Steric-Enhanced, Selective C(CO)-C(α) Bond Cleavage of Ketone by Rhodium Porphyrin Methyl

*Hong Sang Fung, Bao Zhu Li and Kin Shing Chan**

Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, People's Republic of China

E-mail: ksc@cuhk.edu.hk

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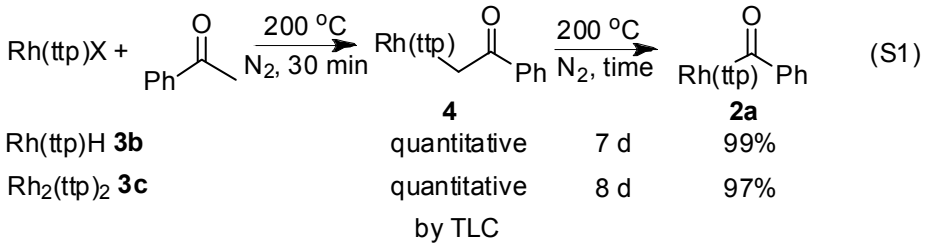
Reactions of Rh(ttp)H (3b) or $Rh_2(ttp)_2$ (3c) with Acetophenone

Rh(ttp)H and $Rh_2(ttp)_2$ quickly reacted with acetophenone at 200 ^oC to give quantitative amount of $Rh(ttp)CH_2COPh$ (observed by TLC analysis) in 30 minutes. Rh(ttp)COPh formed in high yield upon further heating (eq S1).



(S1)

Experimental Section

Unless otherwise noted, all reagents were purchased from commercial suppliers and directly used without further purification. Hexane was distilled from anhydrous calcium chloride. Thin layer chromatography was performed on pre-coated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 mesh) were used for column chromatography. All reactions were carried out in Telfon screw capped tube under N_2 with the mixture degassed for three freeze-thaw-pump cycles and wrapped with aluminum foil to prevent undesired photochemical reactions. The crude mixture was dried under high vacuum. The products were further purified by silica gel column chromatography eluting with a solvent mixture of hexane: CH_2Cl_2.

^1H NMR and ^{13}C NMR spectra were recorded on a Bruker DPX-300 at 300 MHz and 75 MHz or a Bruker AV-400MHz at 400 MHz and 100 MHz respectively. Chemical

Shifts were referenced with the residual solvent protons in chloroform-*d* (δ = 7.26 ppm) or tetramethylsilane (δ = 0.00 ppm) and benzene-d_6 (δ = 7.15 ppm) in ^{1}H NMR spectra, $CDCl_3$ (δ = 77.16 ppm) in ^{13}C NMR spectra as the internal standards. Chemical shifts (δ) were reported as part per million (ppm) in (δ) scale downfield from TMS. Coupling constants (*J*) were reported in Hertz (Hz). High resolution mass spectra (HRMS) were recorded on a ThermoFinnigan MAT 95 XL mass spectrometer. Fast atom bombardment spectra were performed with 3-nitrobenzyl alcohol (NBA) as the matrix. All single crystals were immersed in Paraton-N oil and sealed under N_2 in thin-walled glass capillaries. Data were collected at 123 K on a Bruker SMART 1000 CCD diffractometer using MoK_α radiation. An empirical absorption correction was applied using the SADABS program. All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F2 using the SHELXTL program package. All hydrogen atoms were geometrically fixed using the riding model. Rh(ttp)Me,[1] Rh(ttp)H[2] and $Rh_2(ttp)_2$[2] were synthesized according to the literature methods.

Reaction between Rh(ttp)Me and Acetophenone at 200 ^{o}C for 15 d. Rh(ttp)Me (**1**) (17.4 mg, 0.022 mmol) and acetophenone (1.5 mL) were heated at 200 ^{o}C under N_2 for 15 d. A red product Rh(ttp)COPh (**2a**)[1b] (17.9 mg, 0.021 mmol, 93%) with R_f =

0.43 (hexane/ CH_2Cl_2 = 1:1) was purified and collected by column chromatography. Rh(ttp)COPh (**2a**). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.43 (dd, 2 H, *J* = 8.1 Hz), 2.70 (s, 12 H), 5.95 – 6.00 (m, 2 H), 6.40 (t, 1 H, *J* = 7.8 Hz), 7.52 – 7.56 (m, 8 H), 7.95 – 8.01 (m, 8 H), 8.76 (s, 8 H).

Monitoring the Sequence of Reaction between Rh(ttp)Me and Acetophenone at 200 ^{o}C for 12 d. Rh(ttp)Me (**1**) (17.3 mg, 0.022 mmol) and acetophenone (1.5 mL) were heated at 200 ^{o}C under N_2. Aliquots of the reaction mixture were taken out regularly and analyzed by ^{1}H NMR spectroscopy in benzene-d_6. Rh(ttp)CH_2COPh (**4**) formed quantitatively in 1 hour, which further converted to Rh(ttp)COPh (**2a**) in 94% yield in 12 days. Water, as an immiscible liquid was observed visually and by ^{1}H NMR in 5 days while 28% yield (w.r.t. acetophenone) of 1,3,5-triphenylbenzene was obtained in 12 days. Rh(ttp)CH_2COPh (**4**) R_f = 0.09 (hexane/ CH_2Cl_2 = 1:1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ -4.14 (d, 2 H, *J* = 3.6 Hz), 2.70 (s, 12 H), 4.59 (d, 2 H, *J* = 7.6 Hz), 6.61 (t, 2 H, *J* = 7.7 Hz), 7.06 (t, 1 H, *J* = 7.3 Hz), 7.53 (t, 8 H, *J* = 8.4 Hz), 7.91 (dd, 4 H, *J* = 1.3, 7.4 Hz), 8.01 (dd, 4 H, *J* = 1.5, 7.5 Hz), 8.70 (s, 8 H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 1.0 (d, $^1J_{Rh\text{-}C}$ = 29.7 Hz), 21.7, 123.1, 125.1, 126.9, 127.5, 127.6, 130.8, 131.9, 133.8, 134.2, 137.3, 139.1, 143.2, 196.8. HRMS (FABMS): Calcd. for $C_{50}H_{41}N_4ORh^+$: m/z 890.2486. Found: m/z 890.2472.

