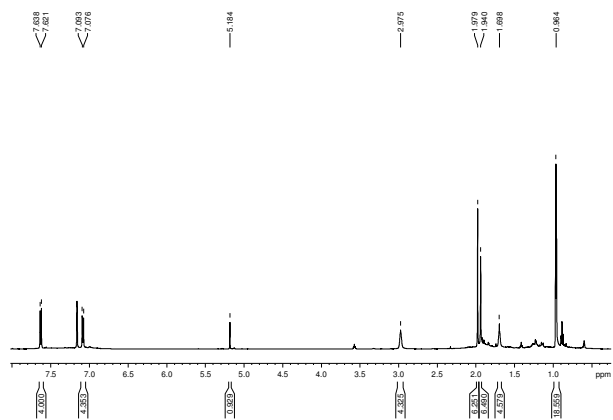




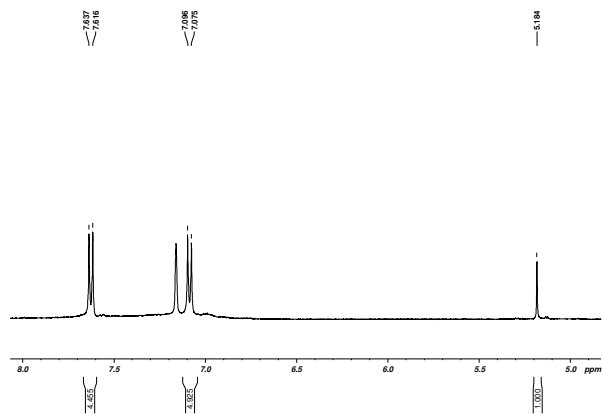
2,5-Bis(*p*-methylthiophenylethynyl)rhodacyclopenta-2,4-diene (3b)



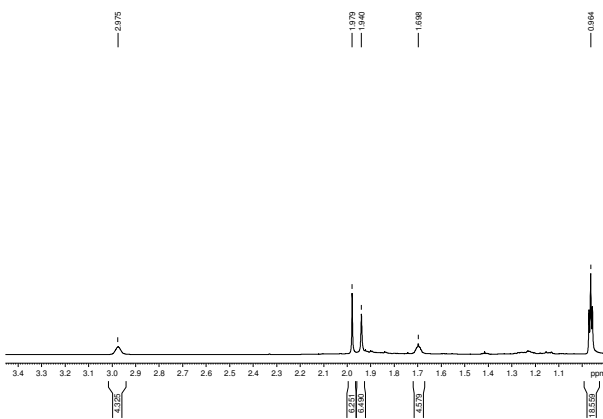
$^{31}\text{P}\{^1\text{H}\}$ NMR, 161 MHz, (C_6D_6).



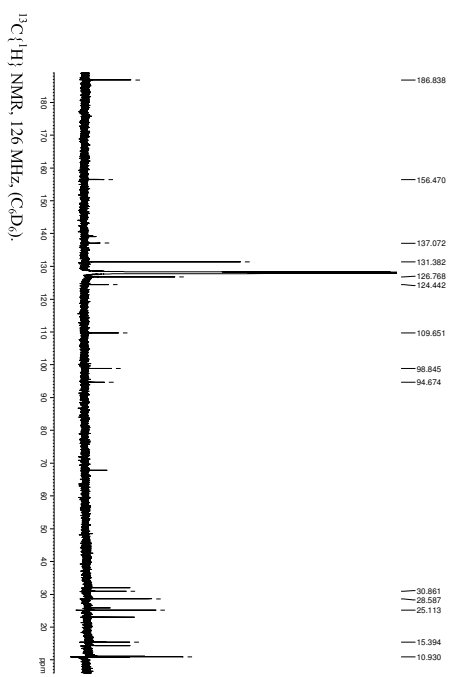
^1H NMR, 400 MHz, (C_6D_6).



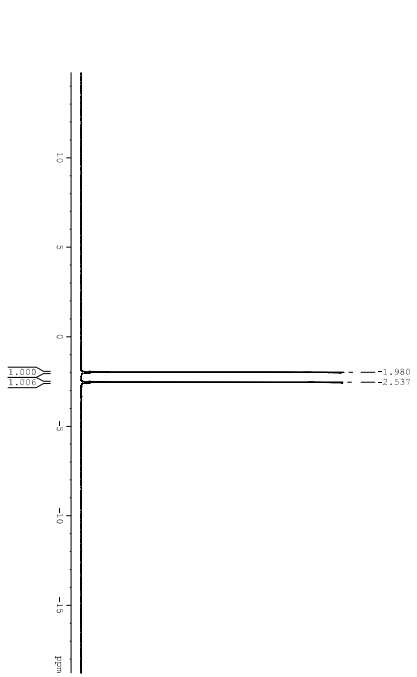
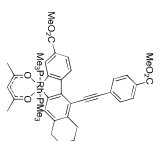
^1H NMR, 400 MHz, (C_6D_6).

