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Supporting Information

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Stabilization of Reactive Organometallic Intermediates inside a Self-Assembled Nanoscale Host

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Experimental Section

General Considerations

All reagents were obtained from commercial suppliers and used without further purification unless stated otherwise. Anhydrous solvents were dried over activated alumina. $K_6(NMe_4)_5[NMe_4 \subset Ga_4L_6]$, $K_{12}[Ga_4L_6]$, $Na_{12}[Al_4L_6]$,[1] CpRu(COD)Cl,[2] and Cp*Ru(COD)Cl[3] were synthesized according to the published procedures. NMR spectra were measured with a Bruker 500 or 400 MHz spectrometer. ^1H NMR chemical shifts are reported as δ in ppm relative to residual protonated solvent resonances; ^{13}C NMR chemical shifts are reported relative to solvent resonances. ^{19}F NMR chemical shifts are reported relative to external $CFCl_3$. Coupling constants are reported in Hz. IR spectra were recorded on an Avatar 370 FT-IR instrument. Samples of encapsulated **1** and **2** for mass spectrometry were prepared using the $Na_{12}[Al_4L_6]$ assembly. Mass spectra were recorded on a triple quadrupole VG Quatttro mass spectrometer in the Mass Spectrometry Laboratory, in the College of Chemistry at the University of California at Berkeley. High resolution TOF mass spectra were recorded at the Waters facility in Dublin, CA, on a Waters QTOF API mass spectrometer equipped with a Z-spray source.

$K_5(NMe_4)_6[CpRu(\mathit{cis}\text{-}1,3,7\text{-octatriene}) \subset Ga_4L_6]$ ($[\mathbf{1} \subset Ga_4L_6]^{11-}$). In the glove box CpRu(COD)Cl (1.80 mg, 5.81 μmol) was dissolved in 1.50 mL Et_2O. To this solution was added a solution of $K_6(NMe_4)_5[NMe_4 \subset Ga_4L_6]$ (20.3 mg, 5.81 μmol) in 1.50 mL H_2O. The biphasic reaction mixture was vigorously stirred for 30 min at room temperature after which the ethereal layer has become colorless. The aqueous layer was separated and all volatile materials removed *in vacuo*. The product was isolated as a yellow solid in 89 % yield (18.7 mg, 5.17 μmol). ^{1}H NMR (500 MHz, D_2O), N-H not observed due to H-D exchange, the two diastereomeric species are denoted A and B and assignments were made based on the TOCSY spectrum: δ 7.97 (d, $^3J_{H\text{-}H} = 7.7$ Hz, 24H, Ar-H), 7.66 (d, $^3J_{H\text{-}H} = 8.5$ Hz, 24H, Ar-H), 7.20 (dd, $^3J_{H\text{-}H} = 8.3$ Hz, $^4J_{H\text{-}H} = 1.6$ Hz, 24H, Ar-H), 6.95 (t, $^3J_{H\text{-}H} = 8.0$ Hz, 24H, Ar-H), 6.59 (d, $^3J_{H\text{-}H} = 7.5$ Hz, 24H, Ar-H), 6.45 (t, $^3J_{H\text{-}H} = 8.0$ Hz, 24H, Ar-H), 2.54 (s, b, 72H, NMe_4, exterior), 2.07 (s, 5H, Cp-H, encaps.), 2.04 (s, 5H, Cp-H, encaps.), 1.47 (t, 1H, =CH, encaps. A), 1.41 (t, 1H, =CH, encaps. B), 1.15 (d, 1H, =CH_2, encaps. A), 1.11 (d, 1H, =CH_2, encaps. B), 0.77 (m, 2H, =CH, encaps. A and B), 0.53 (m, 1H, CH_2, encaps. A), 0.50 (d, 1H, =CH_2, encaps. B), 0.52 (d, 1H, =CH_2, encaps. A), 0.15 (t, 1H, =CH, encaps. B), 0.09 (t, 1H, =CH, encaps. A), 0.02-(-0.31) (m, 4H, CH_2, encaps. A and B), -0.08 (d, 1H, =CH_2, encaps. A), -0.17 (d, 1H, =CH_2, encaps. B), -0.51 (m, 2H, =CH, encaps. A and B), -1.81 (d, 1H, =CH_2, encaps. A), -1.83 (d, 1H, =CH_2, encaps. B), -2.10 (m, 1H, CH_2, encaps. B), -2.23 (m, 1H, CH_2, encaps. A) ppm. ES(-)-MS (65% H_2O, 34 % MeOH, 1 % NaOH), ♦ = $[Al_4L_6]^{12-}$, *m/z*: 603 [♦ $\supset$ CpRu(1,3,7-octatriene)$^+$ + 3Na$^+$ + 3H$^+$]$^{5-}$, 607 [♦ $\supset$ CpRu(1,3,7-octatriene)$^+$ + 4Na$^+$ + 2H$^+$]$^{5-}$, 612 [♦ $\supset$ CpRu(1,3,7-octatriene)$^+$ + 5Na$^+$ + 1H$^+$]$^{5-}$, 616 [♦ $\supset$ CpRu(1,3,7-octatriene)$^+$ + 6Na$^+$]$^{5-}$, 754 [♦ $\supset$ CpRu(1,3,7-octatriene)$^+$ + 3Na$^+$ + 4H$^+$]$^{4-}$, 759 [♦ $\supset$