Reaction between Rh(ttp)H and Acetophenone at 200 ^{o}C for 7 d. Rh(ttp)H (**3b**), freshly prepared from Rh(ttp)Cl (17.8 mg, 0.022 mmol), and acetophenone (1.5 mL) were heated at 200 ^{o}C under N_2. Rh(ttp)CH_2COPh formed quantitatively according to TLC analysis in 30 minutes. After 7 d, a red product Rh(ttp)COPh (**2a**) (19.1 mg, 0.022 mmol, 99%) was purified and collected by column chromatography.

Reaction between Rh_2(ttp)$_2$ and Acetophenone at 200 ^{o}C for 7 d. Rh_2(ttp)$_2$ (**3c**), freshly prepared from Rh(ttp)Cl (17.8 mg, 0.022 mmol), and acetophenone (1.5 mL) were heated at 200 ^{o}C under N_2. Rh(ttp)CH_2COPh formed quantitatively according to TLC analysis in 30 minutes. After 7 d, a red product Rh(ttp)COPh (**2a**) (18.7 mg, 0.021 mmol, 97%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and Propiophenone at 200 ^{o}C for 15 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and propiophenone (1.5 mL) were heated at 200 ^{o}C under N_2 for 15 d. A red product Rh(ttp)COPh (**2a**) (8.5 mg, 0.010 mmol, 44%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and *n*-Butyrophenone at 200 ^{o}C for 19 d. Rh(ttp)Me (**1**) (17.6 mg, 0.022 mmol) and *n*-butyrophenone (1.5 mL) were heated at 200 ^{o}C under N_2 for 19 d. A red product Rh(ttp)COPh (**2a**) (8.3 mg, 0.009 mmol, 43%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and Isobutyrophenone at 200 ^{o}C for 1 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and isobutyrophenone (1.5 mL) were heated at 200 ^{o}C under N_2 for 1 d. A red product Rh(ttp)COPh (**2a**) (18.7 mg, 0.021 mmol, 97%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and Acetone at 200 ^{o}C for 17 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and acetone (1.5 mL) were heated at 200 ^{o}C under N_2 for 17 d. A red product Rh(ttp)COMe (**2b**)[1b] (3.6 mg, 0.004 mmol, 20%) with R_f = 0.38 (hexane/ CH_2Cl_2 = 1:1) was purified and collected by column chromatography. Rh(ttp)COMe (**2b**). ^{1}H NMR ($CDCl_3$, 300 MHz) δ -2.79 (s, 3 H), 2.70 (s, 12 H), 7.54 (t, 8 H, *J* = 7.8 Hz), 8.06 (dd, 8 H, *J* = 3, 6.6 Hz), 8.01 (s, 8 H).

Reaction between Rh(ttp)Me and Diethyl Ketone at 200 ^{o}C for 16 d. Rh(ttp)Me (**1**) (17.4 mg, 0.022 mmol) and diethyl ketone (1.5 mL) were heated at 200 ^{o}C under N_2 for 16 d. A red product Rh(ttp)COEt (**2c**)[1b] (8.2 mg, 0.010 mmol, 45%) with R_f = 0.52 (hexane/ CH_2Cl_2 = 1:1) was purified and collected by column chromatography. Rh(ttp)COEt (**2c**). ^{1}H NMR (300 MHz, $CDCl_3$) δ -3.14 (q, 2 H, *J* = 7.5 Hz), -1.69 (t, 3 H, *J* = 7.2 Hz), 2.70 (s, 12 H), 7.26 (d, 8 H, *J* = 7.8 Hz), 8.05 (d, 8 H, *J* = 6.3 Hz), 8.80 (s, 8 H).

Reaction between Rh(ttp)Me and Methyl Isopropyl Ketone at 200 ^{o}C for 1 d. Rh(ttp)Me (**1c**) (17.6 mg, 0.022 mmol) and methyl isopropyl ketone (1.5 mL) were

