Electronic Supplementary Information

Hydrogenolysis of carbon-carbon σ-bond using water catalyzed by semi-rigid diiridium(III) porphyrins

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General Procedures

Unless otherwise noted, all reagents were purchased from commercial suppliers and directly used without further purification. Hexane was distilled from anhydrous calcium chloride. Benzene and toluene were distilled from sodium. *N,N*-Dimethylformamide (DMF) was distilled from magnesium sulfate under reduced pressure. Thin layer chromatography was performed on Merck pre-coated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230) was used for column chromatography.

All bond activation reactions were carried out inside thick-wall glass tubes equipped with a Rotaflo stopper. The glass tubes were covered by aluminum foil to avoid photochemical reactions. All reactions in 0.5 mL benzene-d_6 were carried out in a flame-sealed NMR tube in vacuum with the reaction mixture degassed with three freeze (77 K)-pump (0.005 mmHg)-thaw cycles, then heated in oven in dark and wrapped with aluminum foil to protect from exposure to room light before ^{1}H NMR measurements. The NMR yields were with benzene residue as the internal standard. Benzene stock solutions of Ir^{III}(linker)(ttp)R_2 (linker = dpmx or dppx, R = Me or ^{i}Pr) were prepared separately, transferred to the reaction vessel and dried under vacuum at room temperature to obtain anhydrous starting materials. Benzene-d_6 stock solution of [2.2]paracyclophane was prepared separately and transferred to the reaction vessel.

Experimental Instrumentation

^{1}H NMR and ^{13}C{^{1}H} NMR spectra were recorded on a Bruker DPX-400 spectrometer at 400 MHz and Bruker DPX-400 at 100 MHz or Bruker DPX-700 at 175 MHz respectively. Chemical shifts were referenced to the residual solvent protons in C_6D_6 (δ = 7.15 ppm), $CDCl_3$ (δ = 7.26 ppm) or tetramethylsilane (δ = 0.00 ppm) in ^{1}H NMR spectra and $CDCl_3$ (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 Bruker SolariX 9.4 Tesla FTICR MS mass spectrometer in electrospray ionization (ESI) mode using chloroform/methanol = 1:1 as solvent or on Bruker Autoflex speed MALDI-TOF instrument using *trans*-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as the matrix and dichloromethane as the solvent.

Synthesis of Various Iridium(III) Diporphyrin

Preparation of 5-(4-hydroxyphenyl)-10,15,20-tritolylporphyrin, H_2(ttp-OH) (1). To the refluxing 4-hydroxybenzaldehyde (4.6 g, 37.7 mmol) and 4-tolualdehyde (13.4 mL, 112.9 mmol) in 250 mL propionic acid, pyrrole (10.5 mL, 150.2 mmol) was added slowly. The colourless solution turned to deep purple quickly. The solution was then turned to dark brown in colour after refluxed for 2 h. The reaction mixture was allowed to cool down and crude purple solid was obtained upon suction filtration with several washings with cold methanol. The crude solid was purified by column chromatography on silica gel (70-230 mesh) eluting with CH_2Cl_2:hexanes = 2:1. The purple fraction was collected and rotary evaporated to obtain purple solid. Recrystallization from CH_2Cl_2/MeOH yields purple solid (1.30 g, 1.98 mmol, 5%). R_f = 0.12 (CH_2Cl_2:hexane = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ -2.78 (s, 2 H), 2.71 (s, 9 H), 7.17 (d, J = 8.3 Hz, 2 H), 7.55 (d, J = 7.7 Hz, 6 H), 8.06 (d, J = 8.3 Hz , 2 H), 8.10 (d, J = 8.2 Hz, 6 H), 8.85 (s, 8 H). HRMS (MALDI/TOF-MS): Calcd. For $(C_{47}H_{36}N_4O)^+$: m/z 672.28891. Found m/z 672.3002.

Preparation of 5,10,15-tritolyl-20-[4-[α,α'-[*p*-(10,15,20-tritolyl-5-porphyrinyl)-phenoxy] -*m*-xyloxy]phenyl]porphyrin, H_4(dpmx)(ttp) (2). A mixture of **1** (541 mg, 0.805 mmol) and α,α'-dibromo-*m*-xylene (106 mg, 0.402 mmol) was stirred with K_2CO_3 (1.11 g, 8.03 mmol) in 125 mL DMF at room temperature for 1 d. Solvent was distilled under high vacuum and the crude solid was purified by column chromatography on silica gel (70-230 mesh) eluting with CH_2Cl_2:hexanes =

2:1. The dark purple fraction was collected and rotary evaporated to obtain dark purple solid. Recrystallization from CH_2Cl_2/MeOH yields dark purple solid (314 mg, 0.217 mmol, 58%). R_f = 0.55 (CH_2Cl_2:hexane = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ -2.76 (s, 4 H), 2.67 (s, 12 H), 2.71 (s, 6 H), 5.47 (s, 4 H), 7.43 (d, J = 8.6 Hz, 4 H), 7.51-7.56 (2 d overlap, 12 H), 7.69-7.71 (m, 3 H), 7.92 (s, 1 H), 8.06-8.10 (2 d overlap, 12 H), 8.17 (d, J = 8.5 Hz, 4 H,), 8.85-8.90 (m, 16 H). HRMS (MALDI/TOF-MS): Calcd. For $(C_{102}H_{78}O_2N_8)^+$: m/z 1447.62477. Found m/z 1446.6534.

Preparation of Ir^{III}_2(dpmx)(ttp)$(CO)_2Cl_2$ (3). In a 100 mL round bottom flask with a reflux condenser, a solution of $[Ir^I(cod)Cl]_2$ (93 mg, 0.138 mmol) and **2** (51 mg, 0.035 mmol) in 50 mL *p*-xylene was refluxed for 2 d. Solvent was distilled under high vacuum and the crude solid was purified by column chromatography on silica gel (70-230 mesh) eluting with CH_2Cl_2:hexanes = 5:1. The red fraction was collected and rotary evaporated to obtain red solid. The major red fraction was collected and rotary evaporated to obtain red solid. Recrystallization from CH_2Cl_2/MeOH yields red solid (42 mg, 0.022 mmol, 62%). R_f = 0.58 (CH_2Cl_2:hexanes = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.73 (s, 18 H), 5.49 (s, 4 H), 7.48 (d, J = 8.1 Hz, 4 H), 7.61 (d, J = 8.1 Hz, 12 H), 7.67-7.74 (m, 3 H), 7.95 (s, 1 H), 8.14 (d, J = 7.2 Hz, 6 H), 8.20 (d, J = 5.7 Hz, 8 H), 8.27 (d, J = 8.2, 2.0 Hz, 2 H), 8.99-9.03 (m, 16 H). HRMS (ESI/FTICR-MS): Calcd. For $(C_{104}H_{74}Cl_2Ir_2N_8O_4 + Na)^+$: m/z 1977.45369. Found m/z 1977.43585.

