Supporting Information

For

A bimetallic iridium(II) catalyst: $[\{Ir(IDipp)(\mu\text{-}H)\}_2][BF_4]_2$ (IDipp = 1,3-bis(2,6-diisopropylphenylimidazol-2-ylidene)

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Table of Contents:

General:

All experiments were carried out under an inert atmosphere by using standard Schlenk techniques. The solvents were dried by known procedures and distilled under argon prior to use or obtained oxygen- and water-free from a Solvent Purification System (Innovative Technologies). The starting complexes[Ir(η^4-COD)(μ-Cl)]$_2$ and [Ir(μ-OMe)(η^4-COD)]$_2$ were prepared according to the literature procedure.[1,2] All other chemicals were used as purchased from Sigma-Aldrich, Merck and J. T. Baker. H_2 gas (>99.5 %) was obtained from Infra. ^{1}H, ^{13}C{^{1}H} and ^{19}F spectra were recorded either on a Bruker ARX 300 MHz or a Bruker Avance 400 MHz instruments. Chemical shifts (expressed in parts per million) are referenced to residual solvent peaks (^{1}H, ^{13}C{^{1}H}). Coupling constants, *J*, are given in Hz. Spectral assignments were achieved by combination of ^{1}H-^{1}H COSY, ^{13}C APT and ^{1}H-^{13}C HSQC/HMBC experiments. C, H, and N analyses were carried out in a Perkin-Elmer 2400 CHNS/O analyzer.

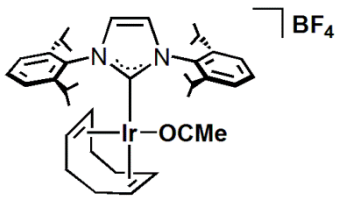
Molecular Structure Determination for Complexes 1 and 3. Intensity data were collected at 100 K on a Bruker APEX-II diffractometer equipped with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) operating at 50 kV and 40 mA. Data reduction of the diffraction images was performed using the APEX2 software.[3] All the structures were solved by direct methods and refined by full-matrix least-squares methods based on F^2 using the SHELXL-97 software.[4] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were positioned geometrically in idealized positions and refined with isotropic displacement parameters according to the riding model, except for the hydrido ligands, which were observed in the difference Fourier map and refined without restraints. All distance and angle calculations were performed using the SHELXL-97 and WinGX programs.[4,5]

Crystal data. Compound **1**: [$C_{35}H_{48}ClIrN_2$], monoclinic, *P21/n*, a = 10.6243(4) Å, b = 19.0191(8) Å, c = 15.8402(6) Å, β = 91.7070(10)º, Z = 4, M_r = 3199.3(2) g mol^{-1}, V = 3199.3(2) Å^3, D_{calcd} = 1.504 g cm^{-3}, λ(Mo Kα) = 0.71073 Å, T = 100 K, μ = 4.282 mm^{-1}, 77782 reflections collected, 7947 unique (R_{int} = 0.0407), 7031 observed, $R1(F_o)$ = 0.0231 [$I > 2\sigma(I)$], $wR2$ (F_o^2) = 0.0723 (all data), GOF = 1.006.

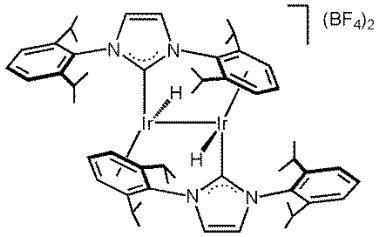
Crystal data. Compound **3**: [$C_{56}H_{78}B_2Cl_4F_8Ir_2N_4$], monoclinic, *C2/c*, a = 19.338(2) Å, b = 16.601(2) Å, c = 18.949(2) Å, β = 95.101(2)º, Z = 4, M_r = 1507.04, V = 6059.0(13) Å^3, D_{calcd} = 1.652 g cm^{-3}, λ(Mo Kα) = 0.71073 Å, T = 100 K, μ = 4.628 mm^{-1}, 27196 reflections collected, 7154 unique (R_{int} = 0.0496), 5661 observed, $R1(F_o)$ = 0.0485 [$I > 2\sigma(I)$], $wR2$ (F_o^2) = 0.1148 (all data), GOF = 1.009.

Preparation of [Ir(IPr)(OCMe$_2$)]BF$_4$ (1). A solution of [Ir(IPr)(Cl)(COD)] (220 mg, 0.30 mmol) in acetone was added 1 equiv of $AgBF_4$ (59 mg, 0.30 mmol), and stirred for 1 h. The resulting suspension was filtered through Celite and evaporated to dryness. The addition of diethyl ether and scratching with a spatula, a yellow solid is obtained. This solid was carefully washed with diethyl ether (3 × 5 mL) and dried in vacuo. Yield: 160 mg (64%). Anal. Cald. for $C_{38}H_{54}N_2BF_4IrO$: C, 54.73; H, 6.53; N, 3.36, found: C, 54.61; H, 6.48; N, 3.26. ^{1}H NMR (300 MHz, CD_2Cl_2, 253 K): δ 7.64 (t, JH-H = 7.4, 2H, Hp-IPr), 7.44 (d, JH-H = 7.4, 4H, Hm-IPr), 7.21 (s, 2H, =CHN), 4.06 and 3.09 (m, 4H =CH_{COD}), 2.69 (sept, JH-H = 6.9, 4H, C<u>H</u>Me$_{IPr}$), 2.15 (s, 6H, C=O<u>Me</u>$_2$), 1.87, 1.63, 1.36, and 1.26 (all m, CH_{2COD}), 1.43 and 1.18 (both d, JH-H = 6.9, 24H, CH<u>Me</u>$_{IPr}$). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, CD_2Cl_2, 253 K): δ 209.9 (s, <u>C</u>=OMe$_2$), 176.1 (s, $C_{Ir\text{-}IPr}$), 145.6 (s, $C_{q\text{-}IPr}$), 134.3 (s, C_{qN}), 130.9 (s, Cp-IPr), 124.7 (s, =CHN), 124.6 (s, Cm-IPr), 83.2 and 53.1 (both s, =CH_{COD}), 32.9 and 27.8 (both s, CH_{2COD}), 31.0 (s,

C=O$\underline{Me}_2$), 28.9 (s, $\underline{C}HMe_{IPr}$), 25.9 and 22.6 (both s, $CH\underline{Me}_{IPr}$). ^{19}F NMR (282 MHz, CD_2Cl_2, 298 K): -150.9 (s, BF_4).



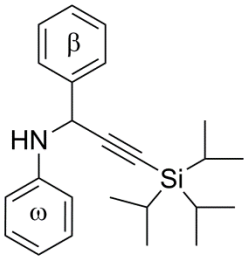
Preparation of [Ir(IPr)(μ-H_2)]$_2$(2BF_4) (2). A solution of **1** (160 mg, 0.1916 mmol) in acetone was stirred under dihydrogen atmosphere (1 bar) for 30 minutes. The resulting pale yellow solution was evaporated to yield an orange oil, which was solidified by the addition of diethyl ether. The resulting orange powder was carefully washed with diethyl ether (3 x 5 mL) and dried in vacuo. Yield: 112 mg (54%). Anal. Cald. for $C_{54}H_{73}B_2F_8Ir_2N_4$: C, 55.79; H, 6.33; N, 4.82, found: C, 55.61; H, 6.33; N, 4.77. ^1H NMR (300 MHz, CD_2Cl_2, 298 K): δ 7.87 and 7.42 (both d, $J_{H\text{-}H}$ = 2.0, 4H, =CHN), 7.80 (t, $J_{H\text{-}H}$ = 7.9, 2H, $H_{p\text{-}Ph\alpha}$), 7.56 (d, $J_{H\text{-}H}$ = 7.9, 4H, $H_{m\text{-}Ph\alpha}$), 6.27 (d, $J_{H\text{-}H}$ = 6.5, 4H, $H_{m\text{-}Ph\beta}$), 4.05 (t, $J_{H\text{-}H}$ = 6.5, 2H, $H_{p\text{-}Ph\beta}$), 2.38 and 2.19 (both, sept, $J_{H\text{-}H}$ = 6.8, 8H, $C\underline{H}Me_{IPr}$), 1.44, 1.37, 1.34, and 1.17 (all d, $J_{H\text{-}H}$ = 6.8, 48H, $CH\underline{Me}_{IPr}$), -15.51 (s, 2H, Ir-H). ^{13}C {^1H}-APT NMR plus HSQC and HMBC (75 MHz, CD_2Cl_2, 298 K): δ 145.8 (s, $C_{qIPr\alpha}$), 135.2 (s, C_qN_α), 132.3 (s, $C_{p\text{-}Ph\alpha}$), 125.1 (s, $C_{m\text{-}Ph\alpha}$), 124.5 and 124.0 (both s, =CHN), 121.2 (s, $C_{qIPr\beta}$), 95.0 (s, $C_{m\text{-}Ph\beta}$), 94.5 (s, $C_{p\text{-}Ph\beta}$), 93.5 (s, C_qN_β), 29.2 and 29.1 (both s, $\underline{C}HMe_{IPr}$), 25.0, 24.2, 22.7, and 22.3 (all s, $CH\underline{Me}_{IPr}$). ^{19}F NMR (282 MHz, CD_2Cl_2, 298 K): 150.9 (s, 2BF_4). Crystals suitable for X-ray diffraction studies were grown by slow evaporation of a diethyl ether solution.