heated at 200 ^{o}C under N_2 for 1 d. A red product Rh(ttp)COMe (**2b**) (17.0 mg, 0.021 mmol, 95%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and Diisopropyl Ketone at 200 ^{o}C for 30 minutes. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and diisopropyl ketone (1.5 mL) were heated at 200 ^{o}C under N_2 for 30 minutes. At the end of the reaction, an aliquot of reaction mixture was added to benzene-d_6 for ^{1}H NMR analysis. Acetone (δ = 1.5 ppm) was observed. A red product Rh(ttp)CO^{i}Pr (**2d**) (15.9 mg, 0.019 mmol, 86%) with R_f = 0.57 (hexane/ CH_2Cl_2 = 1:1) was purified and collected by column chromatography. Rh(ttp)CO^{i}Pr (**2d**) ^{1}H NMR ($CDCl_3$, 400 MHz) δ -3.68 (hept, 1 H, J = 6.8 Hz), -2.14 (d, 6 H, J = 6.8 Hz), 2.69 (s, 12 H), 7.53 (t, 8 H, J = 8.4 Hz), 7.99 (d, 4 H, J = 7.4 Hz), 8.09 (d, 4 H, J = 7.6 Hz), 8.79 (s, 8 H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 12.4, 19.3, 21.6, 29.4, 31.5, 42.6, 48.9, 122.8, 127.4, 127.5, 131.6, 133.7, 134.1, 137.3, 139.1, 143.3, 207.4 (d, $^{1}J_{Rh\text{-}C}$ = 29.8 Hz), 208.1. HRMS (FABMS): Calcd. for $C_{50}H_{41}N_4ORh^+$: m/z 843.2565. Found: m/z 843.2559.

Reaction between Rh(ttp)Me and Isobutyrophenone at 50 ^{o}C for 3 d. Rh(ttp)Me (**1**) (17.6 mg, 0.022 mmol) and isobutyrophenone (1.5 mL) were heated at 50 ^{o}C under N_2 for 3 d. A red product Rh(ttp)COPh (**2a**) (7.9 mg, 0.018 mmol, 41%) was purified and collected by column chromatography. Rh(ttp)Me (5.6 mg, 0.007 mmol, 32%) was recovered.

Reaction between Rh(ttp)Me and Methyl Isopropyl Ketone at 50 ^{o}C for 3 d. Rh(ttp)Me (**1**) (17.6 mg, 0.022 mmol) and methyl isopropyl ketone (1.5 mL) were heated at 50 ^{o}C under N_2 for 3 d. A red product Rh(ttp)COMe (**2b**) (10.2 mg, 0.013 mmol, 57%) was purified and collected by column chromatography. Rh(ttp)Me (6.8 mg, 0.009 mmol, 39%) was recovered.

Reaction between Rh(ttp)Me and Diisopropyl Ketone at 50 ^{o}C for 1 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and diisopropyl ketone (1.5 mL) were heated at 50 ^{o}C under N_2 for 1 d. A red product Rh(ttp)CO^{i}Pr (**2d**) (17.4 mg, 0.021 mmol, 94%) was purified and collected by column chromatography.

Reaction between Rh(ttp)Me and 2,6-Dimethylcyclohexanone at 100 ^{o}C for 4 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol) and 2,6-dimethylcyclohexanone (1.5 mL) were heated at 100 ^{o}C under N_2 for 4 d. A red product Rh(ttp)COCHMe$(CH_2)_3$COMe (**2e**) (17.1 mg, 0.019 mmol, 85%) with R_f = 0.03 (hexane/ CH_2Cl_2 = 1:1) was purified and collected by column chromatography. Rh(ttp)Me (2.4 mg, 0.003 mmol, 14%) was recovered. Rh(ttp)COCHMe$(CH_2)_3$COMe (**2e**) ^{1}H NMR ($CDCl_3$, 400 MHz) δ -3.61 (sext, 1 H, *J* = 5.6 Hz), -2.34 (d, 3 H, *J* = 6.8 Hz), -1.65 (q, 1 H, *J* = 7.8 Hz), -1.39 (m, 2 H), -0.92 (quint, 1 H, *J* = 8.6 Hz), 1.13 (m, 2 H), 1.72 (s, 3 H), 2.72 (s, 12 H), 7.56 (d, 8 H, *J* = 7.9 Hz), 8.04 (dd, 8 H, *J* = 2.0, 7.4 Hz), 8.10 (dd, 8 H, *J* = 2.1, 7.4 Hz), 8.84 (s, 8 H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 15.6, 21.7, 29.8, 43.5, 122.8, 127.5, 127.6,

131.6, 133.7, 134.3, 137.4, 139.3, 143.3, 208 (d, $^1J_{Rh\text{-}C}$ = 29.3 Hz). HRMS (FABMS): Calcd. for $C_{56}H_{49}N_4O_2Rh^+$: m/z 912.2905. Found: m/z 912.2924.

Reaction between Rh(ttp)Me and 2,6-Dimethylcyclohexanone in the Presence of 100 Equivalents of Water at 200 ^{o}C for 1 d. Rh(ttp)Me (**1**) (17.5 mg, 0.022 mmol), H_2O (100 equiv, 40 uL, 2.2 mmol) and 2,6-dimethylcyclohexanone (1.5 mL) were heated at 100 ^{o}C under N_2 for 1 d. A red product Rh(ttp)COCHMe$(CH_2)_3$COMe (**2e**) (18.9 mg, 0.021 mmol, 94%) was purified and collected by column chromatography. Rh(ttp)Me (0.9 mg, 0.001 mmol, 5%) was recovered.

Carbon-Hydrogen Bond Activation of Acetophenone by Rh(ttp)Me. Rh(ttp)Me (**1**) (4.0 mg, 0.005 mmol), acetophenone (60 uL, 0.5 mmol) and benzene-d_6 (500 uL) were added to an NMR tube with a Telfon screw capped. The reaction mixture was degassed for three freeze-thaw-pump cycles and flame sealed. The tube was heated at 200 ^{o}C in dark for 30 minutes and analyzed by ^{1}H NMR spectroscopy. 66% yield of Rh(ttp)CH_2COPh, 33% yield of Rh(ttp)H and 86% of methane were observed in 30 minutes.