Preparation of Ir^{III}_2(dpmx)(ttp)Me_2 (4). A suspension of **3** (47 mg, 0.024 mmol) in 1 mL THF in a Teflon screw head stoppered tube and a solution of $NaBH_4$ (20 mg, 0.53 mmol) in aqueous NaOH (1 M, 1 mL) in a Schlenk tube were purged with N_2 for 15 min separately. The $NaBH_4$ solution was added slowly to the suspension of **3** via a cannula. The mixture was heated at 70 ^{o}C under N_2 for 2 h to give a brown suspension. The reaction was then cooled to room temperature and iodomethane (6 μL, 0.097 mmol) was added under N_2. The reaction mixture was further heated at 70 ^{o}C for 2 h to give a reddish brown suspension. It was worked up by extraction with CH_2Cl_2/H_2O. The organic

layer was rotary evaporated. The crude solid was purified by column chromatography on silica gel eluting with CH_2Cl_2/hexane = 1:1. The major red fraction was collected and dried to give reddish purple solid (33 mg, 0.018 mmol, 73%). R_f = 0.81 (CH_2Cl_2/hexane = 2:1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ -6.29 (s, 6 H), 2.66 (s, 12 H), 2.68 (s, 6 H), 5.42 (s, 4 H), 7.37-7.39 (m, 4 H), 7.49-7.51 (m, 12 H), 7.60-7.62 (m, 1 H), 7.66 (d, J = 7.4 Hz, 2 H), 7.87 (s, 1 H), 7.98-8.03 (m, 12 H), 8.07-8.11 (m, 4 H), 8.51-8.56 (m, 16 H). ^{13}C{^{1}H} NMR ($CDCl_3$, 175 MHz) δ 21.7, 30.3, 70.3, 113.3, 123.5, 124.0, 127.1, 127.6, 127.6, 129.0, 129.1, 131.1, 131.3, 131.4, 131.4, 132.3, 133.7, 133.9, 134.6, 134.9, 135.1, 137.3, 137.6, 138.8, 143.4, 143.5, 158.5. HRMS (ESI/FTICR-MS) calcd. for ($C_{104}H_{80}Ir_2N_8O_2$ + Na)$^+$: m/z 1881.55741. Found: m/z 188155625.

Preparation of Ir^{III}_2(dpmx)(ttp)^{i}Pr$_2$ (5). A suspension of **3** (49 mg, 0.025 mmol) in 1 mL THF in a Teflon screw head stoppered tube and a solution of $NaBH_4$ (20 mg, 0.53 mmol) in aqueous NaOH (1 M, 1 mL) in a Schlenk tube were purged with N_2 for 15 min separately. The $NaBH_4$ solution was added slowly to the suspension of **3** via a cannula. The mixture was heated at 70 ^{o}C under N_2 for 2 h to give a brown suspension. The reaction was then cooled to room temperature and 2-iodopropane (10 μL, 0.10 mmol) was added under N_2. The reaction mixture was further heated at 70 ^{o}C for 2 h to give a reddish brown suspension. It was worked up by extraction with CH_2Cl_2/H_2O. The organic layer was rotary evaporated. The crude solid was purified by column chromatography on silica gel eluting with CH_2Cl_2/hexane = 1:1. The major red fraction was collected and dried to give reddish purple solid (30 mg, 0.016 mmol, 63%). R_f = 0.77 (CH_2Cl_2/hexane = 1:1). δ -5.07 (septet, 2 H), -4.43 (d, 12 H), 2.70 (s, 18 H), 5.42 (s, 4 H), 7.35-7.38 (m, 4 H), 7.48-7.53 (m, 12 H), 7.58 (s, 1 H), 7.61-7.63 (d, 2 H), 7.83 (s, 1 H), 7.98 (d, 6 H), 8.03 (d, 6 H), 8.09 (d, 2 H), 8.48-8.54 (m, 16 H). ^{13}C{^{1}H} NMR ($CDCl_3$, 175 MHz) δ -3.0, 21.5, 21.7, 70.3, 113.2, 113.5, 124.4, 124.8, 124.8, 127.2, 127.6, 127.6, 129.2, 131.3, 131.4, 131.4, 131.5, 133.5, 133.6, 133.9, 134.0, 134.6, 134.7, 135.1, 137.3, 137.6, 138.8, 143.7, 143.7, 143.8, 158.5.

Preparation of 5,10,15-tritolyl-20-[4-[α,α'-[*p*-(10,15,20-tritolyl-5-porphyrinyl)-phenoxy] -*p*-xyloxy]phenyl]porphyrin, H_4(dppx)(ttp) (6). A mixture of **1** (200 mg, 0.297 mmol) and α,α'-dibromo-*m*-xylene (40 mg, 0.150 mmol) was stirred with K_2CO_3 (0.500 g, 3.62 mmol) in 20 mL DMF at room temperature for 3 d. Solvent was distilled under high vacuum and the crude solid was purified by column chromatography on silica gel (70-230 mesh) eluting with chloroform. The dark purple fraction was collected and rotary evaporated to obtain dark purple solid. Recrystallization from CH_2Cl_2/MeOH yields dark purple solid (138.6 mg, 0.0957 mmol, 64%). R_f = 0.34 (CH_2Cl_2:hexanes = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ -2.76 (s, 4 H), 2.70 (s, 9 H), 2.71 (s, 9 H), 5.45 (s, 4 H), 7.41 (d, J = 8.5 Hz, 4 H), 7.54-7.57 (m, 12 H), 7.78 (s, 4 H), 8.08-8.10 (2 d overlap, 12 H), 8.16 (d, J = 8.5 Hz, 4 H), 8.85-8.90 (m, 16 H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz) δ 21.7, 70.3, 113.2, 113.8, 119.8, 120.2, 127.5, 128.3, 129.6, 131.3, 134.7, 135.0, 135.2, 135.8, 137.2, 137.5, 139.4, 158.7. HRMS (MALDI/TOF-MS): Calcd. For $(C_{102}H_{78}O_2N_8)^+$: m/z 1447.62477. Found m/z 1446.7447.

Preparation of Ir^{III}_2(dppx)(ttp)$(CO)_2Cl_2$ (7). In a 100 mL round bottom flask with a reflux condenser, a solution of $[Ir^I(cod)Cl]_2$ (121 mg, 0.180 mmol) and **6** (65 mg, 0.045 mmol) in 50 mL *p*-xylene was refluxed for 2 d. After Solvent was distilled off under high vacuum, the solid was purified by column chromatography on silica gel (70-230 mesh) eluting with $CHCl_3$:hexanes = 5:1. The major red fraction was collected and rotary evaporated to obtain red solid. Recrystallization from CH_2Cl_2/MeOH gave red solid (57 mg, 0.029 mmol, 65%). R_f = 0.24 ($CHCl_3$:hexanes = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.69 (s, 9 H), 2.71 (s, 9 H), 5.44 (d, J = 9.9 Hz, 4 H), 7.38 (d, J = 8.5 Hz, 2 H), 7.43 (d, J = 8.6 Hz, 2 H), 7.51-7.53 (m, 6 H), 7.58 (d, J = 7.7 Hz, 6 H), 7.77-7.79 (m, 4 H), 8.02 (s, 6 H), 8.10 (d, J = 8.2 Hz, 4 H), 8.16 (d, J = 7.7 Hz, 4 H), 8.22 (d, J = 7.7 Hz, 2 H), 8.47-8.50 (m, 8 H), 8.94-8.99 (m, 8 H). ^{13}C{^{1}H} NMR (175 MHz, $CDCl_3$): δ 21.7, 70.2, 113.3, 133.5, 121.8, 122.2, 123.7, 124.1, 127.6, 127.8, 128.0, 128.3, 128.9, 131.4, 131.9, 132.0, 133.4, 133.8, 134.0, 134.3, 134.5, 135.0, 135.5, 135.7, 137.0, 137.2, 137.8, 138.3, 138.8, 138.9, 141.2, 141.4, 143.3,

158.9.