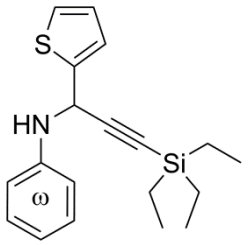
Standard conditions for the preparation of *N*-propargylamines. A NMR tube was charged with 0.01 mmol of catalyst **2**, 0.2 mmol of imine derivative and 0.2 mmol of the alkyne in 0.5 mL of acetone-d_6. After sealing it under argon atmosphere, it was heated at 80 ºC. The reaction course was monitored by ^1H NMR and the conversion was quantified by the integration of the ^1H NMR signals of the imine derivative and the products.

Data analysis of propargylamines.

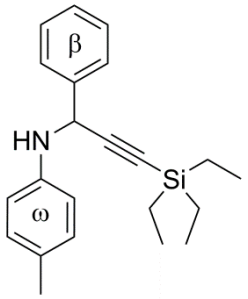
^1H NMR (400 MHz, Acetone-d_6, 298 K): δ 7.09 (d, $J_{H\text{-}H}$ = 7.7, 2H, $H_{o\text{-}Ph\beta}$), 6.93 (dd, $J_{H\text{-}H}$ = 7.7, 7.5, 2H, $H_{m\text{-}Ph\beta}$), 6.85 (t, $J_{H\text{-}H}$ = 7.5, 1H, $H_{p\text{-}Ph\beta}$), 6.64 (dd, $J_{H\text{-}H}$ = 8.5, 6.9, 2H, $H_{m\text{-}Ph\omega}$), 6.24 (d, $J_{H\text{-}H}$ = 8.5, 2H, $H_{o\text{-}Ph\omega}$), 6.17 (t, $J_{H\text{-}H}$ = 6.9, 1H, $H_{p\text{-}Ph\omega}$), 4.57 (s, CH), 3.97 (br, NH), 0.75 (d, $J_{H\text{-}H}$ = 2.1, 9H, Si-CH$\underline{Me}$). 0.73 (sept, $J_{H\text{-}H}$ = 2.1, 4H, Si-C$\underline{H}$Me). ^{13}C {^1H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.9 (s, $C_{q\text{-}Ph\beta}$), 128.7 (s, $C_{m\text{-}Ph\omega}$), 128.4 (s, $C_{m\text{-}Ph\beta}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 116.7 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 96.6 and 83.9 (both s, C≡C), 53.6 (s, CH), 17.9 (s, Si-CH$\underline{Me}$), 10.9 (s, Si-$\underline{C}$HMe).



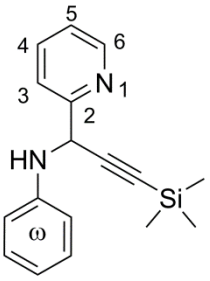
^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.24 (dd, $J_{H\text{-}H}$ = 5.2, 1.3, 1H, $H_{o\text{-}1th}$), 6.93 (dd, $J_{H\text{-}H}$ = 5.2, 3.7, 1H, $H_{m\text{-}th}$), 7.10 (dd, $J_{H\text{-}H}$ = 7.5, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 7.07 (d, $J_{H\text{-}H}$ = 3.7, 1H, $H_{o\text{-}2th}$), 6.70 (d, $J_{H\text{-}H}$ = 7.5, 2H, $H_{o\text{-}Ph\omega}$), 6.61 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 5.25 (s, CH), 3.80 (s, NH), 1.04 (t, $J_{H\text{-}H}$ = 7.6, 9H, Si-$CH_2C\underline{H}_3$), 0.65 (q, $J_{H\text{-}H}$ = 7.6, 6H, Si-$C\underline{H}_2CH_3$). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 148.7 (s, $C_{q\text{-}th}$), 147.5 (s, $C_{q\text{-}Ph\omega}$), 128.8 (s, $C_{m\text{-}Ph\omega}$), 126.6 (s, $C_{m\text{-}th}$), 123.8 (s, $C_{o\text{-}2th}$), 123.7 (s, $C_{o\text{-}1th}$), 117.2 (s, $C_{p\text{-}Ph\omega}$), 113.5 (s, $C_{o\text{-}Ph\omega}$), 94.9 and 81.0 (both s, C≡C), 49.6 (s, CH), 6.8 (s, Si-$CH_2\underline{C}H_3$), 3.9 (s, Si-$\underline{C}H_2CH_3$).



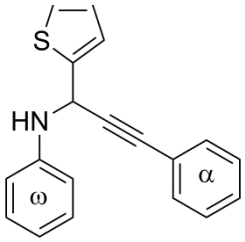
^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.45 (d, $J_{H\text{-}H}$ = 7.8, 2H, , $H_{o\text{-}Ph\beta}$), 7.29 (dd, $J_{H\text{-}H}$ = 7.8, 7.2, 2H, $H_{m\text{-}Ph\beta}$), 7.20 (t, $J_{H\text{-}H}$ = 7.2, 1H, $H_{p\text{-}Ph\beta}$), 6.83 (d, $J_{H\text{-}H}$ = 8.2, 2H, $H_{m\text{-}Ph\omega}$), 6.52 (d, $J_{H\text{-}H}$ = 8.2, 2H, $H_{p\text{-}Ph\omega}$), 4.91 (s, CH), 4.30 (br, NH), 2.12 (s, 3H, Me), 1.02 (t, $J_{H\text{-}H}$ = 8.0, 9H, Si-$CH_2C\underline{H}_3$), 0.65 (q, $J_{H\text{-}H}$ = 8.0, 6H, Si-$C\underline{H}_2CH_3$). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 145.6 (s, $C_{q\text{-}Ph\omega}$), 144.1 (s, $C_{q\text{-}Ph\beta}$), 129.2 (s, $C_{m\text{-}Ph\omega}$), 128.4 (s, $C_{m\text{-}Ph\beta}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 113.6 (s, $C_{o\text{-}Ph\omega}$), 91.2 and 85.6 (both s, C≡C), 53.9 (s, CH), 19.6 (s, Me), 6.7 (s, Si-$CH_2\underline{C}H_3$), 3.9 (s, Si-$\underline{C}H_2CH_3$).



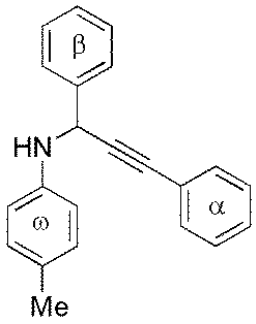
^{1}H NMR (400 MHz, Acetone-d_6, 298 K): δ 8.36 (dq, $J_{H\text{-}H}$ = 4.8, 0.9, 1H, $H_{6\text{-}py}$), 7.49 (ddd, $J_{H\text{-}H}$ = 7.8, 7.6, 1.8, 1H, $H_{4\text{-}py}$), 7.28 (d, $J_{H\text{-}H}$ = 7.8, 1H, $H_{3\text{-}py}$), 7.02 (ddd, $J_{H\text{-}H}$ = 7.6, 4.8, 0.9, 1H, $H_{5\text{-}py}$), 6.86 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 6.49 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\omega}$), 6.40 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 4.87 (s, CH), 3.64 (br, NH), 0.00 (s, 9H, Si-Me). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 162.4 (s, $C_{2\text{-}py}$), 149.1 (s, $C_{6\text{-}py}$), 147.5 (s, $C_{q\text{-}Ph\omega}$), 136.4 (s, $C_{4\text{-}py}$), 128.0 (s, $C_{m\text{-}Ph\omega}$), 122.0 (s, $C_{5\text{-}py}$), 121.2 (s, $C_{3\text{-}py}$), 116.9 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 94.6 and 88.8 (both s, C≡C), 55.0 (s, CH), -0.7 (s, Si-Me).