CpRu(1,3,7-octatriene)$^{+}$ + 4Na^{+} + 3H^{+}]$^{4-}$, 764 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 5Na^{+} + 2H^{+}]$^{4-}$, 770 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 6Na^{+} + 1H^{+}]$^{4-}$, 775 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 7Na^{+}]$^{4-}$, 1027 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 6Na^{+} + 2H^{+}]$^{3-}$, 1034 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 7Na^{+} + 1H^{+}]$^{3-}$, 1042 [♦ ⊃ CpRu(1,3,7-octatriene)$^{+}$ + 8Na^{+}]$^{3-}$.

[CpRu(*cis*-1,3,7-octatriene)]BF$_4$ (1-BF$_4$). In the glove box, CpRu(COD)Cl (62.1 mg, 0.200 mmol) was dissolved in 5 mL CH_2Cl_2. To the orange solution was added AgBF$_4$ (42.9 mg, 0.220 mmol) and the reaction mixture was stirred for 30 min at room temperature. The solution was filtered and all volatile materials were removed *in vacuo*. The product was isolated as an orange solid in 92% yield (66.3 mg, 0.184 mmol). Due to its unstable nature **1**-BF$_4$ was only be characterized in solution. For resonance assignments see also Figure S-2. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 6.07 (ddd, app. dt, $^{3}J_{\text{H-H}}$ = 7.8 Hz, $^{4}J_{\text{H-H}}$ = 2.0 Hz , 1H, H$_a$), 5.44 (s, 5H, Cp-H), 5.43 (m, 1H, H$_b$), 4.49 (d, $^{3}J_{\text{H-H}}$ = 12.0 Hz, 1H, H$_c$), 4.32 (d, $^{3}J_{\text{H-H}}$ = 8.5 Hz, 1H, H$_d$), 4.19 (dd, app. t, $^{3}J_{\text{H-H}}$ = 8.5 Hz, 1H, H$_e$), 3.75 (ddd, $^{3}J_{\text{H-H}}$ = 12.0 Hz, $^{3}J_{\text{H-H}}$ = 8.5 Hz, $^{3}J_{\text{H-H}}$ = 6.5 Hz, 1H, H$_f$), 3.61 (d, $^{3}J_{\text{H-H}}$ = 6.5 Hz, 1H, H$_g$), 3.20 (dddd, app. ddt, $^{2}J_{\text{H-H}}$ = 15.6 Hz, $^{3}J_{\text{H-H}}$ = 13.8 Hz, $^{3}J_{\text{H-H}}$ = 7.7 Hz, 1H, H$_h$), 3.05 (dd, $^{2}J_{\text{H-H}}$ = 15.8 Hz, $^{3}J_{\text{H-H}}$ = 5.5 Hz, 1H, H$_i$), 2.70 (ddd, app. dt, $^{2}J_{\text{H-H}}$ = 13.6 Hz, $^{3}J_{\text{H-H}}$ = 6.8 Hz, 1H, H$_j$), 1.80 (d, $^{3}J_{\text{H-H}}$ = 13.4 Hz, 1H, H$_k$), 1.48 (dddd, app. ddt, $^{2}J_{\text{H-H}}$ = 14.0 Hz, $^{3}J_{\text{H-H}}$ = 11.0 Hz. $^{3}J_{\text{H-H}}$ = 6.5 Hz, 1H, H$_l$) ppm. ^{13}C{^{1}H} NMR (500 MHz, CD_2Cl_2): 98.4 (C$_H$), 96.8 (C$_G$), 89.0 (Cp), 83.2 (C$_F$), 82.5 (C$_E$), 58.1 (C$_D$), 38.6 (C$_B$), 36.6 (C$_A$) ppm. ^{19}F NMR (376.5 MHz, $CDCl_3$): -152.0 ppm.