Preparation of Ir^{III}_2(dppx)(ttp)Me_2 (8). A suspension of **7** (21 mg, 0.011 mmol) in 1 mL THF in a Teflon screw head stoppered tube and a solution of $NaBH_4$ (8.3 mg, 0.22 mmol) in aqueous NaOH (1 M, 1 mL) in a Schlenk tube were purged with N_2 for 15 min separately. The $NaBH_4$ solution was added slowly to the suspension of **7** via a cannula. The mixture was heated at 70 ^oC under N_2 for 2 h to give a brown suspension. The reaction was then cooled to room temperature and iodomethane (3 μL, 0.043 mmol) was added under N_2. The reaction mixture was further heated at 70 ^oC for 2 h to give a reddish brown suspension. It was worked up by extraction with $CHCl_3/H_2O$. The organic layer was rotary evaporated. The crude solid was purified by column chromatography on silica gel eluting with $CHCl_3$/hexane = 2:1. The major red fraction was collected and dried to give reddish purple solid (10 mg, 0.0054 mmol, 50%). R_f = 0.75 (CH_2Cl_2/hexane = 2:1). ^1H NMR ($CDCl_3$, 400 MHz) δ -6.28 (s, 6 H), 2.68 (s, 18 H), 5.41 (s, 4 H), 7.37 (d, J = 8.4 Hz, 4 H), 7.52 (d, J = 7.3 Hz, 12 H), 7.75 (s, 4 H), 7.99-8.04 (m, 14 H), 8.06-8.07 (m, 2 H), 8.52-8.55 (m, 16 H). $^{13}C\{^1H\}$ NMR (175 MHz, $CDCl_3$): δ 21.7, 30.4, 70.1, 113.1, 113.2, 123.5, 124.0, 127.6, 127.6, 128.3, 131.4, 133.7, 133.9, 134.5, 134.8, 135.0, 137.0, 137.3, 138.8, 143.3, 143.5, 158.5. HRMS (ESI/FTICR-MS): Calcd. For $(C_{104}H_{80}Ir_2N_8O_2)^+$: m/z 1858.56764. Found m/z 1858.57146.

Preparation of Ir^{III}_2(dppx)(ttp)$^iPr_2$ (9). A suspension of **7** (21 mg, 0.011 mmol) in 1 mL THF in a Teflon screw head stoppered tube and a solution of $NaBH_4$ (8.3 mg, 0.22 mmol) in aqueous NaOH (1 M, 1 mL) in a Schlenk tube were purged with N_2 for 15 min separately. The $NaBH_4$ solution was added slowly to the suspension of **7** via a cannula. The mixture was heated at 70 ^oC under N_2 for 2 h to give a brown suspension. The reaction was then cooled to room temperature and 2-iodopropane (4 μL, 0.43 mmol) was added under N_2. The reaction mixture was further heated at 70 ^oC for 2 h to give a reddish brown suspension. It was worked up by extraction with $CHCl_3/H_2O$. The organic layer was rotary evaporated. The crude solid was purified by column chromatography on silica gel eluting with

$CHCl_3$/hexane = 2:1. The major red fraction was collected and dried to give reddish purple solid (12 mg, 0.0061 mmol, 56%). R_f = 0.76 (CH_2Cl_2/hexane = 2:1). ^{1}H NMR ($CDCl_3$, 400 MHz) δ -5.07 (septet, 2 H), -4.43 (d, J = 6.5 Hz, 12 H), 2.70 (s, 18 H), 5.42 (s, 4 H), 7.37-7.40 (m, 4 H), 7.52-7.55 (m, 12 H), 7.74-7.75 (m, 4 H), 8.01 (d, J = 6.8 Hz, 6 H), 8.05 (d, J = 6.5 Hz, 8 H), 8.11 (d, J = 7.7 Hz, 2 H), 8.51-8.58 (m, 16 H). ^{13}C{^{1}H} NMR (175 MHz, $CDCl_3$): δ -3.0, 21.5, 21.7, 70.1, 113.1, 113.1, 124.3, 124.7, 124.8, 127.6, 127.6, 128.2, 131.4, 131.4, 131.4, 133.5, 134.0, 134.5, 134.6, 135.1, 137.0, 137.3, 138.8, 143.6, 143.8, 158.4. HRMS (ESI/FTICR-MS): Calcd. For $(C_{104}H_{80}Ir_2N_8O_2)^+$: m/z 1914.63033. Found m/z 1914.63138.

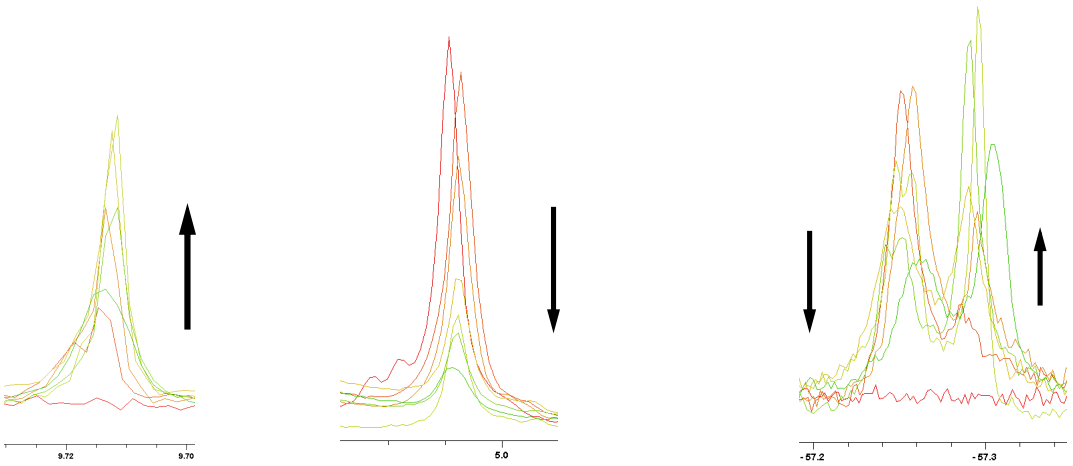
Catalytic Hydrogenation of PCP with Water by Iridium(III) Diporphyrin

With Ir^{III}_2(dpmx)(ttp)Me_2. Ir^{III}_2(dpmx)(ttp)Me_2 (0.45 mg, 0.00024 mmol), H_2O (8.6 μL, 0.48 mmol) and benzene-d_6 stock solution (500 μL) of PCP (1.0 mg, 0.0048 mmol) were added successively to a NMR tube. The orange mixture was degassed for three freeze-pump-thaw cycles and the NMR tube was flame-sealed under vacuum. It was heated at 200 ^{o}C in the dark for 40 h. It was monitored with ^{1}H NMR spectroscopy at particular time intervals and the NMR yields were taken. 4,4'-Dimethylbibenzyl **11** was formed in 27% yield. Some precipitate was observed at the bottom of the sealed tube.

With Ir^{III}_2(dpmx)(ttp)^iPr_2. Ir^{III}_2(dpmx)(ttp)^iPr_2 (0.46 mg, 0.00024 mmol), H_2O (8.6 μL, 0.48 mmol) and benzene-d_6 stock solution (500 μL) of PCP (1.0 mg, 0.0048 mmol) were added successively to a NMR tube. The orange mixture was degassed for three freeze-pump-thaw cycles and the NMR tube was flame-sealed under vacuum. It was heated at 200 ^{o}C in the dark for 40 h. It was monitored with ^{1}H NMR spectroscopy at particular time intervals and the NMR yields were taken. 4,4'-Dimethylbibenzyl **11** was formed in 40% yield. Some precipitate was observed at the bottom of the sealed tube.