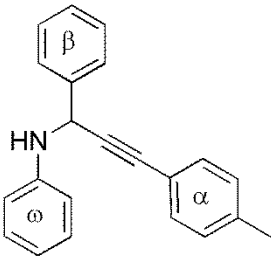
^{1}H NMR (400 MHz, Acetone-d_6, 298 K): δ 7.39 (dd, $J_{H\text{-}H}$ = 8.4, 7.3, 2H, $H_{m\text{-}Ph\alpha}$), 7.38 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\alpha}$), 7.27 (d, $J_{H\text{-}H}$ = 8.4, 2H, $H_{o\text{-}Ph\alpha}$), 7.24 (dd, $J_{H\text{-}H}$ = 5.1, 1.2, 1H, $H_{o\text{-}1th}$), 7.09 (dd, $J_{H\text{-}H}$ = 8.3, 7.3, 2H, $H_{m\text{-}Ph\omega}$), 7.06 (d, $J_{H\text{-}H}$ = 3.5, 1H, $H_{o\text{-}2th}$), 6.93 (dd, $J_{H\text{-}H}$ = 5.1, 3.5, 1H, $H_{m\text{-}th}$), 6.72 (d, $J_{H\text{-}H}$ = 8.3, 2H, $H_{o\text{-}Ph\omega}$), 6.63 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\omega}$), 5.26 (s, CH), 3.60 (br, NH). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (100 MHz, Acetone-d_6, 298 K): δ 152.3 (s, $C_{q\text{-}Ph\alpha}$), 149.6 (s, $C_{q\text{-}th}$), 148.5 (s, $C_{q\text{-}Ph\omega}$), 130.1 (s, $C_{m\text{-}Ph\alpha}$), 129.8 (s, $C_{m\text{-}Ph\omega}$), 128.8 (s, $C_{p\text{-}Ph\alpha}$), 121.9 (s, $C_{o\text{-}Ph\alpha}$), 124.7 and 124.6 (both s, $C_{o\text{-}th}$), 118.2 (s, $C_{p\text{-}Ph\omega}$), 114.5 (s, $C_{o\text{-}Ph\omega}$), 83.9 and 79.3 (both s, C≡C), 50.4 (s, CH).



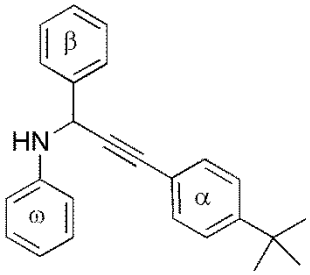
^{1}H NMR (300 MHz, C_6D_6, 298 K): 7.3-7.0 (all m, 10H, H_{Ph}), 6.68 (d, $J_{H\text{-}H}$ = 8.3, 2H, $H_{m\text{-}Ph\omega}$), 6.37 (d, $J_{H\text{-}H}$ = 8.3, 2H, $H_{o\text{-}Ph\omega}$), 4.77 (s, 1H, C<u>H</u>NH), 3.50 (br, 1H, CHN<u>H</u>), 1.96 (s, 3H, Me). ^{13}C{^{1}H}-APT NMR (75 MHz, C_6D_6, 298 K): δ 145.6, 144.0 and 125.5 (all s, C_{qPh}), 131.9, 128.9, 128.6, 128.4, 126.8, and 126.6 (all s, C_{Ph}), 129.3 (s, $C_{m\text{-}Ph\omega}$), 113.7 (s, $C_{o\text{-}Ph\omega}$), 81.2 and 78.4 (both s, C_1 and C_2), 53.9 (s, CHNH), 19.7 (s, Me).



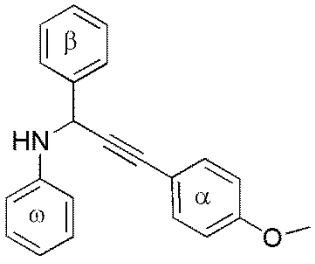
^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.29 (d, $J_{H\text{-}H}$ = 8.0, 2H, $H_{o\text{-}Ph\beta}$), 7.24 (d, $J_{H\text{-}H}$ = 7.4, 2H, $H_{o\text{-}Ph\alpha}$), 7.13 (dd, $J_{H\text{-}H}$ = 8.0, 7.3, 2H, $H_{m\text{-}Ph\beta}$), 7.04 (d, $J_{H\text{-}H}$ = 7.4, 2H, $H_{m\text{-}Ph\alpha}$), 7.02 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\beta}$), 6.85 (dd, $J_{H\text{-}H}$ = 8.6, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 6.44 (d, $J_{H\text{-}H}$ = 8.6, 2H, $H_{o\text{-}Ph\omega}$), 6.37 ((t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 4.79 (s, 1H, CH), 3.64 (br, NH), 2.16 (s, 3H, Me). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.9 (s, $C_{q\text{-}Ph\beta}$), 138.9 (s, $C_{q\text{-}Ph\text{-}Me}$), 129.2 (s, $C_{o\text{-}Ph\alpha}$), 128.8 (s, $C_{m\text{-}Ph\beta}$), 128.7 (s, $C_{m\text{-}Ph\alpha}$), 128.4 (s, $C_{m\text{-}Ph\omega}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 119.2 (s, $C_{q\text{-}Ph\alpha}$), 116.7 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 85.6 and 79.2 (both s, C≡C), 53.4 (s, CH), 20.3 (s, Me).



^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.30 (d, $J_{H\text{-}H}$ = 8.0, 2H, $H_{o\text{-}Ph\beta}$), 7.27 (d, $J_{H\text{-}H}$ = 6.0, 2H, $H_{o\text{-}Ph\alpha}$), 7.25 (d, $J_{H\text{-}H}$ = 6.0, 2H, $H_{m\text{-}Ph\alpha}$), 7.13 (dd, $J_{H\text{-}H}$ = 8.0, 7.3, 2H, $H_{m\text{-}Ph\beta}$), 7.05 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\beta}$), 6.84 (dd, $J_{H\text{-}H}$ = 8.2, 7.3, 2H, $H_{m\text{-}Ph\omega}$), 6.44 (d, $J_{H\text{-}H}$ = 8.2, 2H, $H_{o\text{-}Ph\omega}$), 6.37 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\omega}$), 4.78 (s, 1H, CH), 3.66 (br, NH), 1.14 (s, 9H, ^{t}Bu). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 150.1 (s, $C_{q\text{-}Ph\text{-}^{t}Bu}$), 147.8 (s, $C_{q\text{-}Ph\omega}$), 143.8 (s, $C_{q\text{-}Ph\beta}$), 128.8 (s, $C_{m\text{-}Ph\beta}$), 128.6 (s, $C_{o\text{-}Ph\alpha}$), 128.4 (s, $C_{m\text{-}Ph\omega}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 125.4 (s, $C_{m\text{-}Ph\alpha}$), 119.5 (s, $C_{q\text{-}Ph\alpha}$), 116.7 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 88.4 and 77.5 (both s, C≡C), 53.5 (s, CH), 34.3 (s, $C_{q\text{-}^{t}Bu}$), 30.8 (s, ^{t}Bu).

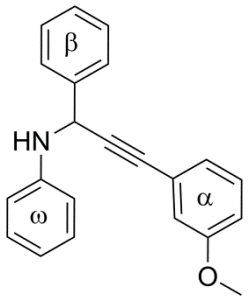


^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.47 (d, $J_{H\text{-}H}$ = 8.4, 2H, $H_{o\text{-}Ph\alpha}$), 7.44 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\beta}$), 7.31 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\beta}$), 7.20 (t, $J_{H\text{-}H}$ = 7.1, 1H, $H_{p\text{-}Ph\beta}$), 7.02 (dd, $J_{H\text{-}H}$ = 8.0, 7.3, 2H, $H_{m\text{-}Ph\omega}$), 6.94 (d, $J_{H\text{-}H}$ = 8.4, 2H, $H_{m\text{-}Ph\alpha}$), 6.62 (d, $J_{H\text{-}H}$ = 8.0, 2H, $H_{o\text{-}Ph\omega}$), 6.54 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\omega}$), 4.95 (s, 1H, CH), 3.81 (s, 3H, OMe), 3.77 (br, NH). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 160.2 ($C_{q\text{-}OMe}$), 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.9 (s, $C_{q\text{-}Ph\beta}$), 133.3 (s, $C_{o\text{-}Ph\alpha}$), 128.7 (s, $C_{m\text{-}Ph\beta}$), 128.4 (s, $C_{m\text{-}Ph\omega}$), 126.9 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 116.7 (s, $C_{p\text{-}Ph\omega}$), 114.2 (s, $C_{q\text{-}Ph\alpha}$), 114.0 (s, $C_{m\text{-}Ph\alpha}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 82.3 and 77.0 (both s, C≡C), 54.0 (s, OMe), 53.5 (s, CH).