$K_5(NMe_4)_6[CpRu(COD)(CO) \subset Ga_4L_6]$ ($[2 \subset Ga_4L_6]^{11-}$). To an aqueous solution of $K_6(NMe_4)_5[NMe_4 \subset Ga_4L_6]$ (22.3 mg, 6.37 μmol) was added 1 equiv. of $[CpRu(COD)(CO)]BF_4$ (2.49 mg, 6.37 μmol). The solution was stirred for 1 h, filtered, and all volatiles removed under reduced pressure. The product was isolated almost quantitatively as a yellow solid (22.4 mg, 6.05 μmol, 95%). IR (KBr pellet): $\nu_{C\text{-}O}$ = 2026 cm^{-1}. ^1H NMR (500 MHz, D_2O), N-H not observed due to H-D exchange: δ 8.02 (d, $^3J_{H\text{-}H}$ = 7.7 Hz, 12H, napht-H), 7.66 (d, $^3J_{H\text{-}H}$ = 8.5 Hz, 12H, napht-H), 7.25 (dd, $^3J_{H\text{-}H}$ = 8.2 Hz, $^4J_{H\text{-}H}$ = 1.5 Hz, 12H, cat-H), 6.90 (t, $^3J_{H\text{-}H}$ = 8.2 Hz, 12H, napht-H), 6.64 (dd, $^3J_{H\text{-}H}$ = 7.4 Hz, $^4J_{H\text{-}H}$ = 1.5 Hz, 12H, cat-H), 6.51 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 12H, cat-H), 2.66 (s, b, 60H, NMe_4, exterior), 2.31 (s, 5H, Cp-H, encaps.), 1.16 (m, 1H, COD C=C-H, encaps.), 1.12 (m, 1H, COD C=C-H, encaps.), 0.43 (m, 1H, COD C=C-H, encaps.), 0.35 (m, 1H, COD C=C-H, encaps.), 0.01 (m, 1H, COD $–CH_2–$, encaps.), -0.28 (m, 1H, COD $–CH_2–$, encaps.), -0.46 (m, 1H, COD $–CH_2–$, encaps.), -0.52 (m, 2H, COD $–CH_2–$, encaps.), -0.93 (m, 1H, COD $–CH_2–$, encaps.), -1.00 (m, 1H, COD $–CH_2–$, encaps.), -1.33 (m, 1H, COD $–CH_2–$, encaps.) ppm. ES(-)-MS (65% H_2O, 34 % MeOH, 1 % NaOH), ♦ = $[Al_4L_6]^{12-}$, *m/z*: 608 $[♦ \supset CpRu(COD)(CO)^+ + 3Na^+ + 3H^+]^{5-}$, 613 $[♦ \supset CpRu(COD)(CO)^+ + 4Na^+ + 2H^+]^{5-}$, 617 $[♦ \supset CpRu(COD)(CO)^+ + 5Na^+ + 1H^+]^{5-}$, 622 $[♦ \supset CpRu(COD)(CO)^+ + 6Na^+]^{5-}$, 766 $[♦ \supset CpRu(COD)(CO)^+ + 4Na^+ + 3H^+]^{4-}$, 772 $[♦ \supset CpRu(COD)(CO)^+ + 5Na^+ + 2H^+]^{4-}$, 777 $[♦ \supset CpRu(COD)(CO)^+ + 6Na^+ + 1H^+]^{4-}$, 782 $[♦ \supset CpRu(COD)(CO)^+ + 7Na^+]^{4-}$, 1051 $[♦ \supset CpRu(COD)(CO)^+ + 8Na^+]^{3-}$.