With Ir^{III}_2(dppx)(ttp)Me_2. Ir^{III}_2(dppx)(ttp)Me_2 (0.45 mg, 0.00024 mmol), H_2O (8.6 μL, 0.48 mmol) and benzene-d_6 stock solution (500 μL) of PCP (1.0 mg, 0.0048 mmol) were added successively to a NMR tube. The orange mixture was degassed for three freeze-pump-thaw cycles and the NMR tube was flame-sealed under vacuum. It was heated at 200 °C in the dark for 40.5 h. It was monitored with ^{1}H NMR spectroscopy at particular time intervals and the NMR yields were taken. 4,4'-Dimethylbibenzyl **11** was formed in 59% yield. Some precipitate was observed at the bottom of the sealed tube.

With Ir^{III}_2(dppx)(ttp)$^i Pr_2$. Ir^{III}_2(dpmx)(ttp)$^i Pr_2$ (0.46 mg, 0.00024 mmol), H_2O (8.6 μL, 0.48 mmol) and benzene-d_6 stock solution (500 μL) of PCP (1.0 mg, 0.0048 mmol) were added successively to a NMR tube. The orange mixture was degassed for three freeze-pump-thaw cycles and the NMR tube was flame-sealed under vacuum. It was heated at 200 °C in the dark for 31.5 h. It was monitored with ^{1}H NMR spectroscopy at particular time intervals and the NMR yields were taken. 4,4'-Dimethylbibenzyl **11** was formed in 66% yield. Some precipitate was observed at the bottom of the sealed tube.



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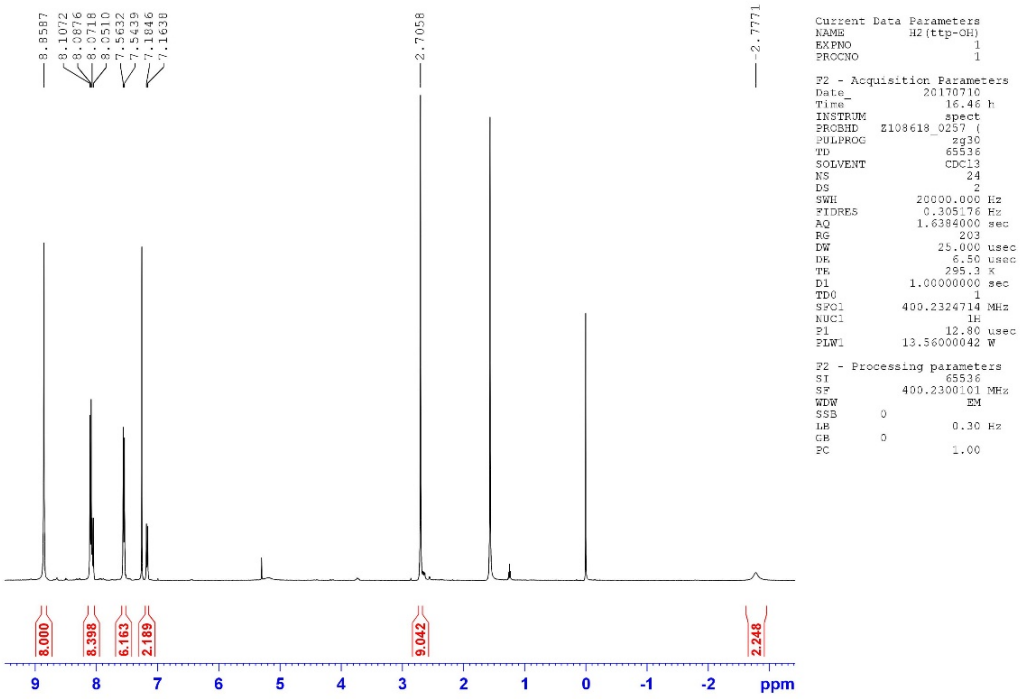
Iridium Hydride Signal

$\delta \sim 5$ ppm
Tether Xylyl Proton Signal

^{1}H NMR Reaction Progress of the Independent Experiment in the Absence of PCP

^{1}H NMR and ^{13}C Spectra

^{1}H NMR Spectrum of H_2(ttp-OH)



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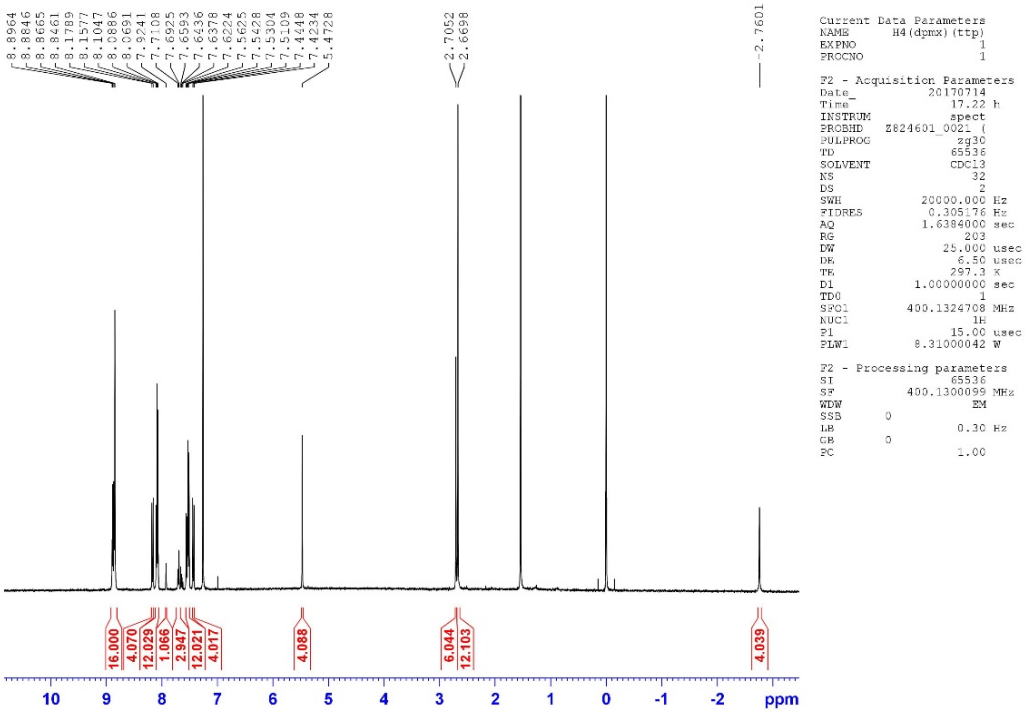