Determine the Yield of CH_4 Formation[3]

The molar concentration of methane in benzene as a function of temperature and methane pressure is given by the following expression: $[CH_4]_{T,\,P}$ = [3.871x10^{-2} mol L^{-1} - (5.143x10^{-5})T] P, where P is the CH_4 pressure in atmospheres at 296 K, and T is

the temperature when taking the NMR (296 K).[4,5]

Mole of Rh(ttp)Me used = 5.08×10^{-6} mol

The yield of CH_4 formed in benzene-d_6 solvent = 8% (NMR yield, Me signal of the excess acetophenone as the internal standard)

Mole of CH_4 formed in benzene-d_6 = 5.08×10^{-6} x 8% = 4.06×10^{-7} mol

Conc. of CH_4 in benzene-d_6 = 4.06×10^{-7} mol/0.5×10^{-3} dm^3 *(volume of benzene-d_6 used is 0.5×10^{-3} dm^3)*

= 8.13×10^{-4} M

Pressure of CH_4 in gas phase = (8.13×10^{-4} M)/[3.871×10^{-2} mol L^{-1} - (5.143×10^{-5})(296 K)]

= 0.0346 atm

Mole of CH_4 in gas phase = [(0.0346 atm)(2.8×10^{-6} m^3)]/(8.205×10^{-5} m^3 atm K^{-1} mol^{-1})(296 K) *(volume of gas phase is 2.8×10^{-6} m^3)* = 3.99×10^{-6} mol

Total mole of CH_4 formed = 3.99×10^{-6} mol + 4.06×10^{-7} mol = 4.40×10^{-6} mol

Total yield of CH_4 formed = (4.40×10^{-6} mol/ 5.08×10^{-6} mol) x100% = 87%

Hydrolysis of Rh(ttp)CH_2COPh. Rh(ttp)CH_2COPh (**4**) (4.0 mg, 0.004 mmol), H_2O (100 equiv, 8.0 uL, 0.45 mmol) and benzene-d_6 (500 uL) were added to an NMR tube with a Telfon screw capped. The reaction mixture was degassed for three freeze-thaw-pump cycles and flame sealed. The tube was heated at 200 ^oC in dark for

5 minutes and analyzed by ^{1}H NMR spectroscopy. 42% of yield Rh(ttp)H, 13% yield of $Rh_2(ttp)_2$, 57% yield of acetophenone and 42% recovery yield of $Rh(ttp)CH_2COPh$ were obtained in 5 minutes.

References

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2. Wayland, B. B.; Van Voorhees, S. L.; Wilker, C. *Inorg. Chem.* **1986**, *25*, 4039-4042.
3. Choi, K. S.; Chiu, P. F.; Chan, K. S. *Organometallics* **2010**, *29*, 624-629.
4. (a) Evans, F. C.; Battino, R. *J. Chem. Thermodyn.* **1971**, *3*, 753. (b) Brunel, R. F.; Van Bibber, K. *Int. Crit. Tables 3*, 27.
5. Wayland, B. B.; Ba, S.; Sherry, A. E. *J. Am. Chem. Soc.* **1991**, *113*, 5305-5311.

6. X-ray Structures

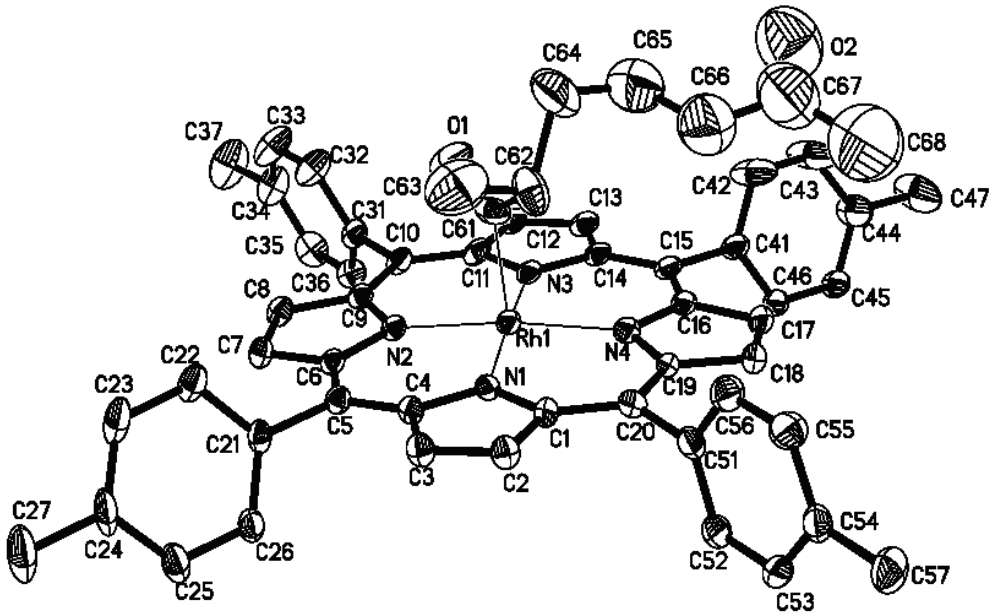


Figure S1a. ORTEP presentation of the molecular structure with numbering scheme for Rh(ttp)COCHMe$(CH_2)_3$COMe (**2e**) (30% probability displacement ellipsoids).