[Cp*Ru(*cis*-1,3,7-octatriene)]BF_4 (3-BF_4). To generate **3**-BF_4 in solution, Cp*Ru(COD)Cl (31.0 mg, 81.6 μmol) was dissolved in 0.75 mL CD_2Cl_2 in the glove box. To the orange solution was added $AgBF_4$ (17.5 mg, 89.8 μmol) and the reaction mixture was stirred for 15 min at room temperature. The solution was filtered and the filtrate, an orange solution, was placed in an NMR tube and the spectra recorded. Decomposition of the complex starts after 2 h and is complete within 30 h. ^1H NMR (500 MHz, $CDCl_3$): δ 4.93 (ddd, app. dt, $^3J_{H\text{-}H}$ = 7.6 Hz, $^3J_{H\text{-}H}$ = 2.5 Hz , 1H, =CH-), 4.27 (dddd, $^3J_{H\text{-}H}$ = 4.9 Hz, $^3J_{H\text{-}H}$ = 8.6 Hz, $^3J_{H\text{-}H}$ = 10.8 Hz, $^3J_{H\text{-}H}$ = 13.3 Hz, 1H, =CH-), 4.19 (d, $^3J_{H\text{-}H}$ = 6.4 Hz, 1H, $=CH_2$), 3.79 (ddd, $^3J_{H\text{-}H}$ = 11.5 Hz, $^3J_{H\text{-}H}$ = 8.3 Hz, $^3J_{H\text{-}H}$ = 6.6 Hz, 1H, =CH-), 3.22 (d, $^3J_{H\text{-}H}$ = 11.6 Hz, 1H, $=CH_2$), 3.14 (dd, app. t, $^3J_{H\text{-}H}$ = 8.3 Hz, 1H, =CH-), 3.07 – 2.95 (m, 2H, $-CH_2-$), 2.69 (ddd, app. dt, $^2J_{H\text{-}H}$ = 13.4 Hz, $^3J_{H\text{-}H}$ = 6.2 Hz, 1H, $-CH_2-$), 2.52 (d, $^3J_{H\text{-}H}$ = 8.6 Hz, 1H, $=CH_2$), 1.94 (d, $^3J_{H\text{-}H}$ = 13.1 Hz, 1H, $=CH_2$), 1.73 (s, 15H, Cp-CH_3), 1.54 (dddd, $^2J_{H\text{-}H}$ = 13.3 Hz, $^3J_{H\text{-}H}$ = 13.3 Hz, $^3J_{H\text{-}H}$ = 10.8 Hz, $^3J_{H\text{-}H}$ = 7.0 Hz, 1H, =CH-) ppm. $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): 104.8 (=CH-), 101.4 ($\underline{Cp}$-CH_3), 97.2 (=CH-), 90.3 (=CH-), 89.5 (=CH-), 67.3 ($=CH_2$), 62.9 ($=CH_2$), 38.4 ($-CH_2-$), 37.3 ($-CH_2-$), 9.8 (Cp-$\underline{C}H_3$) ppm. ^{19}F NMR (376.5 MHz, $CDCl_3$): -151.6 ppm.