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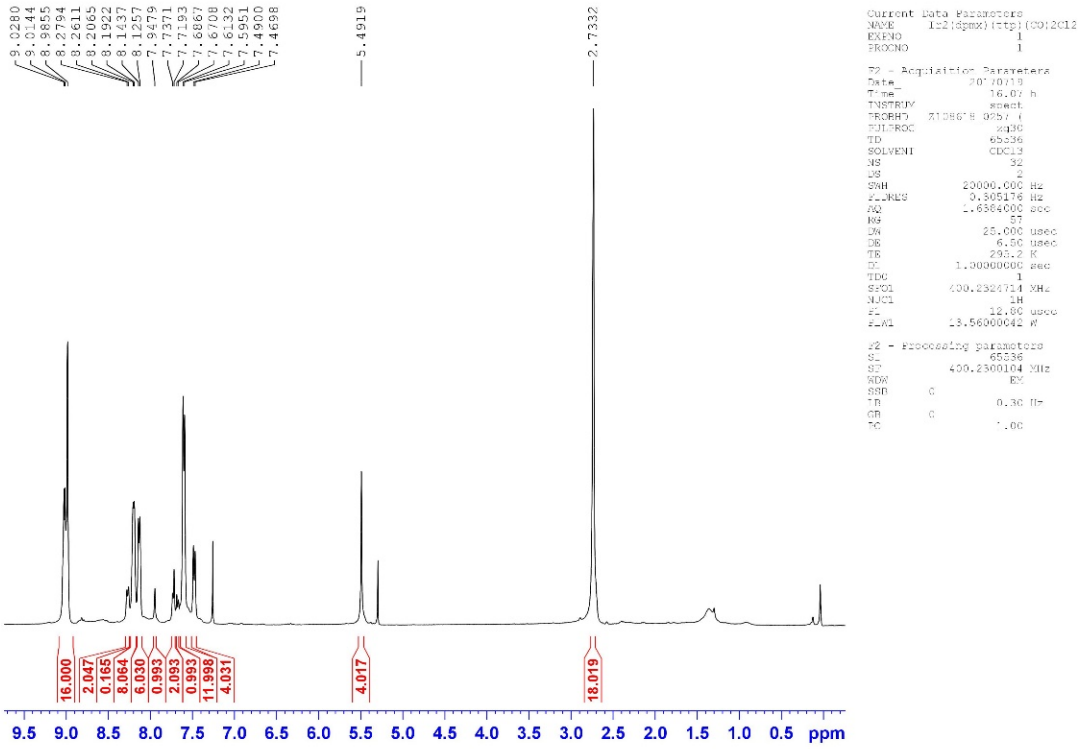

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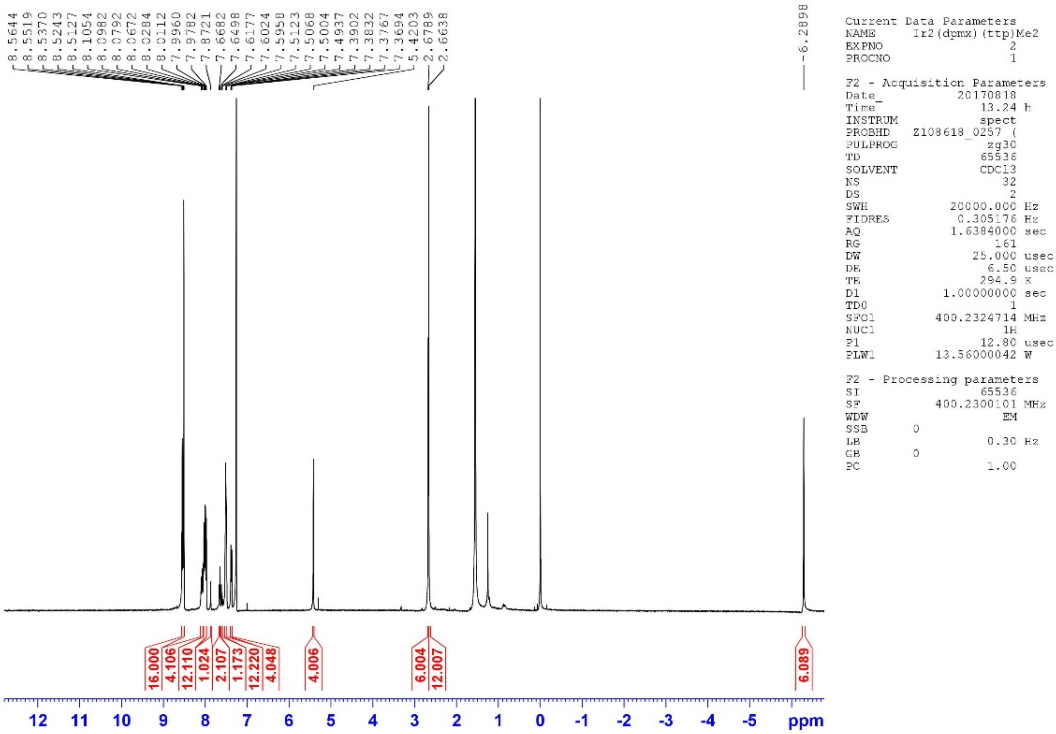
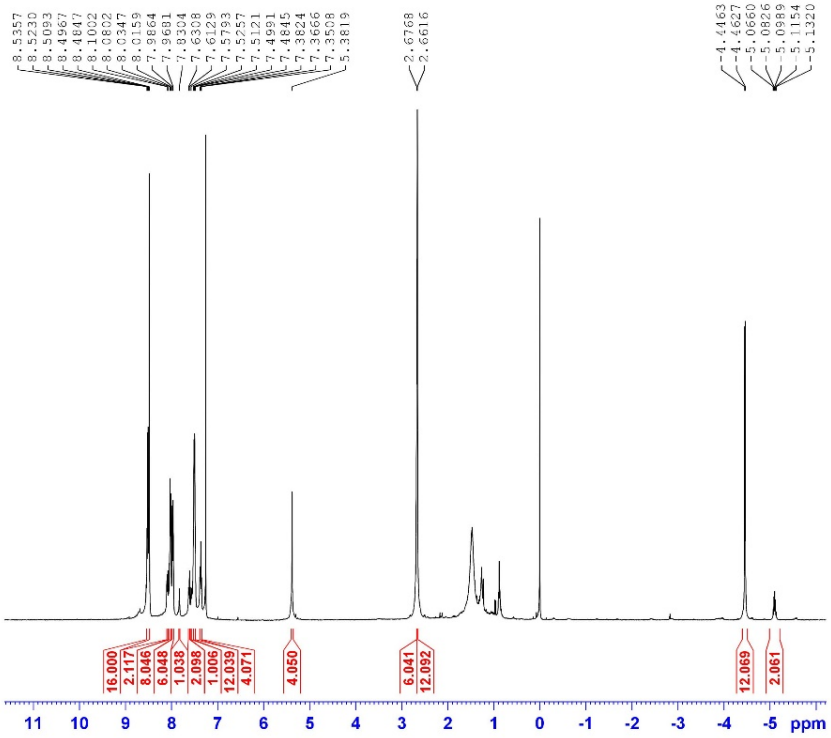


^{1}H NMR Spectrum of $Ir^{III}_{2}(dpmx)(ttp)^{i}Pr_{2}$

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PROCNO                       1

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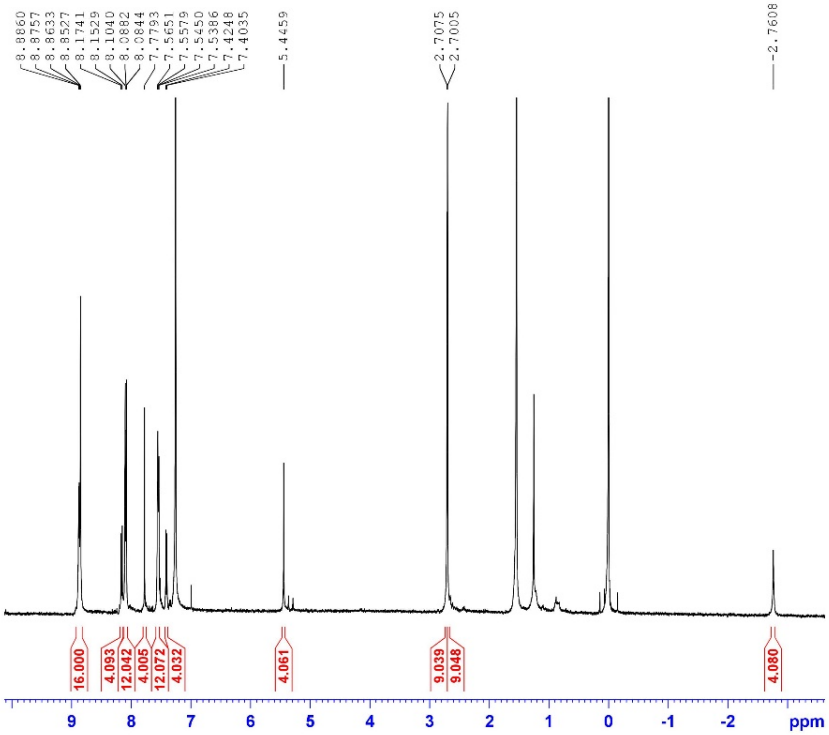
^{1}H NMR Spectrum of $H_{4}(dppx)(ttp)$