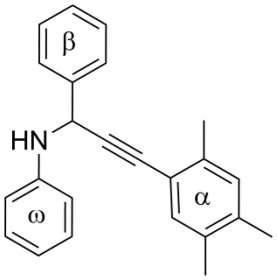


^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.47 (d, $J_{H\text{-}H}$ = 7.6, 2H, $H_{o\text{-}Ph\beta}$), 7.33 (dd, $J_{H\text{-}H}$ = 7.6, 7.4, 2H, $H_{m\text{-}Ph\beta}$), 7.31 (dd, $J_{H\text{-}H}$ = 7.6, 7.1, 1H, $H_{m\text{-}Ph\alpha}$), 7.21 (t, $J_{H\text{-}H}$ = 7.1, 1H, $H_{p\text{-}Ph\beta}$), 7.09 (d, $J_{H\text{-}H}$ = 7.6, 1H, $H_{o\text{-}Ph\alpha}$),7.05 (m, 1H, $H_{o\text{-}Ph\alpha}$), 7.03 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 6.95 (d, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\alpha}$), 6.62 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\omega}$), 6.56 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 4.96 (s, 1H, CH), 3.80 (s, 3H, OMe), 3.69 (br, NH). ^{13}C {^{1}H}-APT NMR plus HSQC and

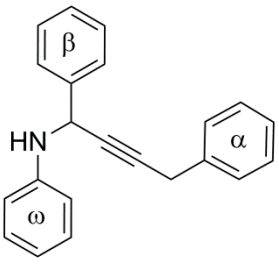
HMBC (75 MHz, Acetone-d_6, 298 K): δ 160.2 (s, $C_{q\text{-}OMe}$), 147.8 (s, $C_{q\text{-}Ph\omega}$), 143.9 (s, $C_{q\text{-}Ph\beta}$), 128.8 (s, $C_{m\text{-}Ph\beta}$), 128.7 (s, $C_{m\text{-}Ph\alpha}$), 128.4 (s, $C_{m\text{-}Ph\omega}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 124.2 (s, $C_{o\text{-}Ph\alpha}$), 123.3 (s, $C_{q\text{-}Ph\alpha}$), 116.9 (s, $C_{o\text{-}Ph\alpha}$), 116.8 (s, $C_{p\text{-}Ph\omega}$), 115.2 (s, $C_{p\text{-}Ph\alpha}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 82.8 and 78.1 (both s, C≡C), 54.8 (s, OMe), 53.5 (s, CH).



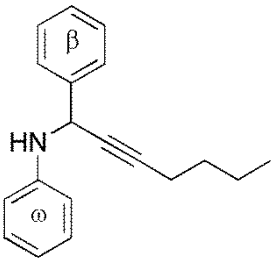
^{1}H NMR (400 MHz, Acetone-d_6, 298 K): δ 7.48 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\beta}$), 7.30 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\beta}$), 7.23 (s, 2H, $H_{Ph\alpha}$), 7.20 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\beta}$), 7.03 (dd, $J_{H\text{-}H}$ = 8.5, 7.3, 2H, $H_{m\text{-}Ph\omega}$), 6.63 (d, $J_{H\text{-}H}$ = 8.5, 2H, 6.62 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\omega}$), 6.55 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\omega}$), 4.97 (s, 1H, CH), 2.22 (s, 9H, Me), 3.70 (br, NH). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 148.6 (s, $C_{q\text{-}Ph\omega}$), 144.7 (s, $C_{q\text{-}Ph\beta}$), 138.5, 138.4, 137.9 and 137.8 (all s, $C_{q\text{-}Ph\alpha}$), 134.0 (s, $C_{Ph\alpha}$), 129.7 (s, $C_{m\text{-}Ph\omega}$), 129.4 (s, $C_{m\text{-}Ph\beta}$), 127.8 (s, $C_{p\text{-}Ph\beta}$), 127.4 (s, $C_{o\text{-}Ph\beta}$), 83.1 and 80.0 (both s, C≡C), 117.7 (s, $C_{p\text{-}Ph\omega}$), 114.3 (s, $C_{o\text{-}Ph\omega}$), 54.5 (s, CH), 19.5 (br, Me).



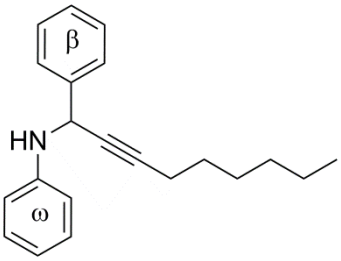
^{1}H NMR (400 MHz, Acetone-d_6, 298 K): δ 7.48 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\beta}$), 7.43 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\alpha}$), 7.34 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\alpha}$), 7.31 (dd, $J_{H\text{-}H}$ = 7.8, 7.4, 2H, $H_{m\text{-}Ph\beta}$), 7.28 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\alpha}$), 7.21 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\beta}$), 7.04 (dd, $J_{H\text{-}H}$ = 8.6, 7.2, 2H, $H_{m\text{-}Ph\omega}$), 6.64 (d, $J_{H\text{-}H}$ = 8.6, 2H, $H_{o\text{-}Ph\omega}$), 6.56 (t, $J_{H\text{-}H}$ = 7.2, 1H, $H_{p\text{-}Ph\omega}$), 4.97 (s, 1H, CH), 4.44 (br, NH), 3.34 (s, 2H, C$\underline{H}_2$-Ph). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (100 MHz, Acetone-d_6, 298 K): δ 148.7 (s, $C_{q\text{-}Ph\omega}$), 144.8 (s, $C_{q\text{-}Ph\beta}$), 137.5 (s, $C_{q\text{-}Ph\alpha}$), 129.7 (s, $C_{m\text{-}Ph\alpha}$), 129.6 (s, $C_{m\text{-}Ph\omega}$), 129.3 (s, $C_{m\text{-}Ph\beta}$), 129.2 (s, $C_{o\text{-}Ph\alpha}$), 127.8 (s, $C_{p\text{-}Ph\beta}$), 127.4 (s, $C_{o\text{-}Ph\beta}$), 126.8 (s, $C_{p\text{-}Ph\alpha}$), 117.6 (s, $C_{p\text{-}Ph\omega}$), 114.4 (s, $C_{o\text{-}Ph\omega}$), 78.2 and 75.0 (both s, C≡C), 54.6 (s, CH), 39.3 (s, $\underline{C}H_2$-Ph).



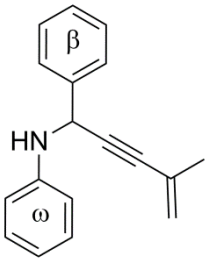
^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.43 (d, $J_{H\text{-}H}$ = 7.5, 2H, $H_{o\text{-}Ph\beta}$), 7.26 (dd, $J_{H\text{-}H}$ = 7.5, 7.0, 2H, $H_{m\text{-}Ph\beta}$), 7.19 (t, $J_{H\text{-}H}$ = 7.0, 1H, $H_{p\text{-}Ph\beta}$), 6.98 (dd, $J_{H\text{-}H}$ = 8.6, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 6.58 (d, $J_{H\text{-}H}$ = 8.6, 2H, $H_{o\text{-}Ph\omega}$), 6.51 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 4.92 (s, 1H, CH), 3.79 (br, NH), 1.6-1.1 (m, 6H, CH_2), 0.88 (t, $J_{H\text{-}H}$ = 7.3, 3H, CH_3). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.9 (s, $C_{q\text{-}Ph\beta}$), 128.8 (s, $C_{m\text{-}Ph\beta}$), 128.7 (s, $C_{m\text{-}Ph\omega}$), 126.7 (s, $C_{p\text{-}Ph\beta}$), 126.4 (s, $C_{o\text{-}Ph\beta}$), 116.8 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 88.2 and 70.2 (both s, C≡C), 53.5 (s, CH), 31.7, 28.8, and 22.3 (all s, CH_2), 13.3 (s, CH_3).



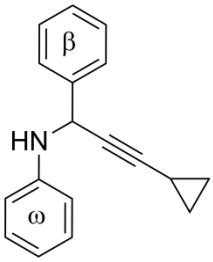
^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.47 (d, $J_{H\text{-}H}$ = 7.7, 2H, $H_{o\text{-}Ph\beta}$), 7.33 (dd, $J_{H\text{-}H}$ = 7.7, 7.2, 2H, $H_{m\text{-}Ph\beta}$), 7.23 (t, $J_{H\text{-}H}$ = 7.2, 1H, $H_{p\text{-}Ph\beta}$), 7.02 (dd, $J_{H\text{-}H}$ = 8.2, 7.5, 2H, $H_{m\text{-}Ph\omega}$), 6.62 (d, $J_{H\text{-}H}$ = 8.2, 2H, $H_{o\text{-}Ph\omega}$), 6.55 (t, $J_{H\text{-}H}$ = 7.5, 1H, $H_{p\text{-}Ph\omega}$), 4.96 (s, 1H, CH), 3.72 (br, NH), 1.5-1.2 (m, 10H, CH_2), 0.91 (m, 3H, CH_3). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.8 (s, $C_{q\text{-}Ph\beta}$), 128.7 (s, $C_{m\text{-}Ph\beta}$), 128.3 (s, $C_{m\text{-}Ph\omega}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 116.7 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 88.3 and 70.4 (both s, C≡C), 53.6 (s, CH), 31.6, 31.5, 31.2, 28.9, and 22.4 (all s, CH_2), 13.5 (s, CH_3).