K_{11}[Cp*Ru(*cis*-1,3,7-octatriene) ⊂ Ga_4L_6] ([3 ⊂ Ga_4L_6]$^{11-}$). To a solution of $K_{12}[Ga_4L_6]$ (50.0 mg, 14.7 μmol) in 5 mL of water was added an ethereal solution (6 mL) of Cp*Ru(COD)Cl (5.58 mg, 14.7 μmol) in equimolar concentration. Vigorous stirring at room temperature for 2 h led to loss of the yellow color of the organic layer. The two layers were separated. All volatile materials were removed from the aqueous solution under reduced pressure, yielding a yellow solid (47.8 mg, 13.2 μmol, 90%). ^1H NMR (500 MHz, D_2O), N-H not observed due to H-D exchange, aromatic region broad: δ 1.70 (d, $^3J_{H\text{-}H}$ = 6.4 Hz, 1H, triene $=CH_2$, encaps.), 1.64 (m, 1H, triene, encaps.), 1.60 (m, 1H, triene, encaps.), 1.47 (d, $^3J_{H-H}$ = 6.4 Hz, 1H, triene =CH_2, encaps.), 1.23 (m, 1H, triene, encaps.), 0.98 (dt, $^3J_{H-H}$ = 8.0 Hz, 1H, triene =CH, encaps.), 0.89 (m, 1H, triene, encaps.), 0.80 – 0.68 (m, 2H, triene, encaps.), 0.55 (m, 1H, triene, encaps.), 0.36 (m, 1H, triene, encaps.), 0.18 – 0.04 (m, 2H, triene, encaps.), -0.03 (m, 1H, triene, encaps.), -0.07 (d, $^3J_{H-H}$ = 11.5 Hz, 1H, triene =CH_2, encaps.), -0.33 (d, $^3J_{H-H}$ = 11.8 Hz, 1H, triene =CH_2, encaps.), -0.48 (t, $^3J_{H-H}$ = 8.4 Hz, 1H, triene =CH, encaps.), -0.65 (t, $^3J_{H-H}$ = 8.3 Hz, 1H, triene =CH, encaps.), -0.71 (s, 15H, Cp-CH_3, encaps.), -0.73 (s, 15H, Cp-CH_3, encaps.), -0.84 (d, $^3J_{H-H}$ = 8.0 Hz, 1H, triene =CH_2, encaps.), -0.90 (m, 1H, triene, encaps.), -1.06 (d, $^3J_{H-H}$ = 8.1 Hz, 1H, triene =CH_2, encaps.), -1.33 (d, $^3J_{H-H}$ = 13.8 Hz, 1H, triene =CH_2, encaps.), -1.35 (d, $^3J_{H-H}$ = 13.4 Hz, 1H, triene =CH_2, encaps.), -2.15 (m, 1H, triene, encaps.) ppm. ES(-)-MS (65% H_2O, 34 % MeOH, 1 % NaOH), ♦ = $[Ga_4L_6]^{12-}$, *m/z*: 660 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 3Na$^+$ + 3H$^+$]$^{5-}$, 668 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 4K$^+$ + 2H$^+$]$^{5-}$, 676 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 5K$^+$ + 1H$^+$]$^{5-}$, 683 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 6K$^+$]$^{5-}$, 825 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 3K$^+$ + 4H$^+$]$^{4-}$, 835 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 4K$^+$ + 3H$^+$]$^{4-}$, 845 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 5K$^+$ + 2H$^+$]$^{4-}$, 854 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 6K$^+$ + 1H$^+$]$^{4-}$, 864 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 7K$^+$]$^{4-}$, 1114 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 4K$^+$ + 4H$^+$]$^{3-}$, 1127 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 5K$^+$ + 3H$^+$]$^{3-}$, 1139 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 6K$^+$ + 2H$^+$]$^{3-}$, 1152 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 7K$^+$ + 1H$^+$]$^{3-}$, 1165 [♦ $\supset$ Cp*Ru(1,3,7-octatriene)$^+$ + 8K$^+$]$^{3-}$.

K_{11}[Cp*Ru(COD)(CO) $\subset$ Ga_4L_6] ([4 $\subset$ Ga_4L_6]$^{11-}$). To a solution of K_{11}[Cp*Ru(1,3,7-octatriene) $\subset$ Ga_4L_6] (4) (25.0 mg, 6.92 μmol) in 600 μL D_2O in a J. Young tube was added 1 atm of CO. The NMR spectrum was monitored over several days, indicating that formation of the carbonyl complex is quantitative after 2 days. All volatile materials were removed under reduced pressure and the product isolated quantitatively as a yellow solid. IR (KBr pellet): $\nu_{C\text{-}O}$ = 2005 cm^{-1}. ^{1}H NMR (500 MHz, D_2O), N-H not observed due to H-D exchange, aromatic region broad: δ 0.97 (m, 1H, COD, encaps.), 0.66 – 0.43 (m, 4H, COD, encaps.), 0.16 (m, 3H, COD, encaps.), -0.29 (m, 1H, COD, encaps.), -0.33 (s, 15H, Cp-CH_3, encaps.), -0.44 (m, 1H, COD, encaps.), -0.96 (m, 1H, COD, encaps.), -1.33 (m, 1H, COD, encaps.) ppm. TOF MS ES(-) (75% H_2O, 25 % MeOH), ♦ = [Ga_4L_6]$^{12-}$, calcd. (found), *m/z*: 851.791 (851.787) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 5K$^+$ + 2H$^+$]$^{4-}$, 861.280 (861.276) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 6K$^+$ + 1H$^+$]$^{4-}$, 870.769 (870.770) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 7K$^+$]$^{4-}$, 1148.707 (1148.706) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 6K$^+$ + 2H$^+$]$^{3-}$, 1161.361 (1161.363) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 7K$^+$ + 1H$^+$]$^{3-}$, 1174.347 (1174.344) [♦ $\supset$ Cp*Ru(COD)(CO)$^+$ + 8K$^+$]$^{3-}$.