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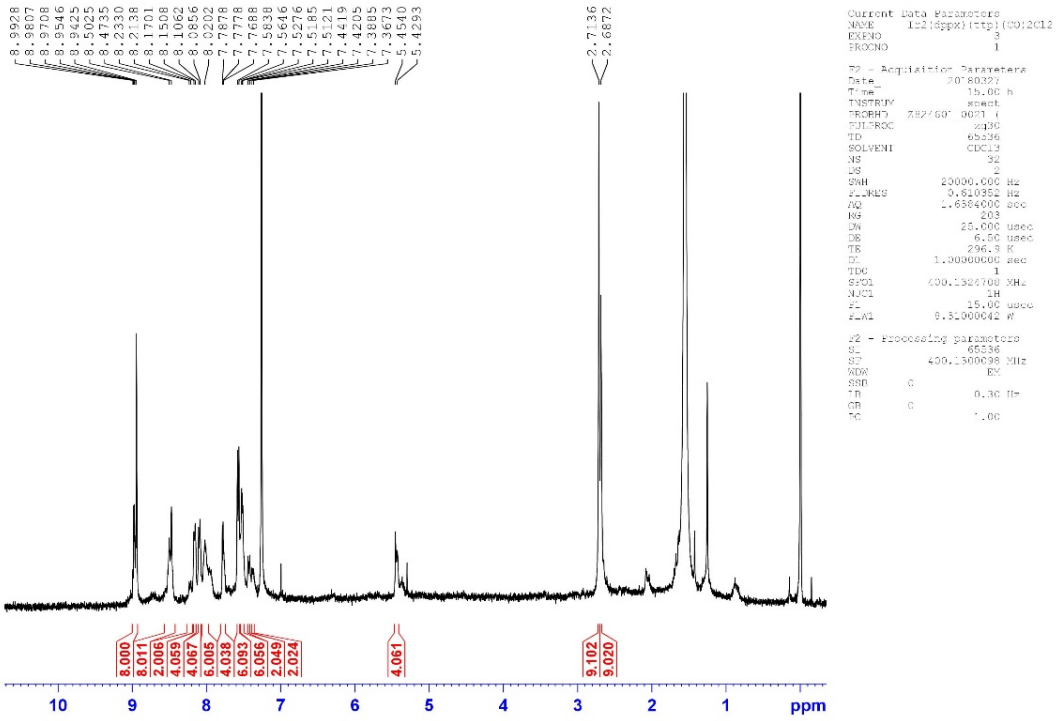
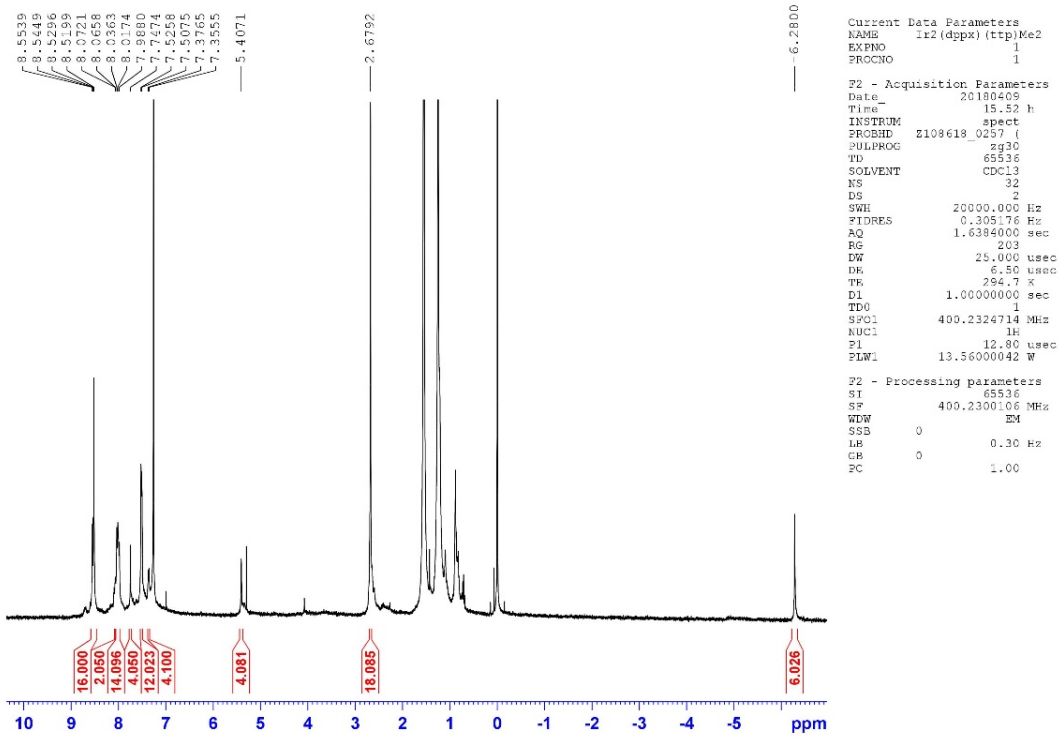
LB                    0.30 Hz
GB           0
PC                    1.00
```

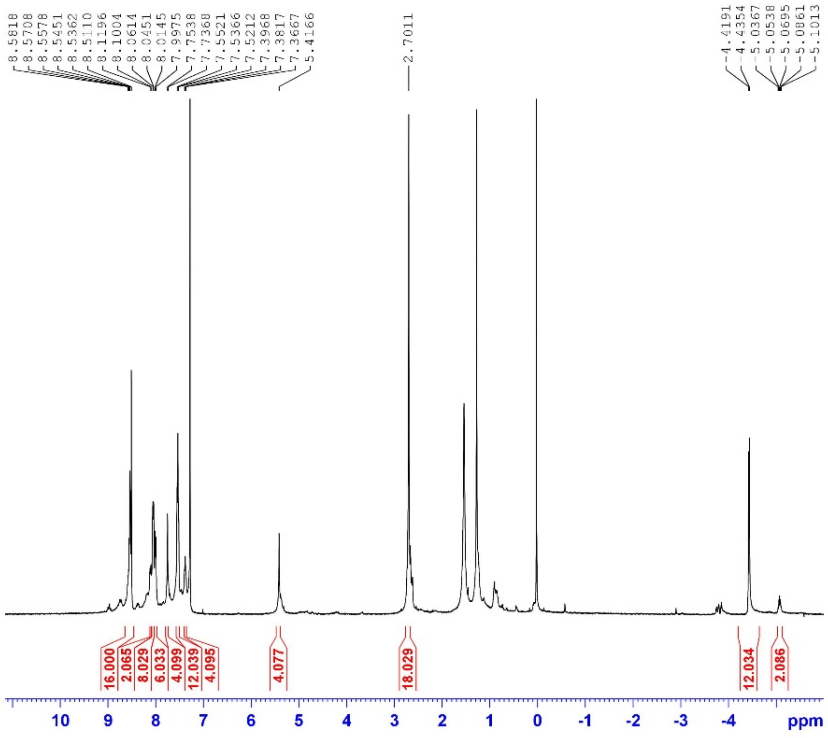
^{1}H NMR Spectrum of $Ir^{III}_{2}(dppx)(ttp)(CO)_{2}Cl_{2}$



^{1}H NMR Spectrum of $Ir^{III}_{2}(dppx)(ttp)Me_{2}$



^{1}H NMR Spectrum of $Ir^{III}_{2}(dppx)(ttp)^{i}Pr_{2}$

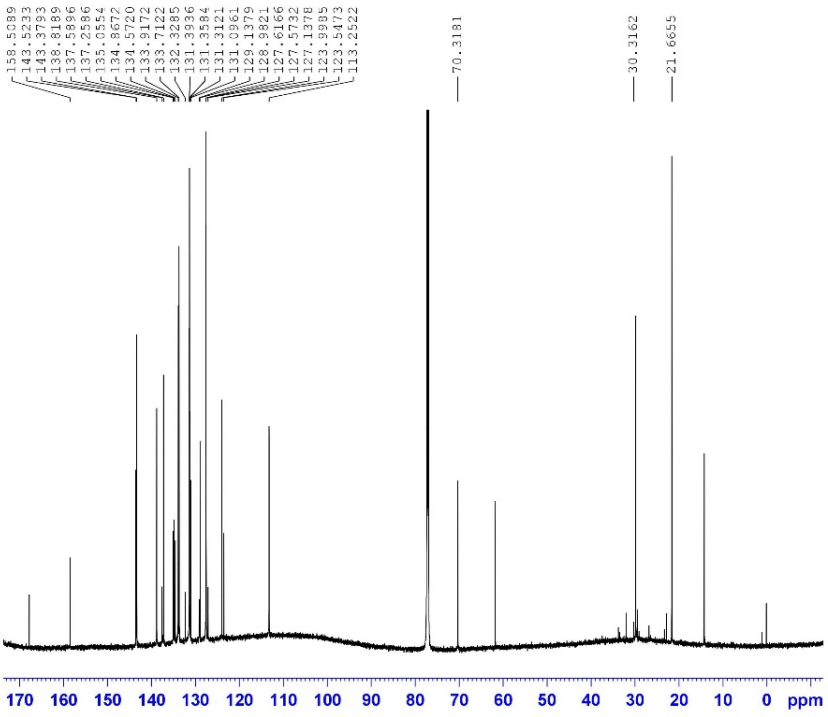


Current Data Parameters
NAME Ir2(dppx)(ttp)iPr2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180312
Time 15.05 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 20000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384000 sec
RG 203
DW 25.000 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR Spectrum of $Ir^{III}_{2}(dpmx)(ttp)Me_{2}$



Current Data Parameters
NAME Ir2(dpmx)(ttp)Me2
EXPNO 2
PROCNO 1

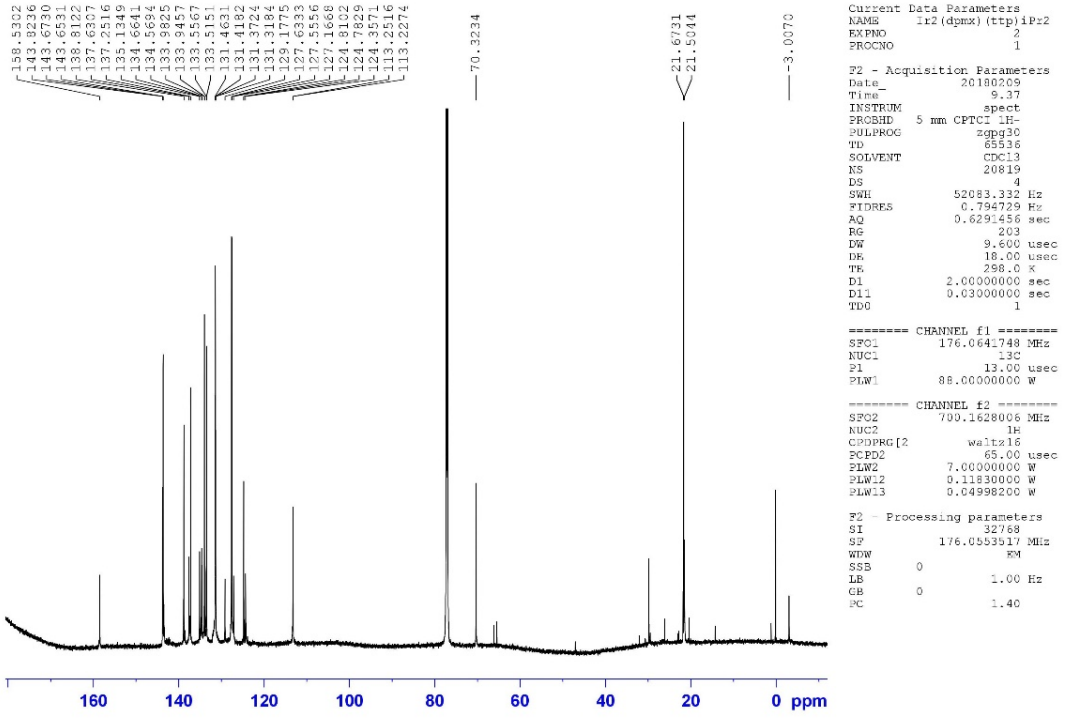
F2 - Acquisition Parameters
Date_ 20180208
Time 16.11