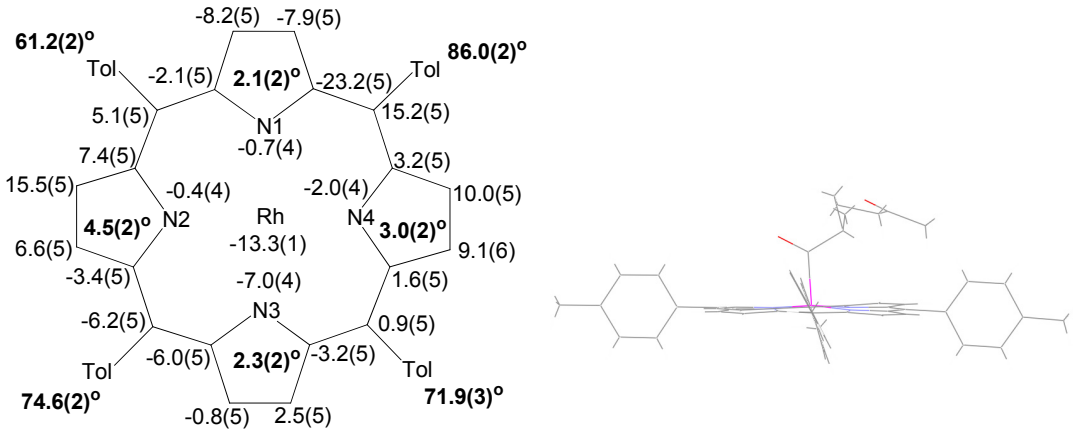


Figure S1b-c. (**S1b**)The conformations of porphyrins in **2e**, showing the displacement of the core atoms and of Rh from the 24-atom least squares plane of porphyrin core (in pm; positive value correspond to displacement towards

$COCHMe(CH_2)_3COMe$ ligand). Absolute values of the angles between pyrrole rings and least-squares plane and angles between tolyl substituents and the least-squares plane are shown in bold. (**S1c**) Wireframe presentation of the molecular structure for **2e**.

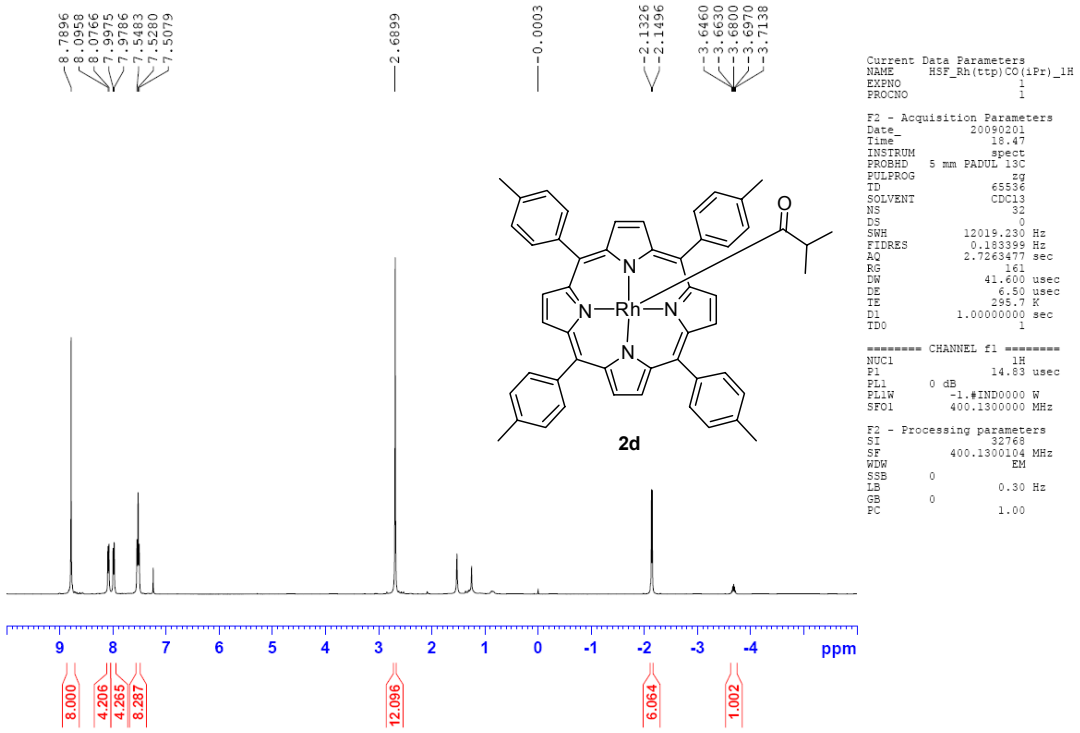
Table S1. Crystal Data and Summary of Data Collection and Refinement for 2e