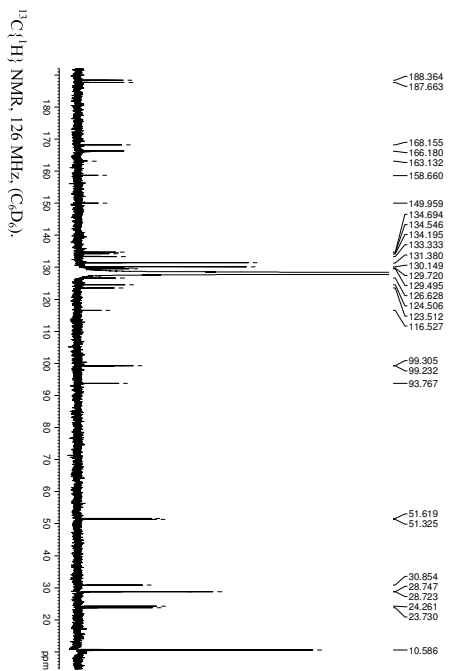
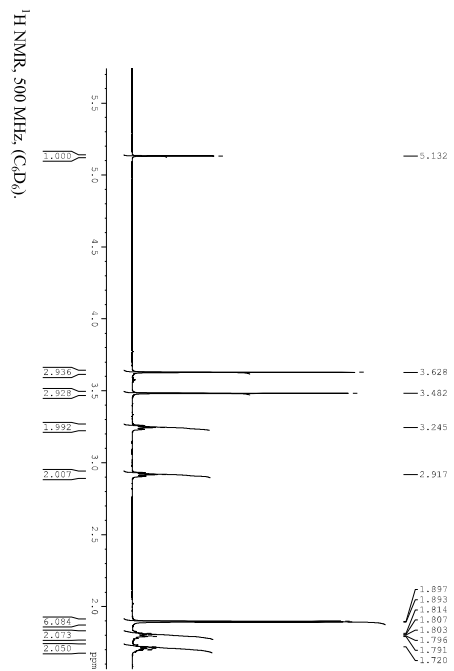


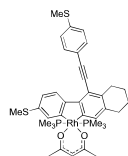
^1H NMR, 400 MHz, (C_6D_6).



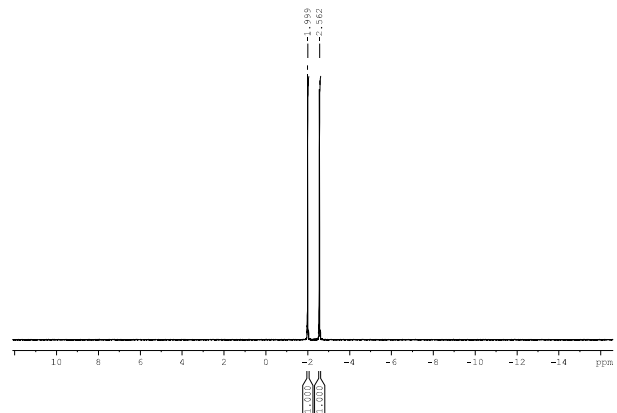
Rhodium biphenyl complex (4a)



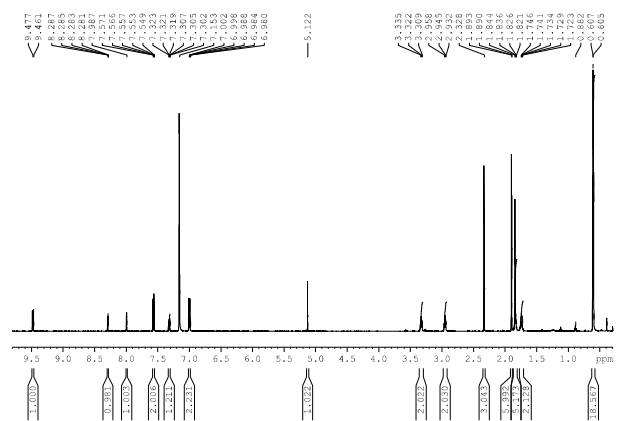




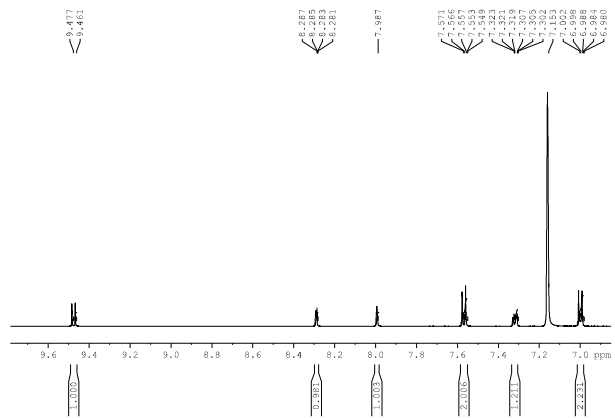
Rhodium biphenyl complex (4b)



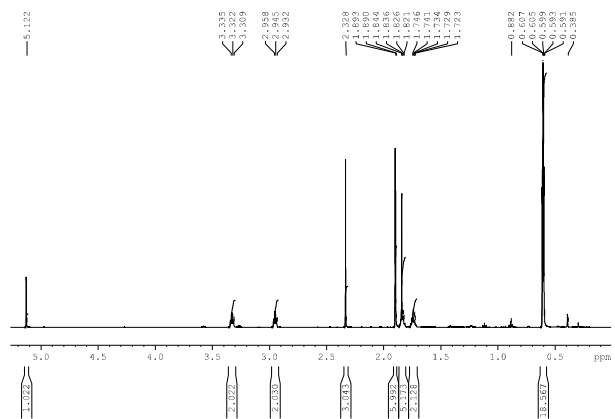
$^{31}\text{P}\{^1\text{H}\}$ NMR, 202 MHz, (C_6D_6).