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5750
DS 4
SWH 52083.332 Hz
FIDRES 0.794729 Hz
AQ 0.6291456 sec
RG 203
DW 9.600 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 176.0641748 MHz
NUC1 13C
P1 13.00 usec
PLW1 88.00000000 W

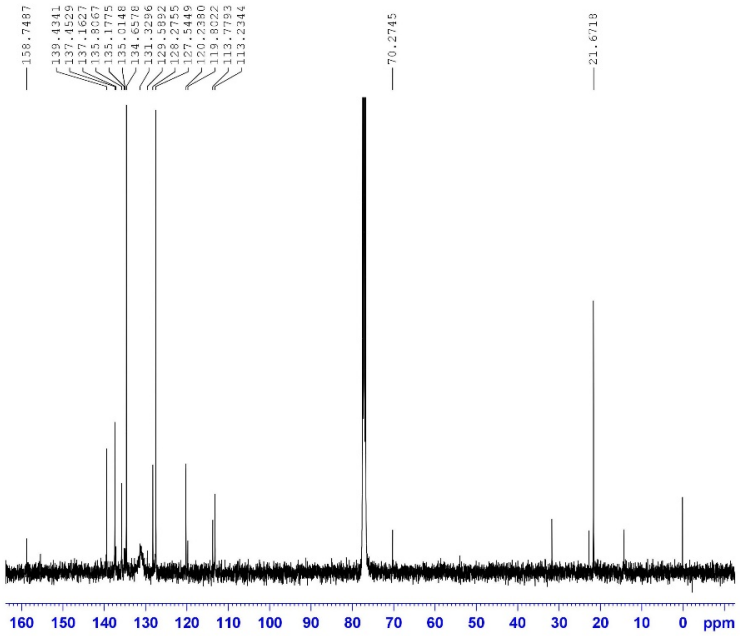
======== CHANNEL f2 ========
SFO2 700.1628006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 7.00000000 W
PLW12 0.11830000 W
PLW13 0.04998200 W

F2 - Processing parameters
SI 32768
SF 176.0553530 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C NMR Spectrum of Ir^{III}_2(dpmx)(ttp)$^{i}Pr_2$



^{13}C NMR Spectrum of H_4(dppx)(ttp



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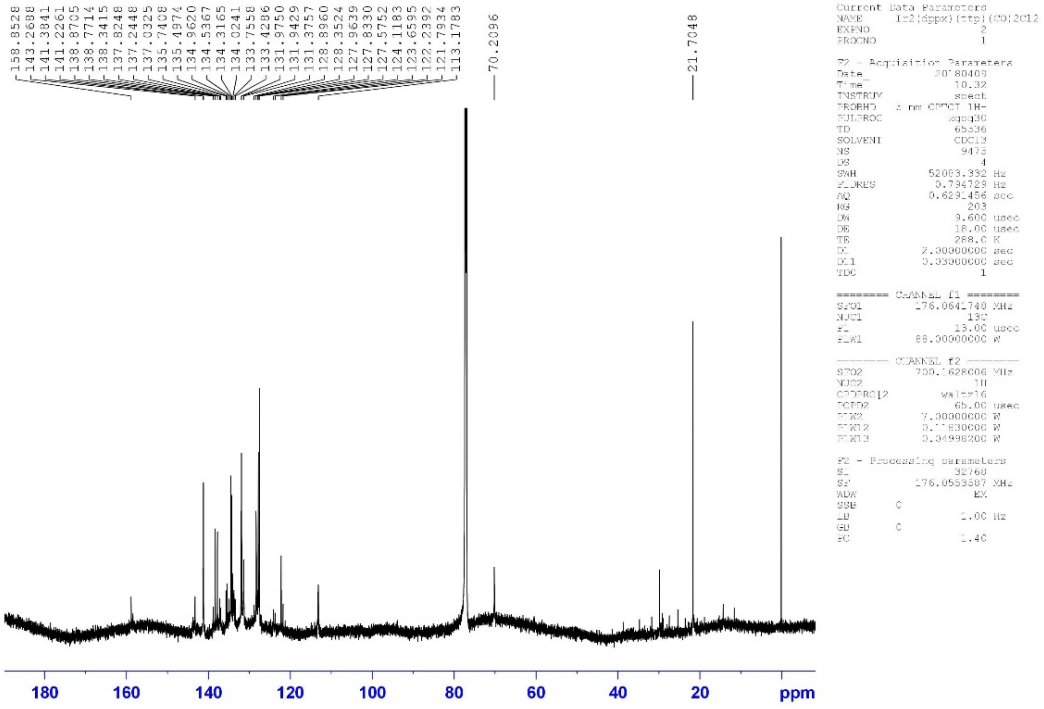
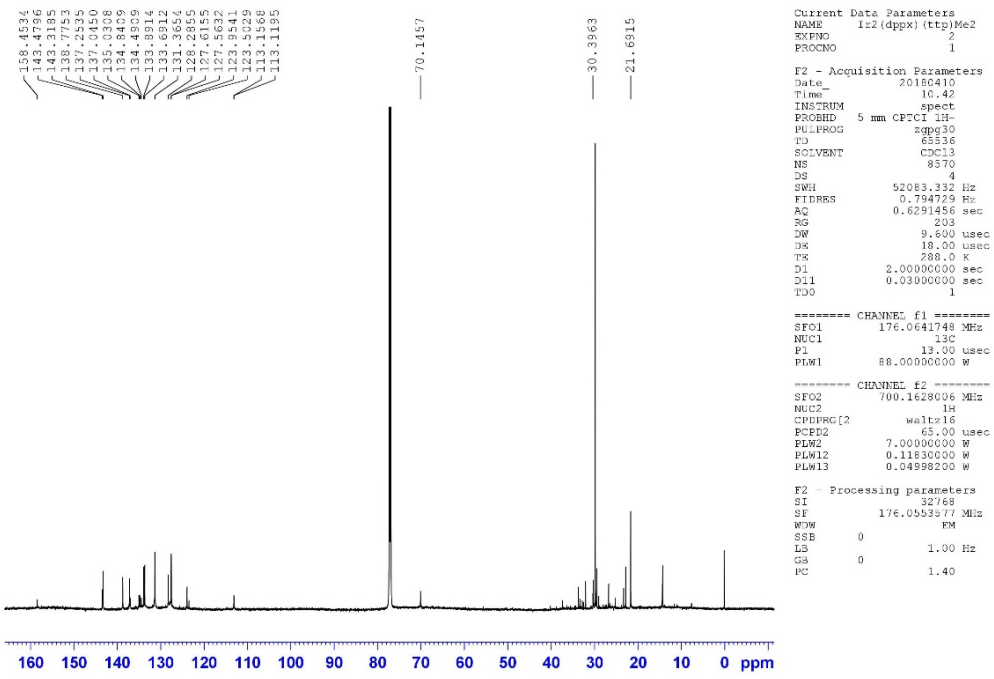
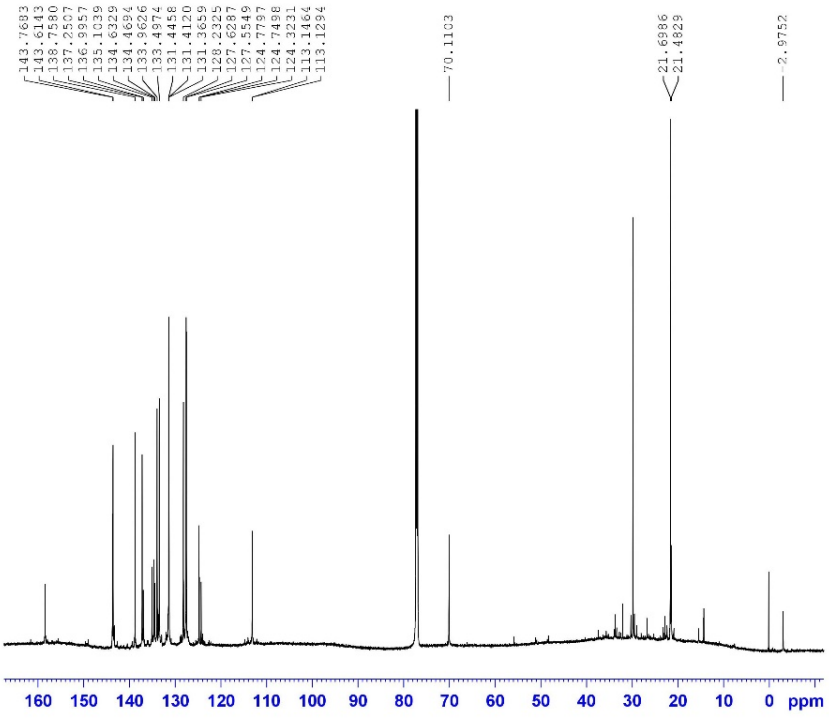
^{13}C NMR Spectrum of $Ir^{III}_2(dppx)(ttp)(CO)_2Cl_2$



^{13}C NMR Spectrum of $Ir^{III}_2(dppx)(ttp)Me_2$



^{13}C NMR Spectrum of $Ir^{III}_2(dppx)(ttp)^iPr_2$

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Current Data Parameters
NAME      1z2(dppx)(ttp)iPr2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180411
Time                 13.19
INSTRUM              spect
PROBHD   5 mm CPTCI 1H-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  26931
DS                      4
SWH           52083.332 Hz
FIDRES         0.794729 Hz
AQ             0.6291456 sec
RG                    203
DW                9.600 usec
DE                18.00 usec
TE                288.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         176.0641748 MHz
NUC1                  13C
P1                 13.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         700.1628006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              65.00 usec
PLW2          7.00000000 W
PLW12         0.11830000 W
PLW13         0.04998200 W

F2 - Processing parameters
SI                   32768
SF           176.0553580 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
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