^{1}H NMR (300 MHz, Acetone-d_6, 298 K): δ 7.52 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\beta}$), 7.36 (dd, $J_{H\text{-}H}$ = 7.8, 7.2, 2H, $H_{m\text{-}Ph\beta}$), 7.27 (t, $J_{H\text{-}H}$ = 7.2, 1H, $H_{p\text{-}Ph\beta}$), 7.07 (dd, $J_{H\text{-}H}$ = 8.0, 7.4, 2H, $H_{m\text{-}Ph\omega}$), 6.67 (d, $J_{H\text{-}H}$ = 8.0, 2H, $H_{o\text{-}Ph\omega}$), 6.60 (t, $J_{H\text{-}H}$ = 7.4, 1H, $H_{p\text{-}Ph\omega}$), 5.40 and 5.38 (both m, 2H, $=CH_2$), 5.01 (s, 1H, =CH), 3.90 (s, NH), 1.93 (dd, $J_{H\text{-}H}$ = 1.6, 1.1, 3H, Me). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (75 MHz, Acetone-d_6, 298 K): δ 147.7 (s, $C_{q\text{-}Ph\omega}$), 143.8 (s, $C_{q\text{-}Ph\beta}$), 128.8 (s, $C_{m\text{-}Ph\omega}$), 128.4 (s, $C_{m\text{-}Ph\beta}$), 126.8 (s, $C_{p\text{-}Ph\beta}$), 126.5 (s, $C_{o\text{-}Ph\beta}$), 122.6 (s, $C_{q\text{-}Me}$), 122.6 (s, $=CH_2$), 116.8 (s, $C_{p\text{-}Ph\omega}$), 113.4 (s, $C_{o\text{-}Ph\omega}$), 82.6 and 77.4 (both s, C≡C), 53.6 (s, =CH), 22.6 (s, Me).

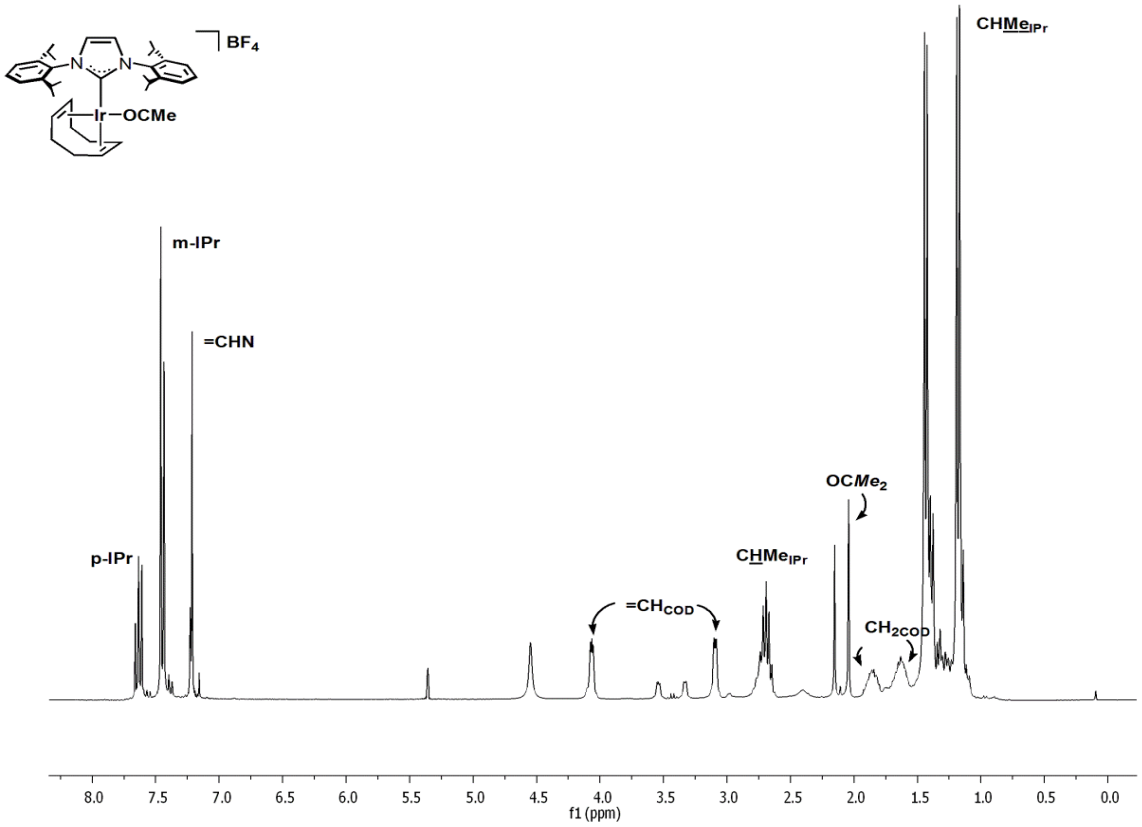


^{1}H NMR (400 MHz, Acetone-d_6, 298 K): δ 7.38 (d, $J_{H\text{-}H}$ = 7.8, 2H, $H_{o\text{-}Ph\beta}$), 7.22 (dd, $J_{H\text{-}H}$ = 7.8, 7.3, 2H, $H_{m\text{-}Ph\beta}$), 7.11 (t, $J_{H\text{-}H}$ = 7.3, 1H, $H_{p\text{-}Ph\beta}$), 6.93 (dd, $J_{H\text{-}H}$ = 8.5, 7.2, 2H, $H_{m\text{-}Ph\omega}$), 6.53 (d, $J_{H\text{-}H}$ = 8.5, 2H, $H_{o\text{-}Ph\omega}$), 6.46 (t, $J_{H\text{-}H}$ = 7.2, 1H, $H_{p\text{-}Ph\omega}$), 4.87 (s, 1H, CH), 4.26 (br, NH), 1.17 (m, 1H, C<u>H</u>-CH_2), 0.68 and 0.53 (both m, 4H, C<u>H</u>-CH_2). ^{13}C {^{1}H}-APT NMR plus HSQC and HMBC (100 MHz, Acetone-d_6, 298 K): δ 149.0 (s, $C_{q\text{-}Ph\omega}$), 145.1 (s, $C_{q\text{-}Ph\beta}$), 129.9 (s, $C_{m\text{-}Ph\omega}$), 129.6 (s, $C_{m\text{-}Ph\beta}$), 127.9 (s, $C_{p\text{-}Ph\beta}$), 127.7 (s, $C_{o\text{-}Ph\beta}$), 117.9 (s, $C_{p\text{-}Ph\omega}$), 114.6 (s, $C_{o\text{-}Ph\omega}$), 88.0 and 84.0 (both s, C≡C), 54.7 (s, <u>C</u>H), 23.7 (s, <u>C</u>H-CH_2), 8.6 (s, CH-<u>C</u>H_2).