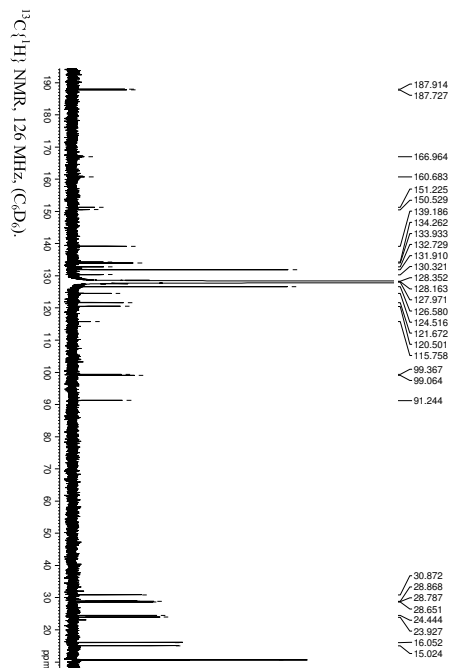
^1H NMR, 500 MHz, (C_6D_6).



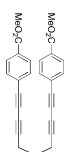
^1H NMR, 500 MHz, (C_6D_6).



^1H NMR, 500 MHz, (C_6D_6).



1,11-Bis(p-carbonmethoxyphenyl)undeca-1,3,9,11-tetrayne (5a)



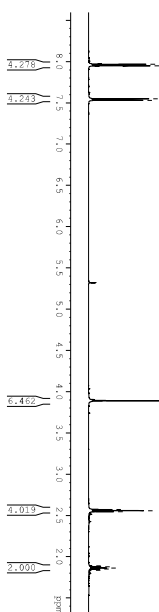
7.967
7.949

5.548
5.531

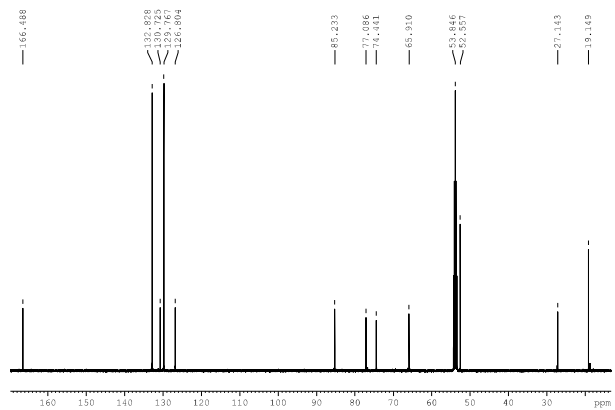
3.888

2.571
2.557
2.543

0.890
0.877
0.863
0.849
0.835

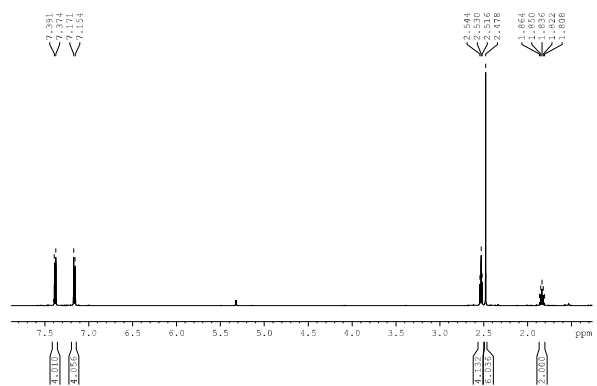


¹H NMR, 500 MHz, (CD₂Cl₂)

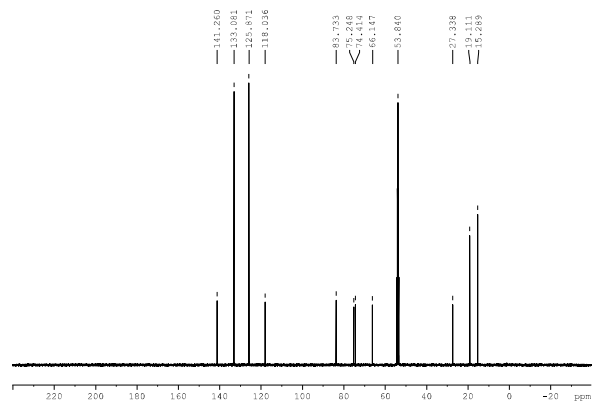


$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (CD_2Cl_2).

1,11-Bis(*p*-methylthiophenyl)undeca-1,3,9,11-tetrayne (5b)

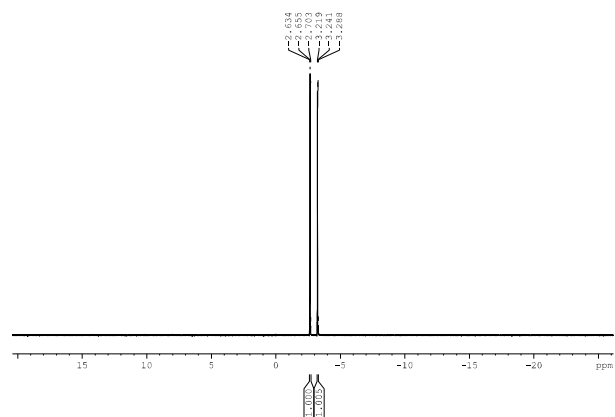
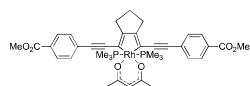


^1H NMR, 500 MHz, (CD_2Cl_2).