Supporting Figures

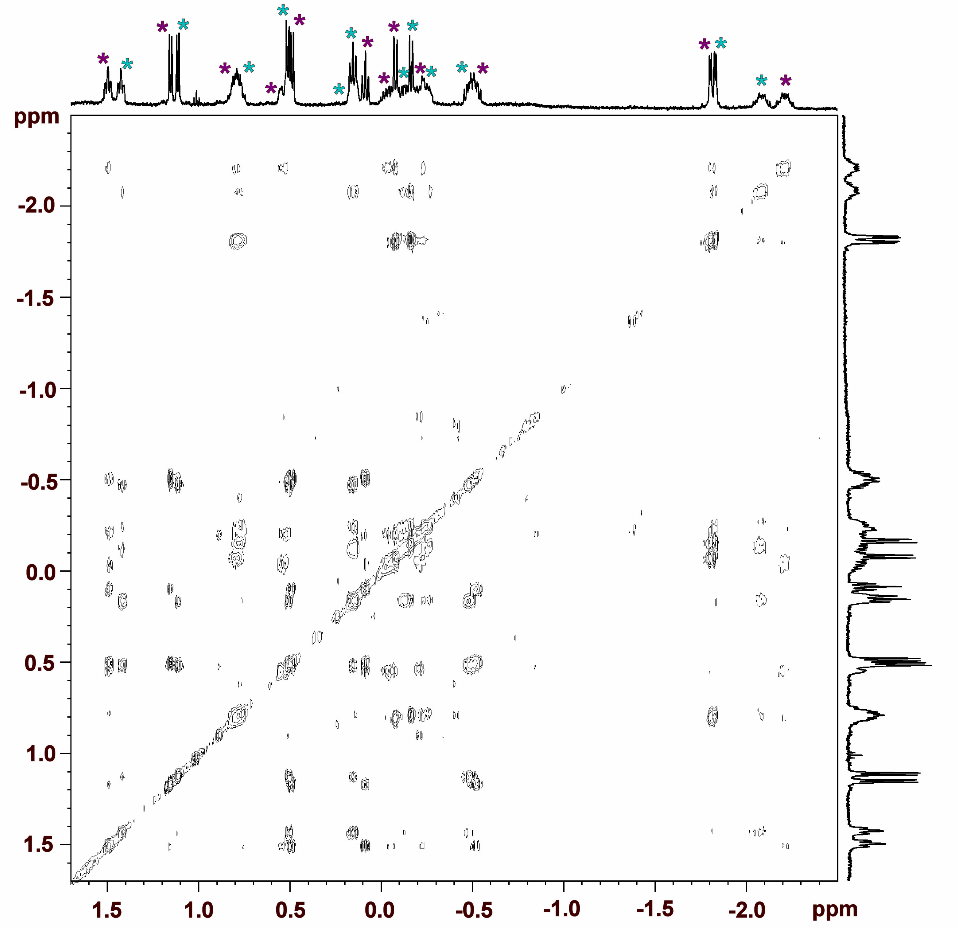

Figure S-1. 2D TOCSY spectrum of [$\mathbf{1} \subset Ga_4L_6$]$(NMe_4)_5K_6$. Two independent spin systems (* and *) with 12 resonances each can be identified.