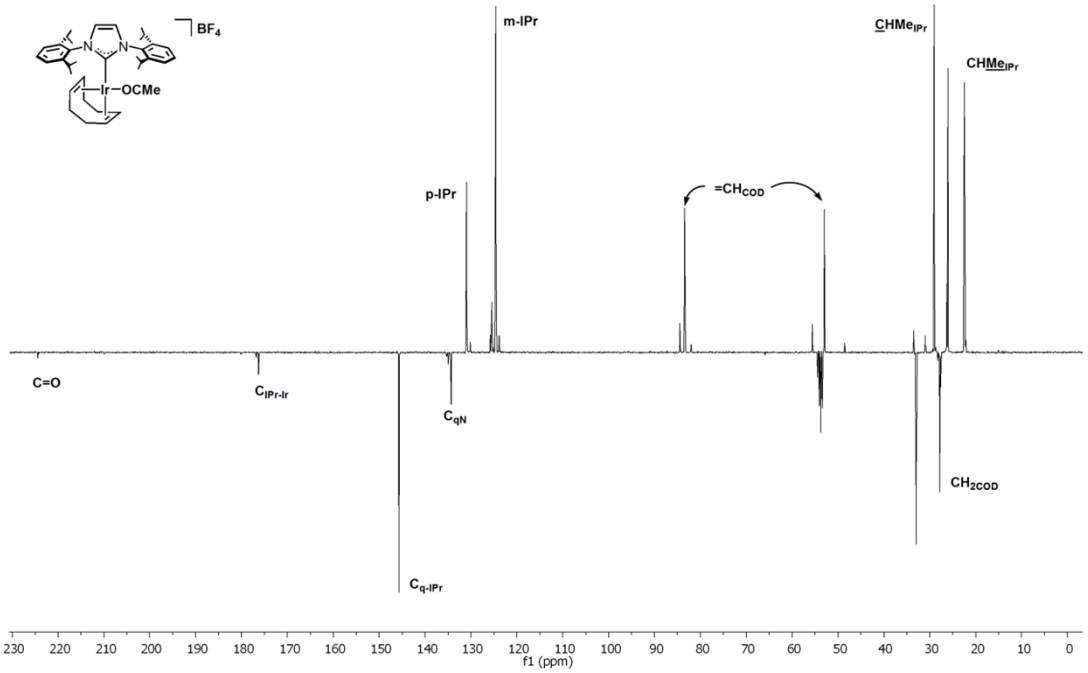


NMR Spectra of Complexes

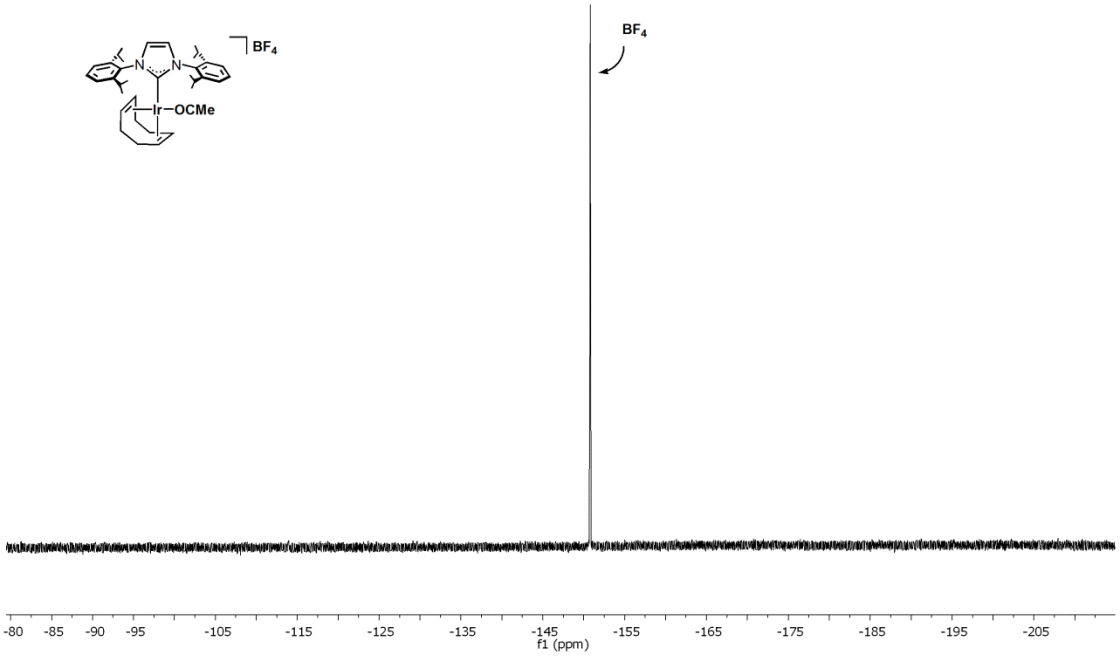
^{1}H NMR



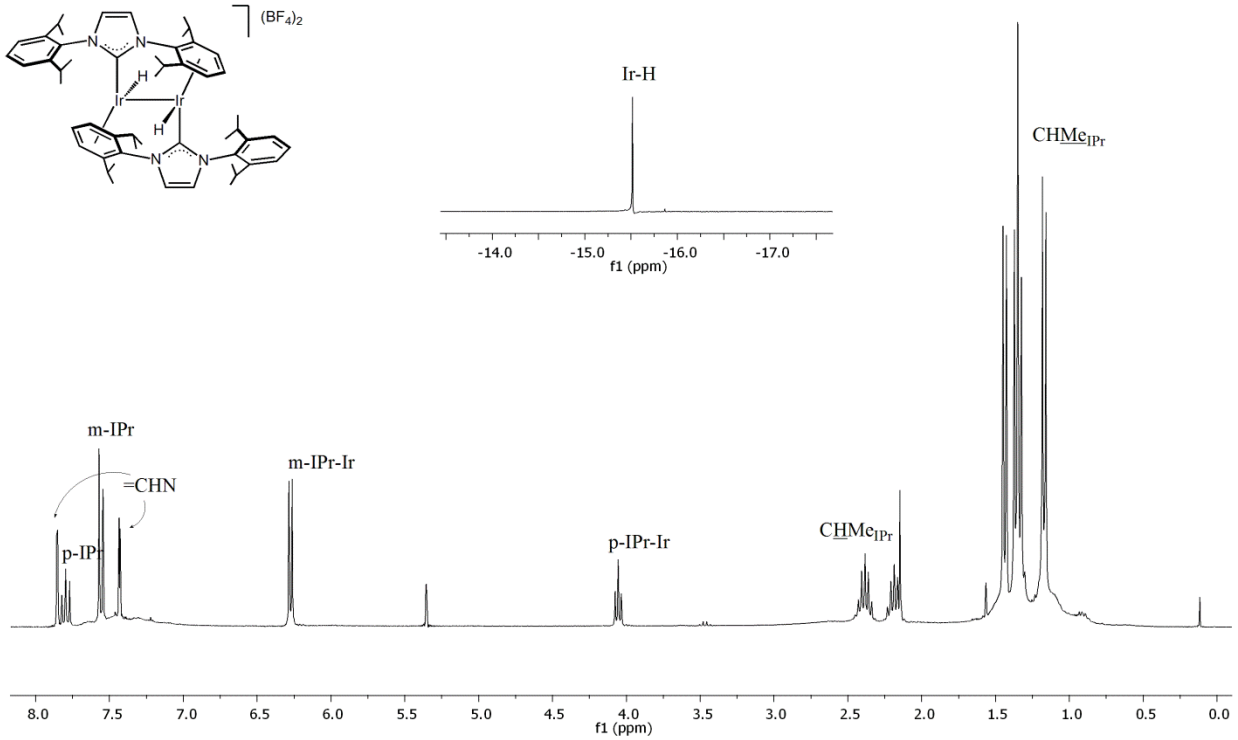
^{13}C NMR



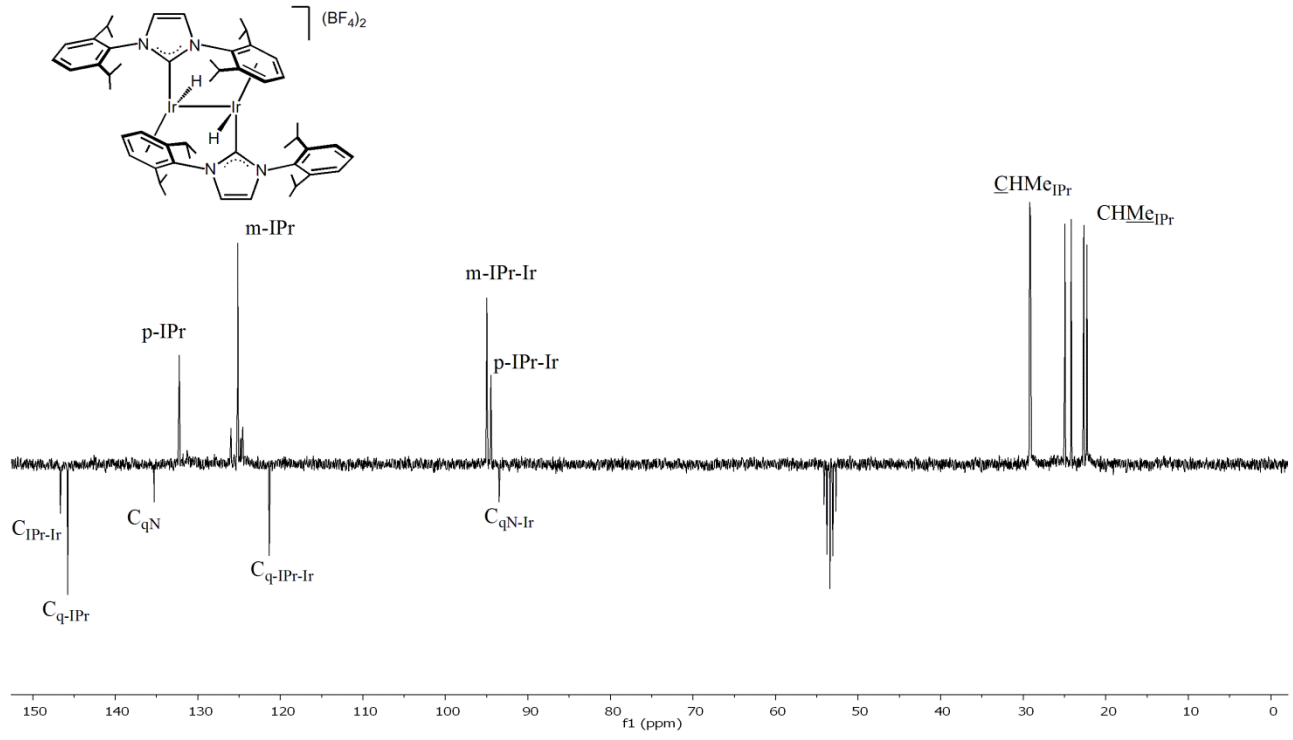
^{19}F NMR


BF4
Ir–OCMe
BF4
-80
-85
-90
-95
-105
-115
-125
-135
-145
-155
-165
-175
-185
-195
-205
f1 (ppm)