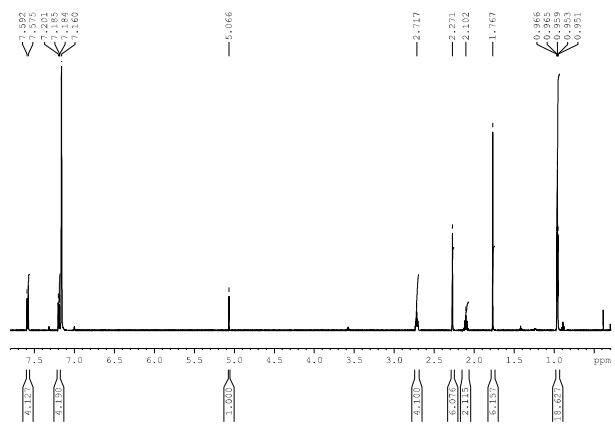


$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (CD_2Cl_2).

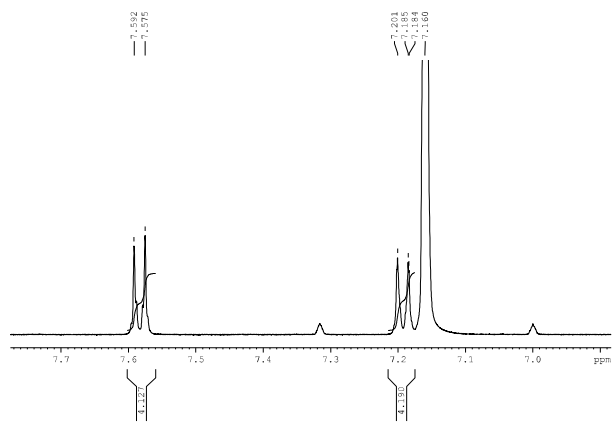
2,5-Bis(*p*-carbomethoxyphenylethynyl)rhodacyclopenta-2,4-diene (6a)



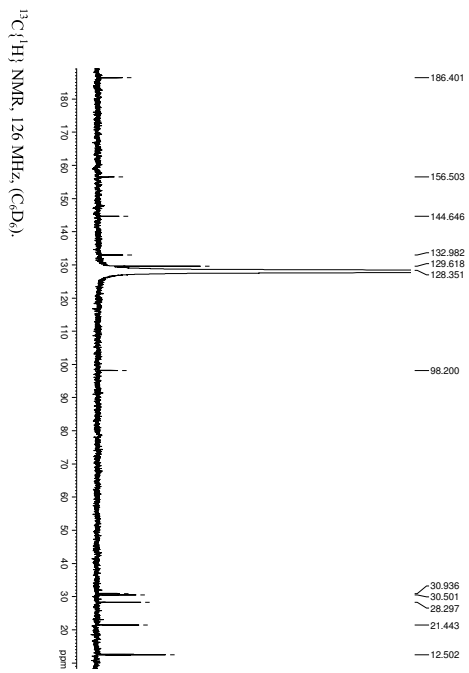
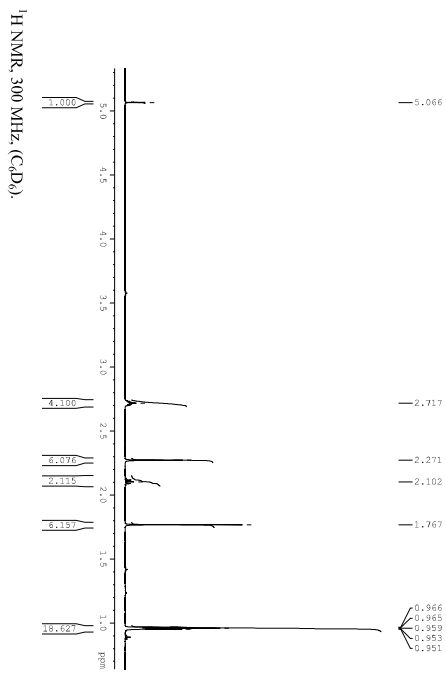
$^{31}\text{P}\{^1\text{H}\}$ NMR, 121 MHz, (C_6D_6).



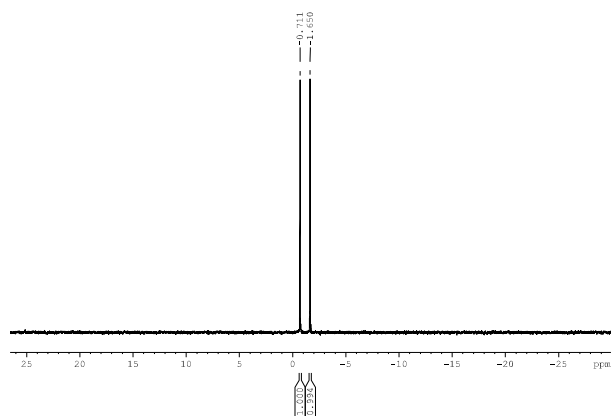
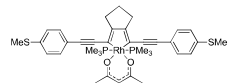
^1H NMR, 300 MHz, (C_6D_6).