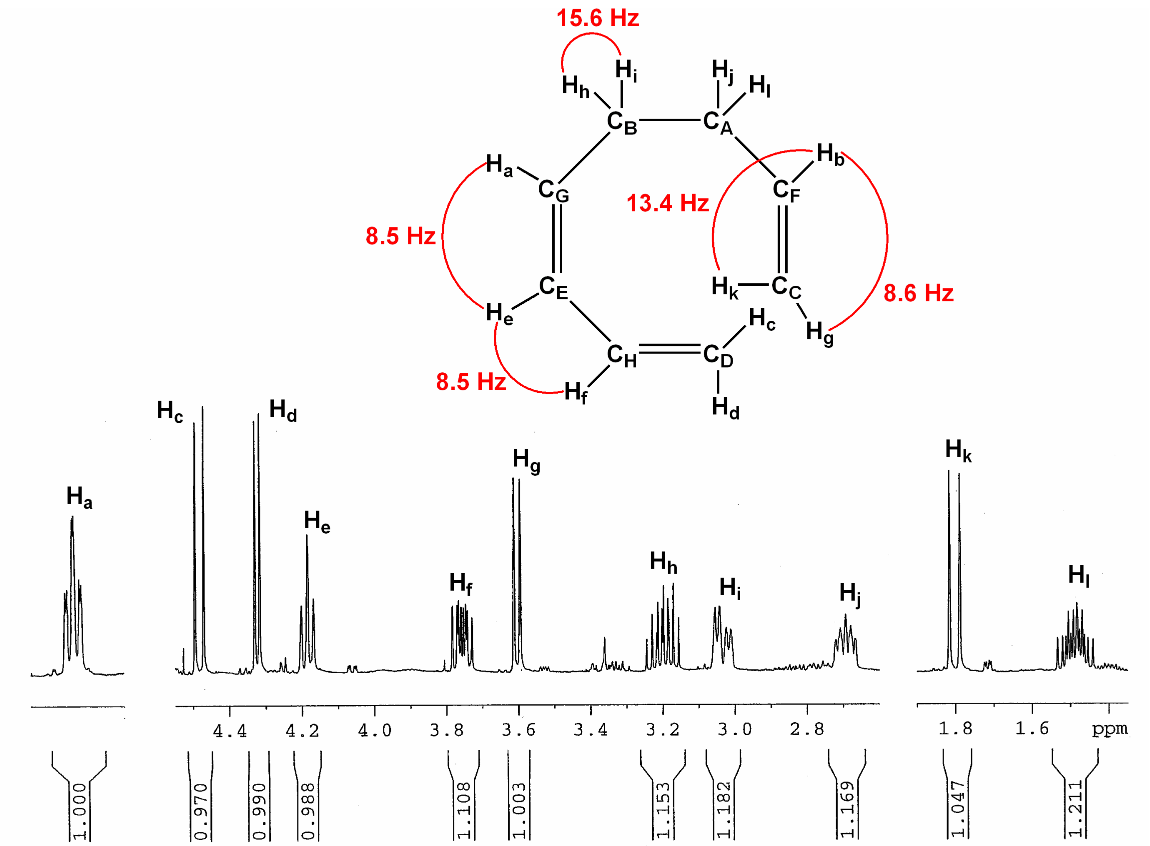

Figure S-2. ^{1}H NMR spectrum of **1**-BF_4. A very distinct feature in the spectrum are the doublets for H_c, H_d, H_g and H_k, the protons on the terminal methylene groups. Their orientation with respect to the adjacent protons can be assigned based on the coupling constants: H_k is *trans* to H_b ($^3J_{Hb\text{-}Hk}$ = 13.4 Hz) and H_g is *cis* to H_b ($^3J_{Hb\text{-}Hk}$ = 8.6 Hz). The fact that H_e appears as a triplet shows that $^3J_{He\text{-}Hf}$ = $^3J_{He\text{-}Ha}$ = 8.5 Hz. This allows for the conclusion that the configuration around C_E-C_G is *cis*. The geminal coupling constants for the methylene protons H_h, H_i and H_j, H_l are 15.6 Hz and 14.0 Hz, respectively, and are of common magnitude.