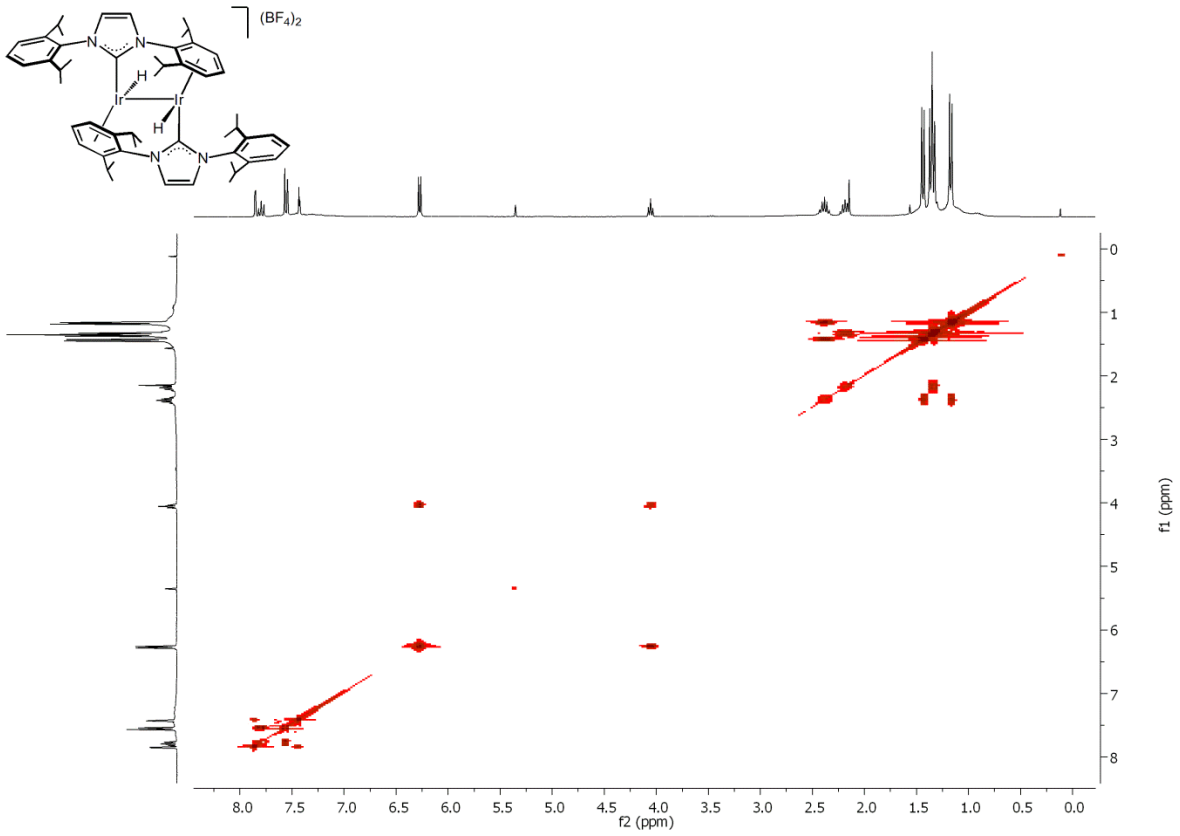
^{1}H NMR



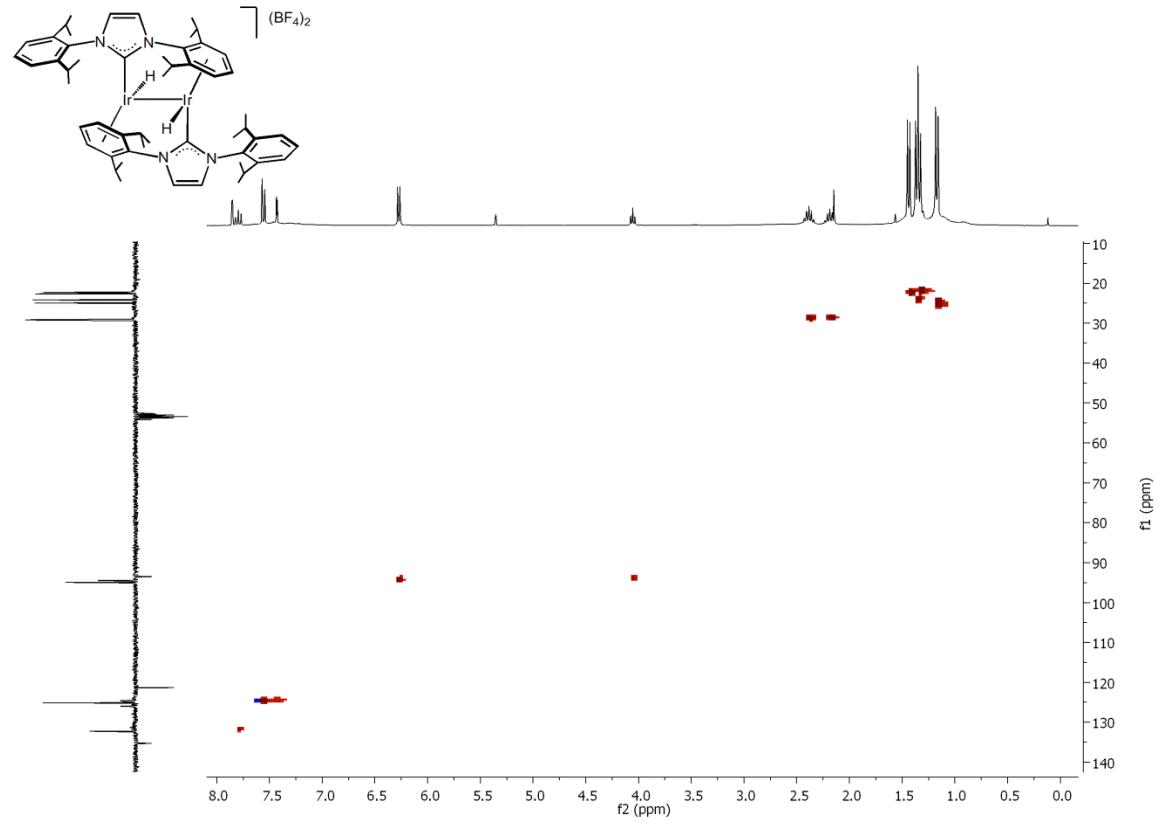
^{13}C NMR



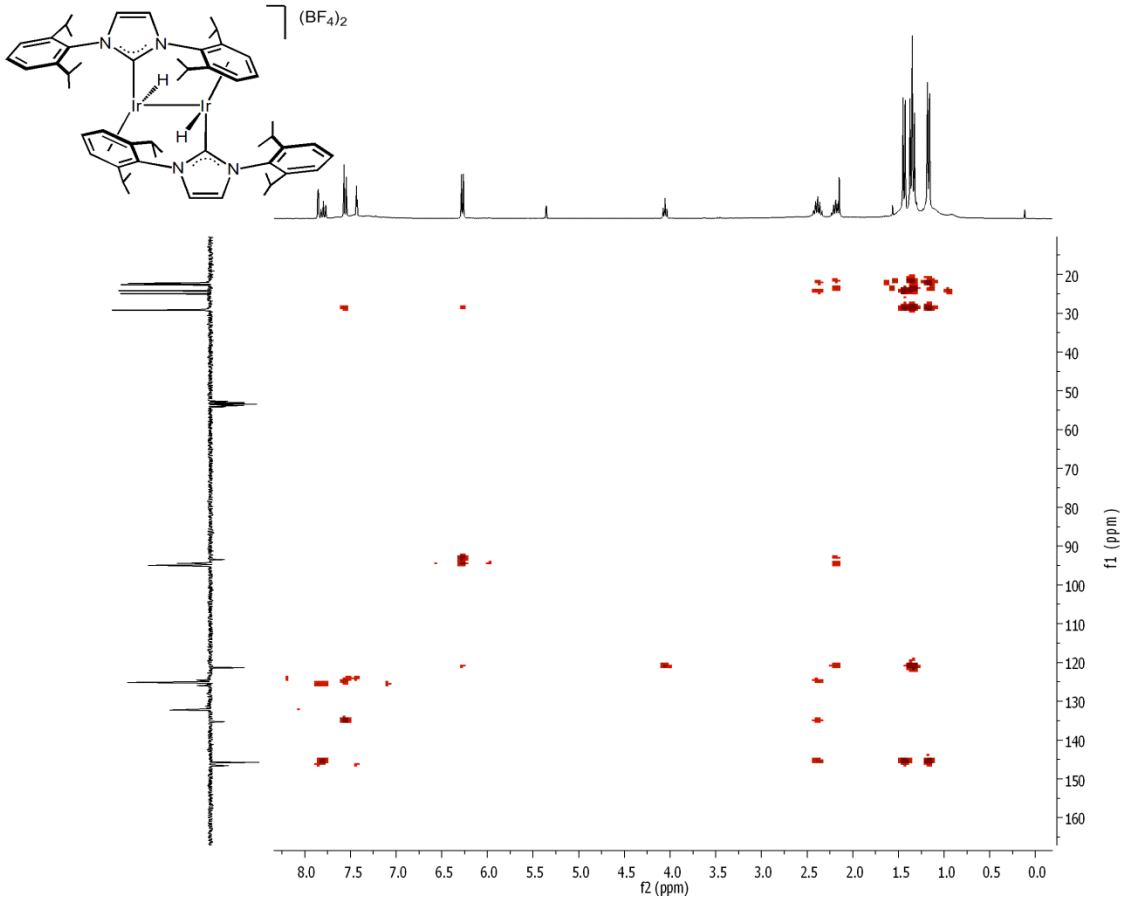
^{1}H-^{1}H COSY



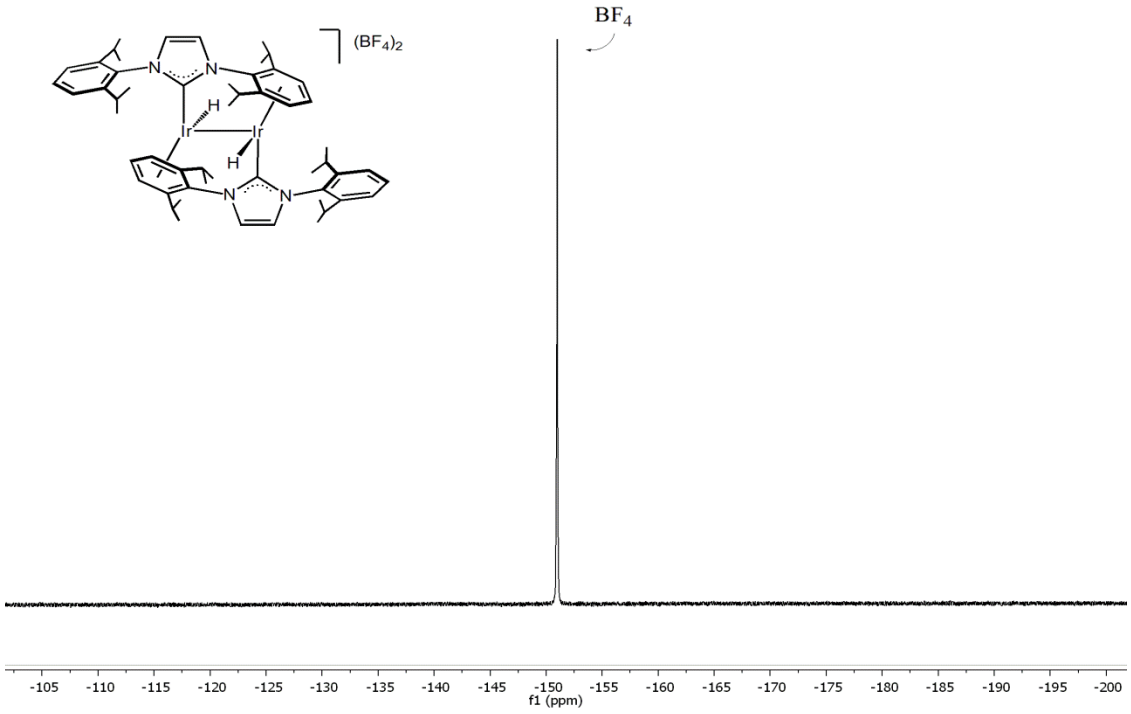
^{1}H-^{13}C HSQC



^{1}H-^{13}C HMBC



^{19}F NMR



Computational details:

All calculations have been carried out at the DFT level using the Gaussian 09.D1 package.[6] The B3LYP-D3[7,8] functional has been used with Becke-Johnson damping[9] and the "ultrafine" grid in combination with the def2-SVP basis set[10] for all atoms and single point calculations at the same level have been done using the PCM model[11] for acetone in order to simulate the solvent effects.

Table S1. Absolute and relative energies and Gibbs free energies (at standard conditions) for all DFT calculated structures in gas phase and solvent.

Structure	E (a.u.)	E(PCM) (a.u.)	ΔE(PCM) (kcalmol^{-1})	G(a.u.)	□G(PCM) (kcalmol^{-1})