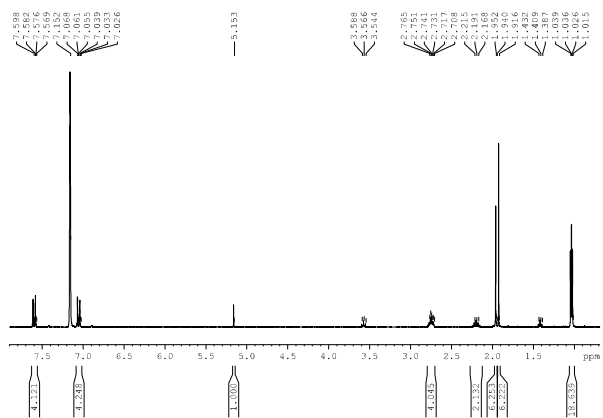
^1H NMR, 300 MHz, (C_6D_6).



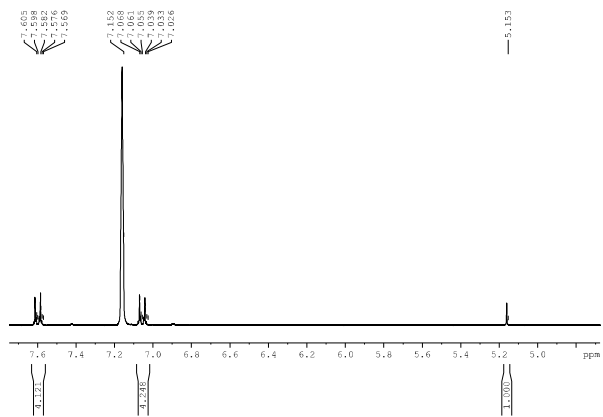
2,5-Bis(*p*-methylthiophenylethynyl)rhodacyclopenta-2,4-diene (6b)



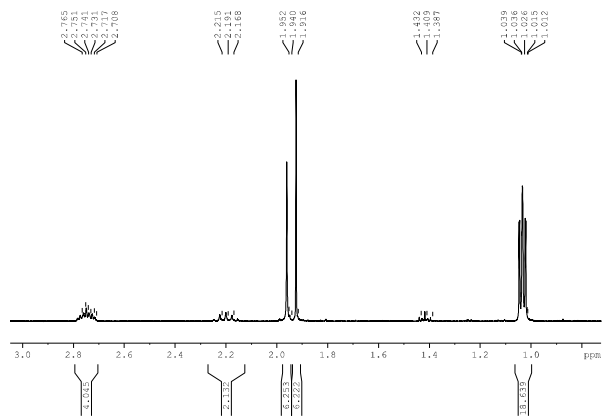
$^{31}\text{P}\{^1\text{H}\}$ NMR, 121 MHz, (C_6D_6).



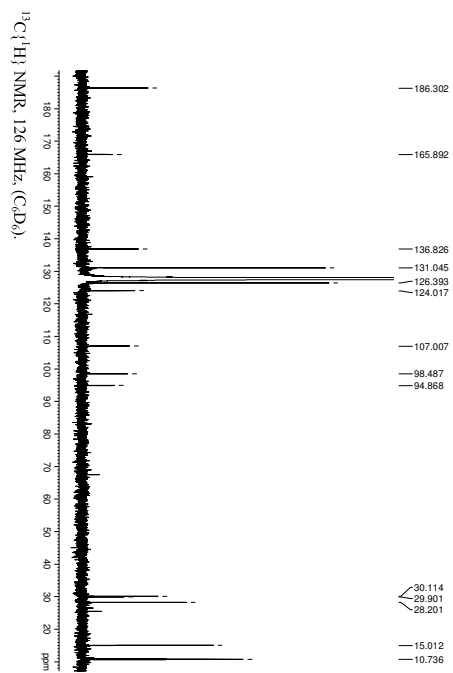
^1H NMR, 300 MHz, (C_6D_6).



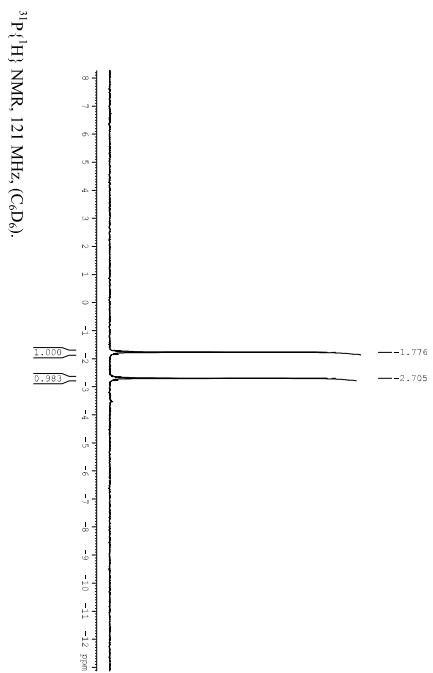
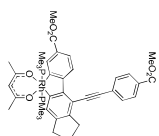
^1H NMR, 300 MHz, (C_6D_6).