	Rh(ttp)COCHMe$(CH_2)_3$COMe **2e**
Color, shape	Purple Prism
Empirical formula	$C_{56}H_{49}N_4O_2Rh$
Formula wt	912.90
Temp (K)	123(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	
a (Å)	13.8403(15)
b (Å)	24.524(3)
c (Å)	15.6200(17)
α (deg)	90
β (deg)	95.666(2)
γ (deg)	90
Volumn ($Å^3$)	5275.9(10)
Z	4
Calcd density (g cm^{-3})	1.149
abs coeff (mm^{-1})	0.365
F(000)	1896
Crystal size (mm)	0.50 x 0.30 x 0.20
θ range for data collection (deg)	1.48 to 25.25
Limiting indices	-16<=h<=16

	-29<=k<=29
	-16<=l<=18
No. of reflections collected/ unique	74777 / 9208 [R(int) = 0.0731]
completeness to θ	96.3 (θ = 25.25)
Absorption correction	multi-scan
Max. and min. transmission	0.7456 and 0.5779
Refinement method	Full-matrix least-squares on F^2
No. of data/ restraints/ parameters	9208 / 39 / 568
GOF	1.067
Final R indices [I>2s (I)]	R_1 = 0.0731
	$_wR_2$ = 0.1911
R indices (all data)	R_1 = 0.0983
	$_wR_2$ = 0.2057
Largest diff peak and hole (e Å^3)	1.385 and -0.818

[a] $R_1 = \sum(||F_0|-|F_c||)/\sum|F_0|$. [b] $_wR_2 = \{\sum[_w(F_0^2 - F_c^2)^2]/\sum[_w(F_0^2)^2]\}^{1/2}$. [c] Weighting scheme $w^{-1} = \sigma^2(F_0^2) + (w_1P)^2 + w_2P$ where $P = (F_0^2 + 2F_c^2)/3$.