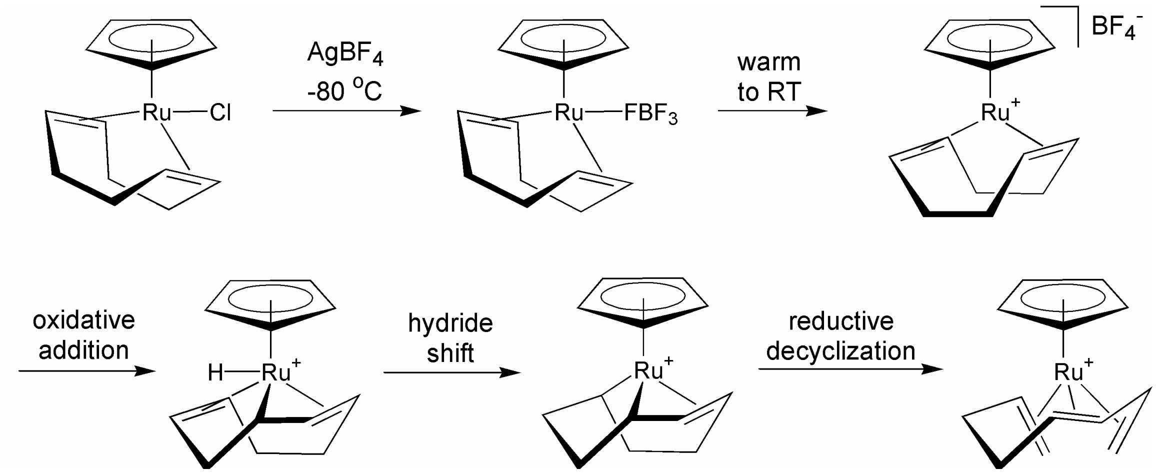

Figure S-3. Proposed mechanism for the formation of **1**, based on Variable Temperature NMR studies: At -80 °C an intermediate with C_s symmetry is observed, presumably CpRu(COD)F-BF_3 (with one of the four fluorines coordinated to the Ru-center). This complex is stable up to 0 °C. At this point formation of **1** starts, along with decomposition to the cyclooctatriene complex. A weak hydride signal at -12.3 ppm is also observed. A possible mechanism for the formation of **1** starts with an insertion of the metal into a methylene C-H bond. A hydride migration gives rise to 9-ruthenal(IV)bicyclo[4.2.1]-2-nonene and a reductive decyclization leads to the product.

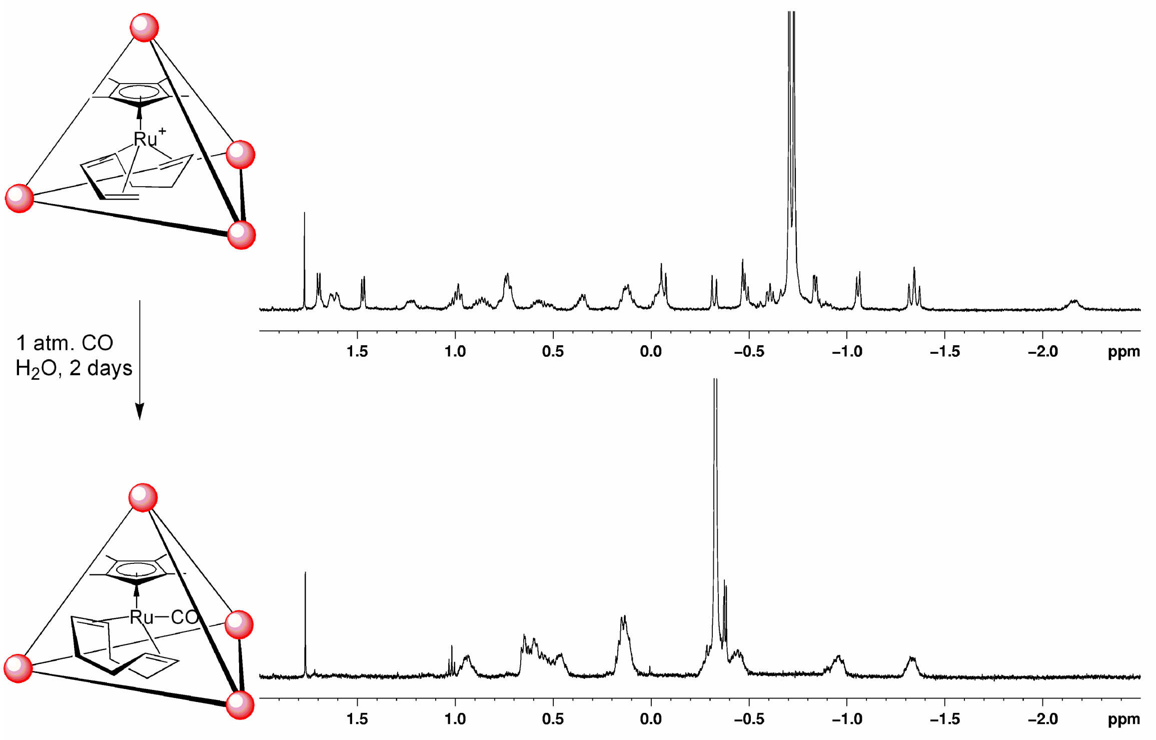

Figure S-4. Reaction of $K_{11}[Cp^*Ru(\textit{cis}\text{-}1,3,7\text{-octatriene}) \subset Ga_4L_6]$ with CO, monitored by ^{1}H NMR spectroscopy.

References

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