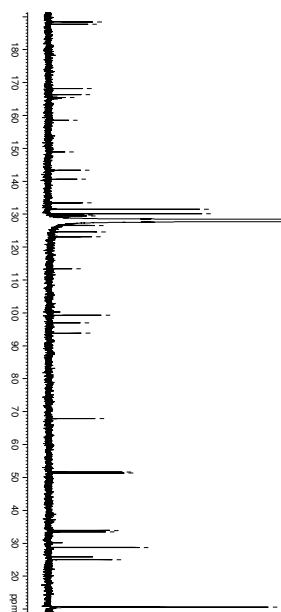
^1H NMR, 300 MHz, (C_6D_6).



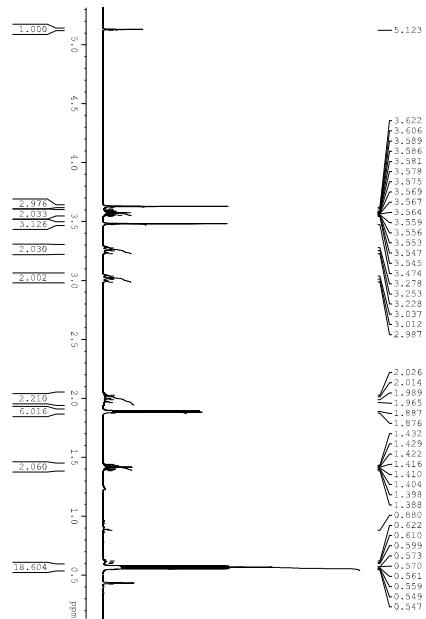
Rhodium biphenyl complex (7a)



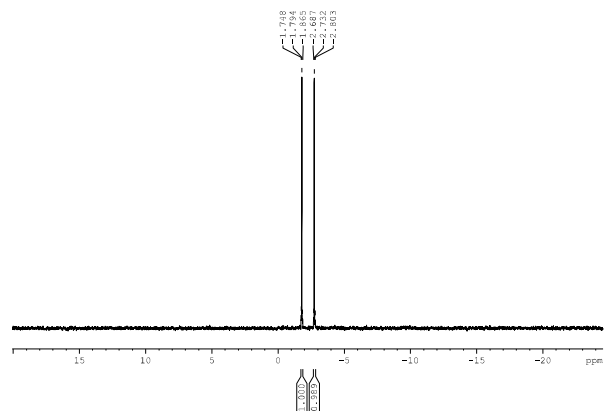
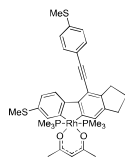
$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (C_6D_6).



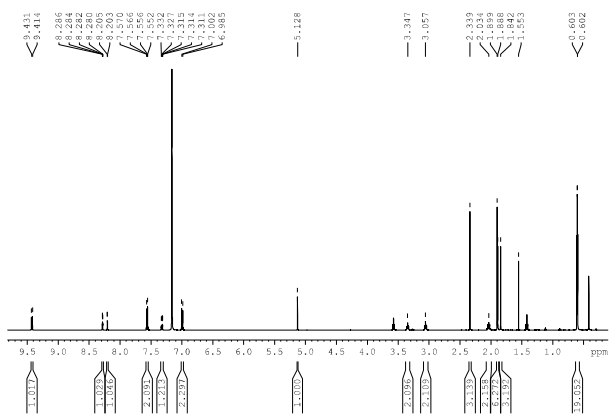
^1H NMR, 300 MHz, (C_6D_6).



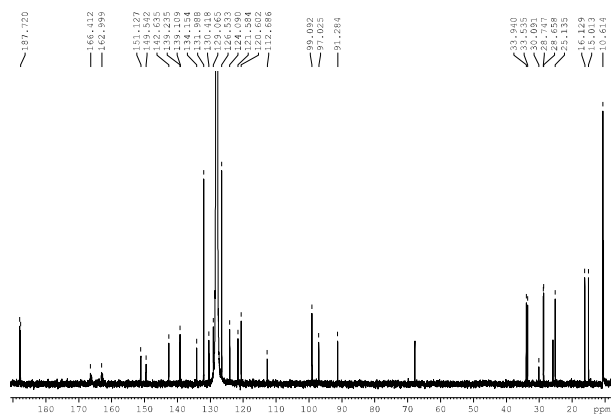
Rhodium-biphenyl-complex (7b)



$^{31}\text{P}\{^1\text{H}\}$ NMR, 121 MHz, (C_6D_6).

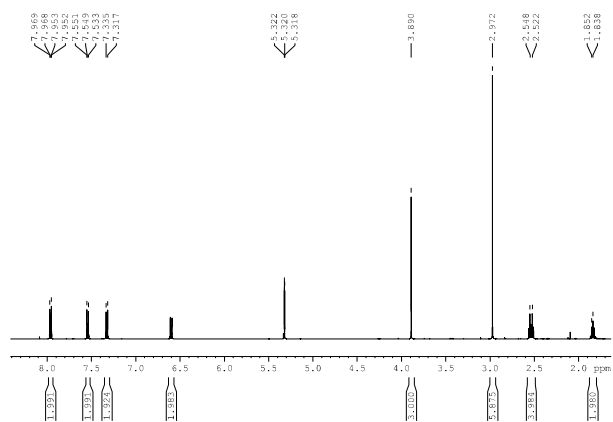
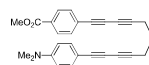


^1H NMR, 500 MHz, (C_6D_6).