NMR Spectra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2d
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PROCNO 1
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SOLVENT CDCl3
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DE 6.50 usec
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D1 1.00000000 sec
TD0 1
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PL1 0 dB
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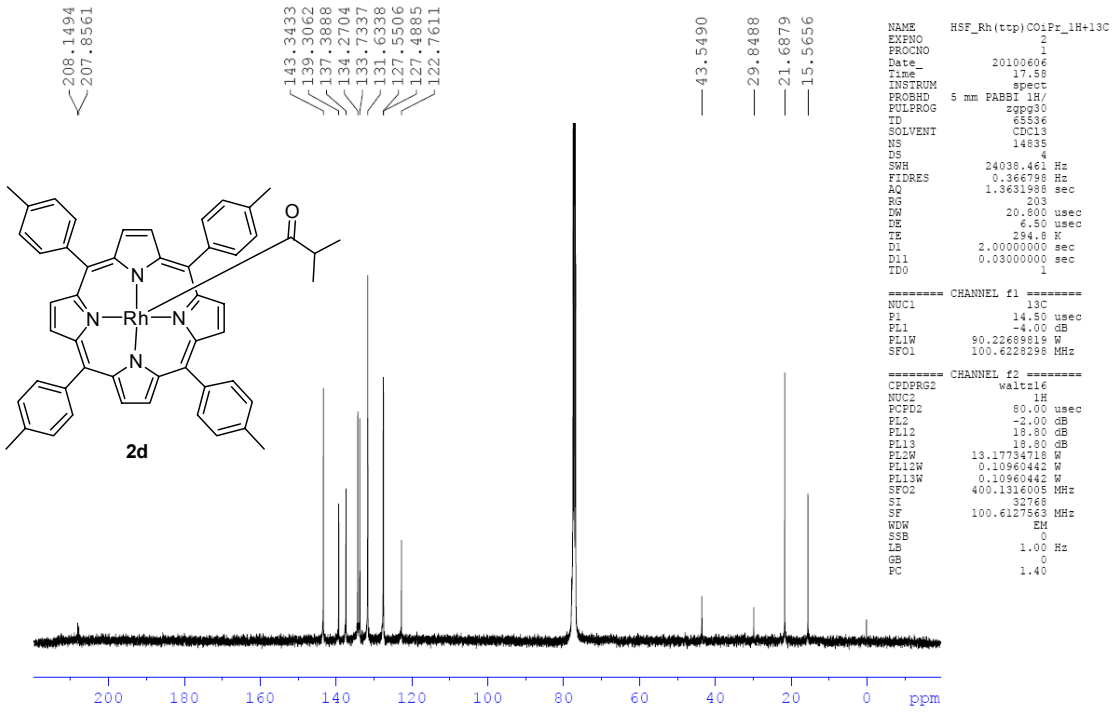
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PL13 18.80 dB
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SSB 0
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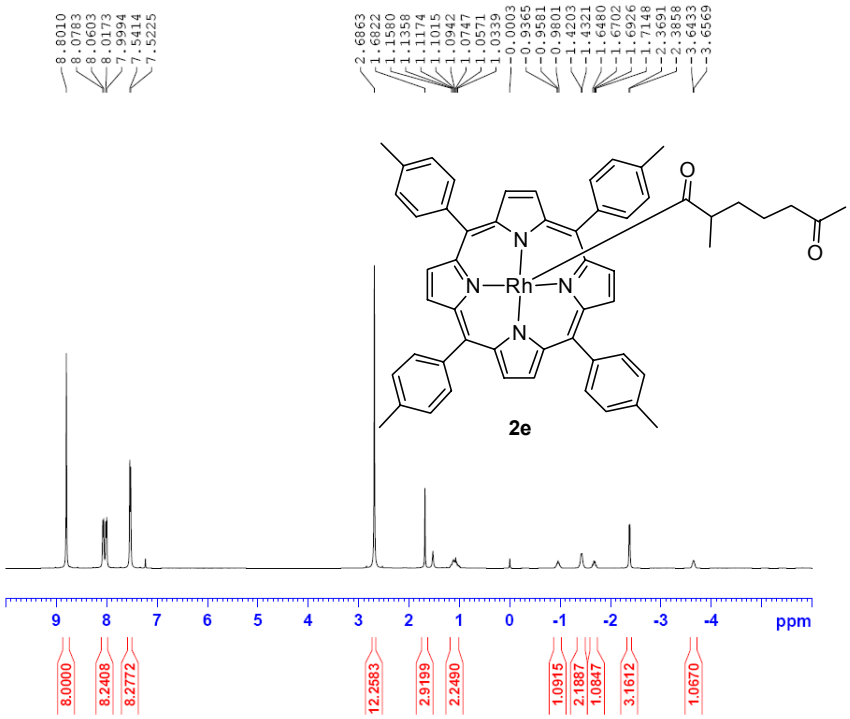
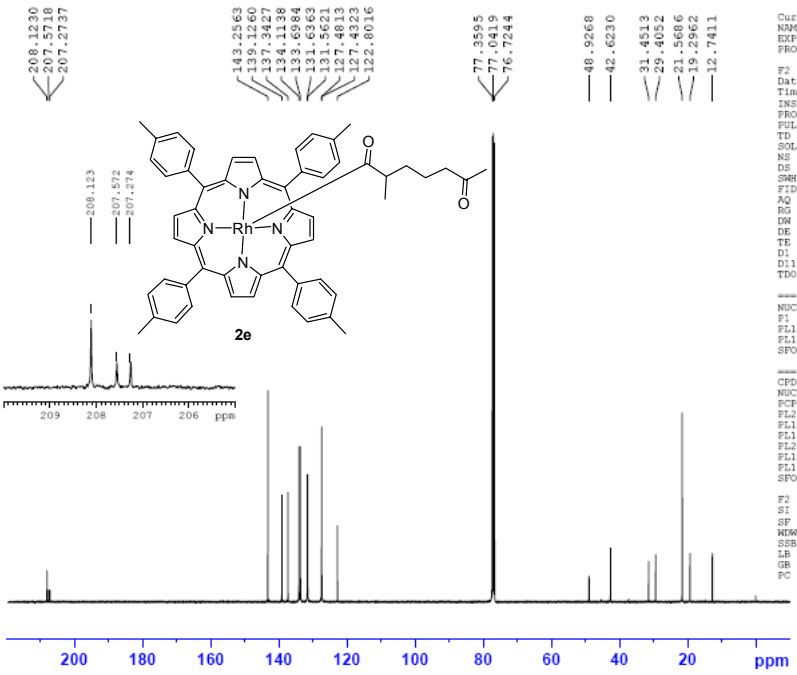
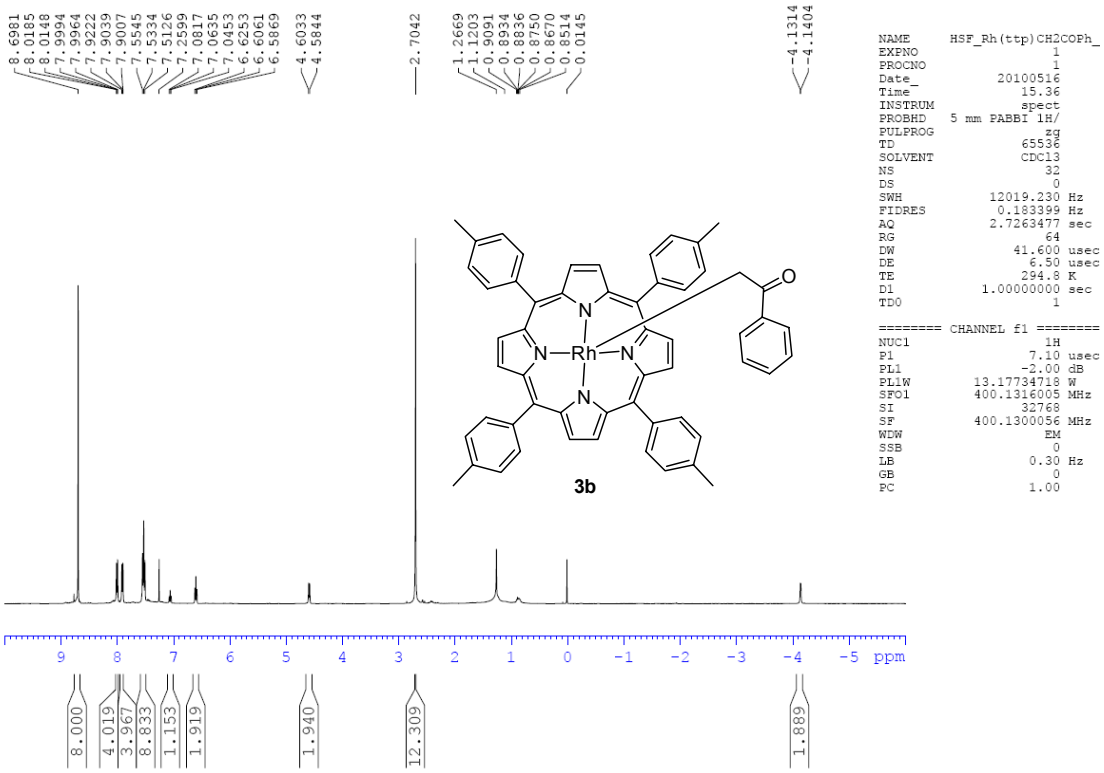
GB 0
PC 1.40