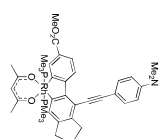
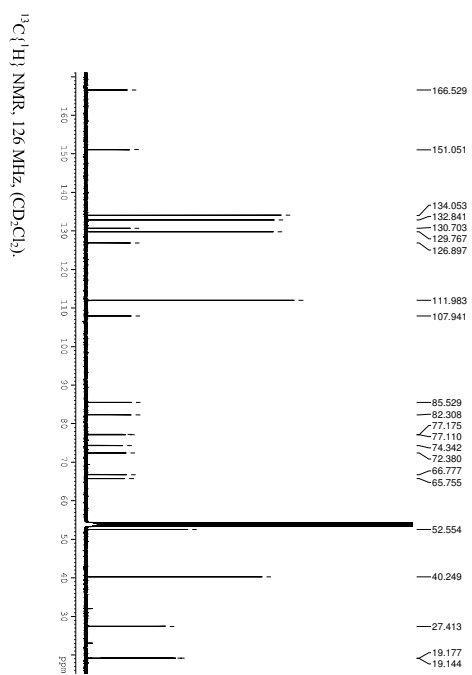


$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (C_6D_6).

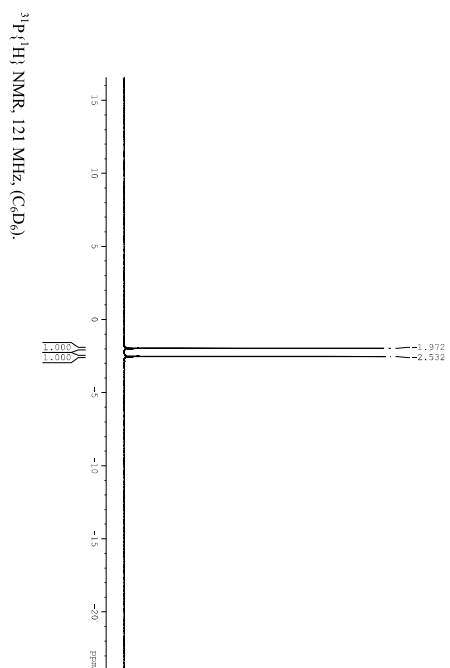
D/A-substituted α,ω -bis(phenylbutadiynyl)alkane (8)

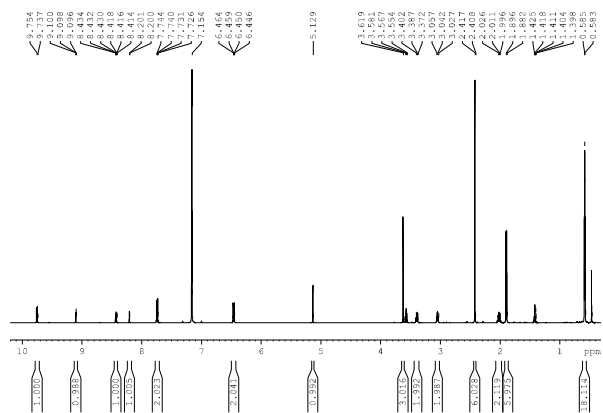


^1H NMR, 500 MHz, (CD_2Cl_2).

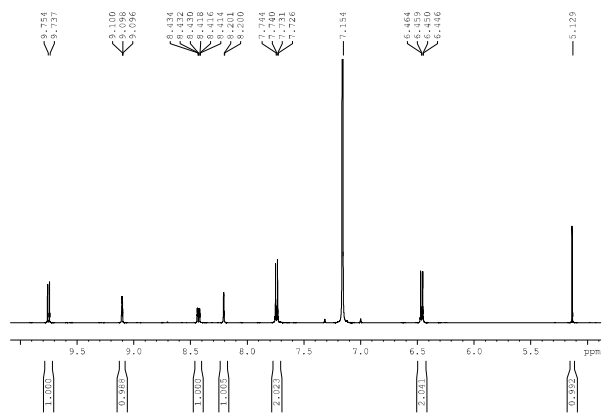


$\text{Me}_2\text{N}/\text{CO}_2\text{Me}$ substituted rhodium bipyridyl complex (9)