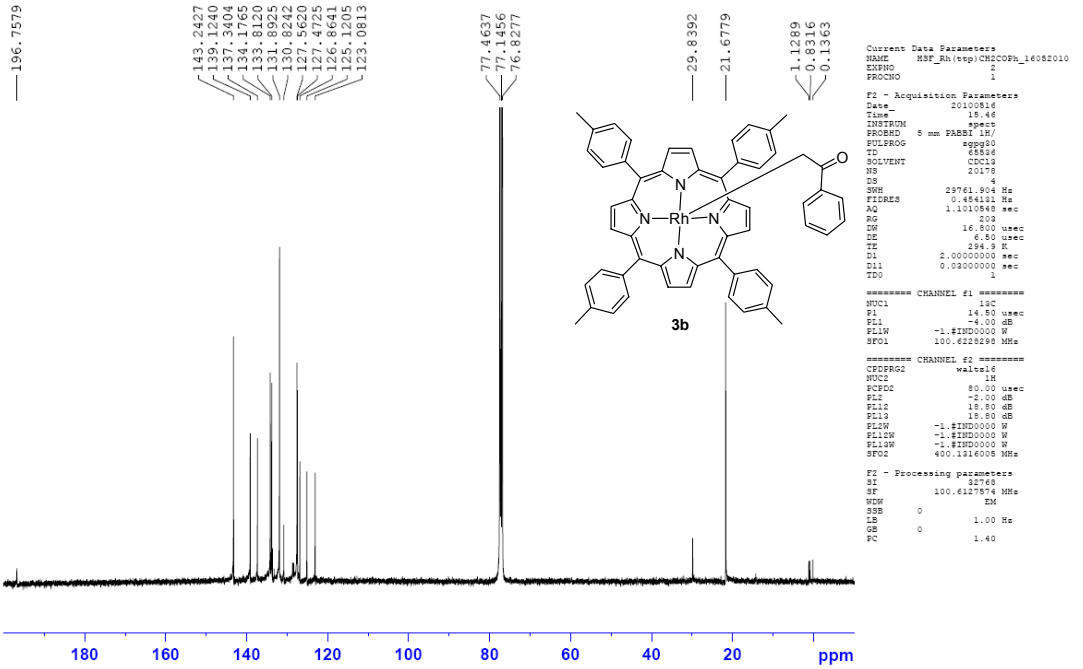



```
Current Data Parameters
NAME                 1H NMR
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_             20091229
Time                 16.27
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       32
DS                        0
SWH              12019.230 Hz
FIDRES            0.183399 Hz
AQ               2.7263477 sec
RG                       64
DW                  41.600 usec
DE                    6.50 usec
TE                   295.0 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   14.83 usec
PL1        0 dB
PL1W          -1.#IND0000 W
SFO1          400.1300000 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300159 MHz
WDW                      EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```




```
Current Data Parameters
NAME      HSF_Rh(ttp)COCH(Me)(CH2)3COMe_01012010
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_             20100101
Time                 15.10
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     6149
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                      203
DW                  20.800 usec
DE                    6.50 usec
TE                   296.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.68 usec
PL1                  -0.60 dB
PL1W          -1.#IND0000 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                     1H
PCPD2                90.00 usec
PL2        0 dB
PL12                 15.66 dB
PL13                 15.92 dB
PL2W          -1.#IND0000 W
PL12W         -1.#IND0000 W
PL13W         -1.#IND0000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB        0
LB                    1.00 Hz
GB         0
PC                    1.40
```


8.6981
8.0185
8.0148
7.9994
7.9964
7.9222
7.9039
7.9007
7.5545
7.5334
7.5126
7.2599
7.0817
7.0635
7.0453
6.6253
6.6061
6.5869
4.6033
4.5844
2.7042
1.2669
1.1203
0.9091
0.8934
0.8836
0.8750
0.8670
0.8514
0.0145
-4.1314
-4.1404
NAME HSF_Rh(ttp)CH2COPh_
EXPNO 1
PROCNO 1
Date_ 20100516
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.10 usec
PL1 -2.00 dB
PL1W 13.17734718 W
SFO1 400.1316005 MHz
SI 32768
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3b
9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 ppm
8.000
4.019
3.967
8.833
1.153
1.919
1.940
12.309
1.889


196.7579
143.2427
139.1240
137.3404
134.1765
133.8120
131.8925
130.8242
127.5620
127.4725
126.8641
125.1205
123.0813
77.4637
77.1456
76.8277
29.8392
21.6779
1.1289
0.8316
0.1363
Current Data Parameters
NAME HSF_Rh(ttp)CH2COPh_16082010
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100816
Time 15.46
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 20178
DS 4
SWH 29761.904 Hz
FIDRES 0.454121 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 14.50 usec
PL1 -4.00 dB
PL1W -1.#IND0000 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.80 dB
PL13 18.80 dB
PL2W -1.#IND0000 W
PL12W -1.#IND0000 W
PL13W -1.#IND0000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127874 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
3b
180 160 140 120 100 80 60 40 20 ppm