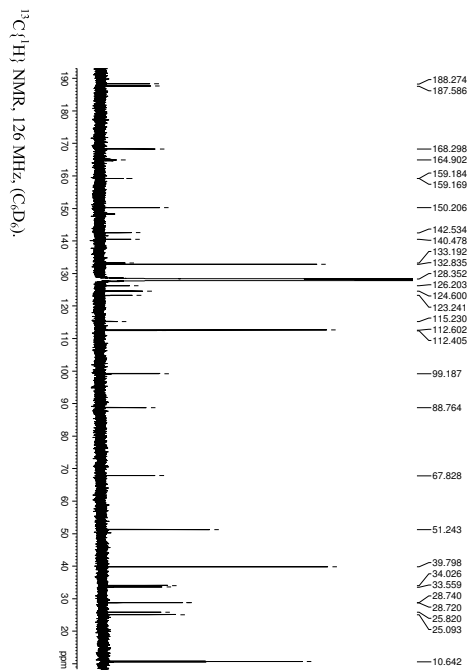
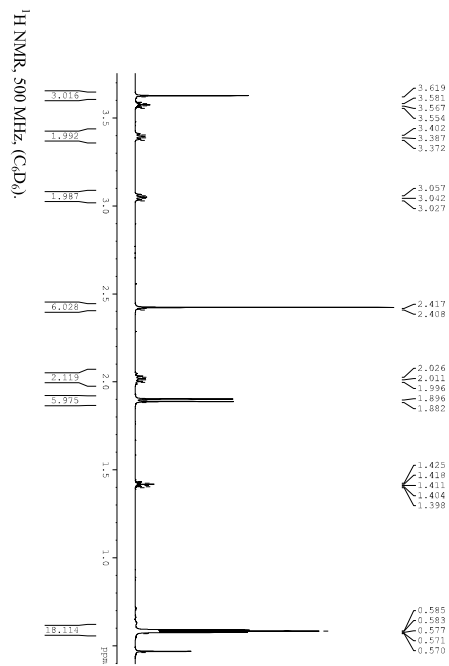




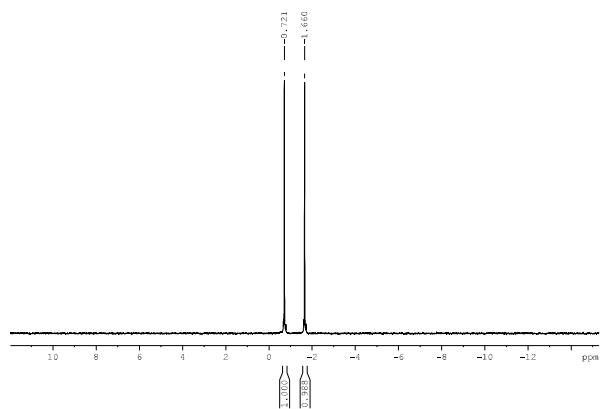
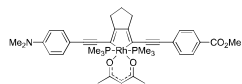
^1H NMR, 500 MHz, (C_6D_6).



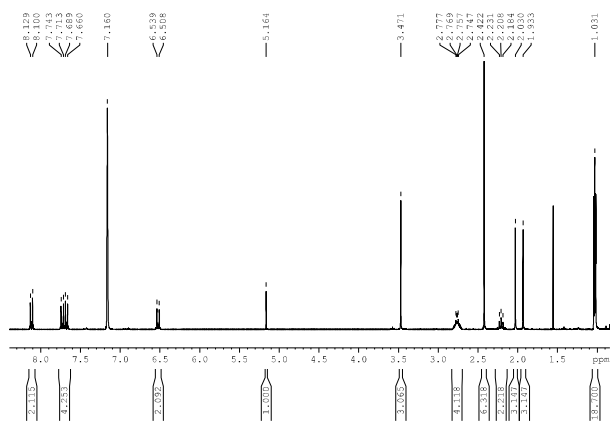
^1H NMR, 500 MHz, (C_6D_6).



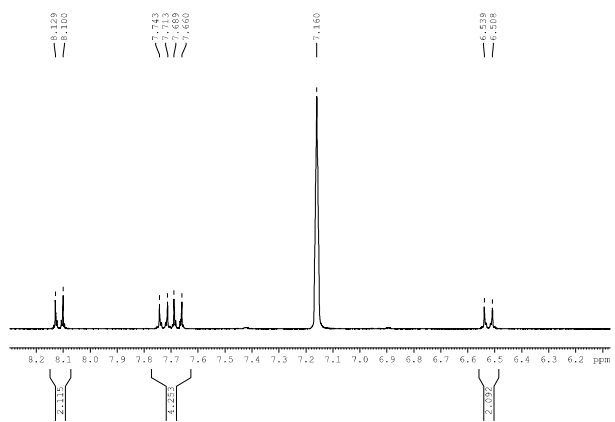
Me₂N/ CO₂Me substituted 2,5-Bis(phenylethynyl)rhodacyclopenta-2,4-diene (11)



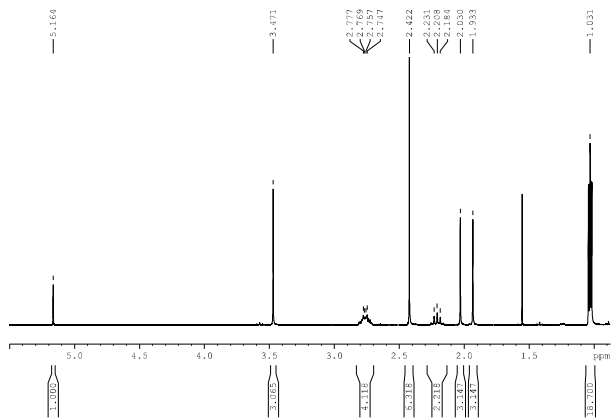
³¹P{¹H} NMR, 121 MHz, (C₆D₆).



¹H NMR, 300 MHz, (C₆D₆).



^1H NMR, 300 MHz, (C_6D_6).



^1H NMR, 300 MHz, (C_6D_6).

$^{13}\text{C}\{^1\text{H}\}$ NMR, 126 MHz, (C_6D_6).