A	-1202.11399	-1202.31691	0.0	-1201.78634	0.00
B	-1510.04773	-1510.11912	-28.1	-1509.6518	-20.78
C	-2066.80802	-2066.99146	-38.3	-2066.20429	-7.90
TSC/D	-2066.79747	-2066.97234	-26.3	-2066.19805	1.40
D	-2066.82265	-2067.01090	-50.5	-2066.2002	-8.35
product	-864.63576	-864.64312	-18.6	-864.38013	-1.00
phenylacetylene	-308.19997	-308.20369		-308.12776	
imine	-556.40466	-556.40976		-556.24931	

Geometrical representation of the DFT optimized molecular structures. Key geometrical parameters (distances in Å, angles in degrees) for all DFT calculated structures

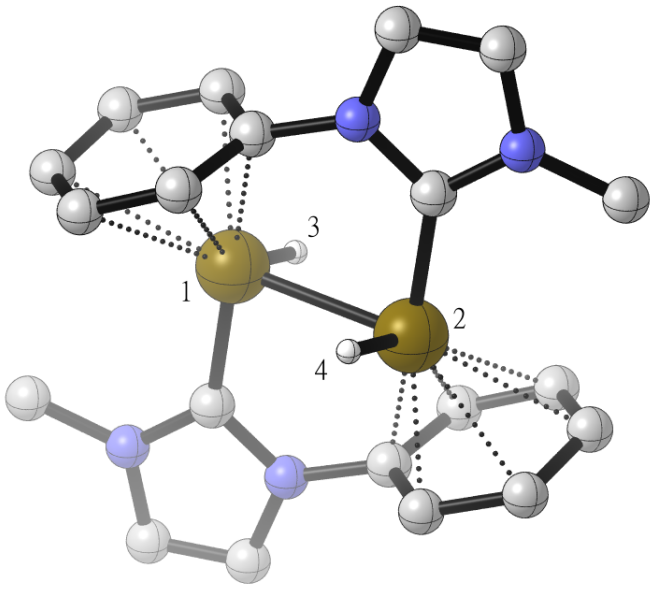


Figure S1. Complex **A**. Ci symmetry group, dIr1-Ir2 2.629, dIr1-H3 1.549, aIr1-Ir2-H4 82.7º

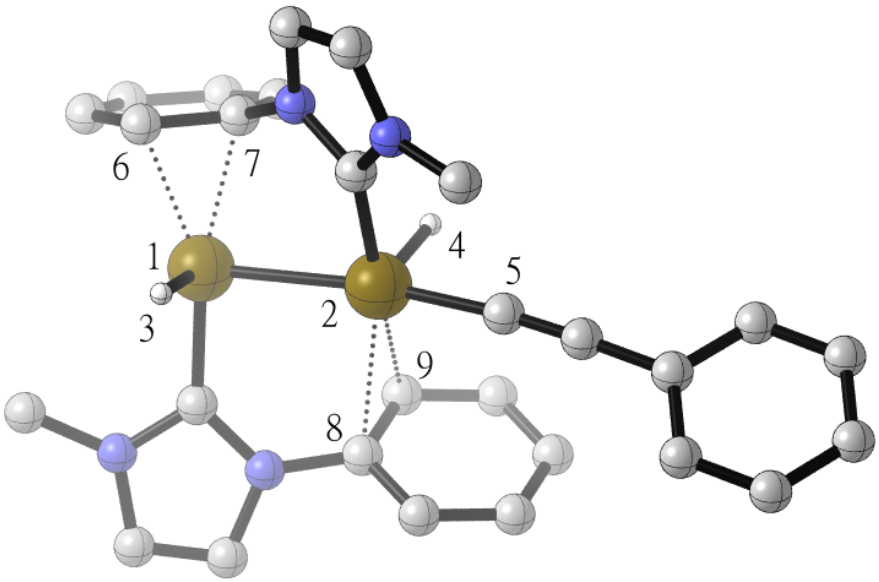


Figure S2. Complex **B**. dIr1-Ir2 2.697, dIr1-H3 1.544, dIr2-H4 1.536, aH3Ir1Ir2 91.9, aH4Ir2Ir1 102.6, dIr2-C5 1.967, dIr1-C6 2.283, dIr1-C7 2.299, dIr2-C8 2.739, dIr2-C9 2.693

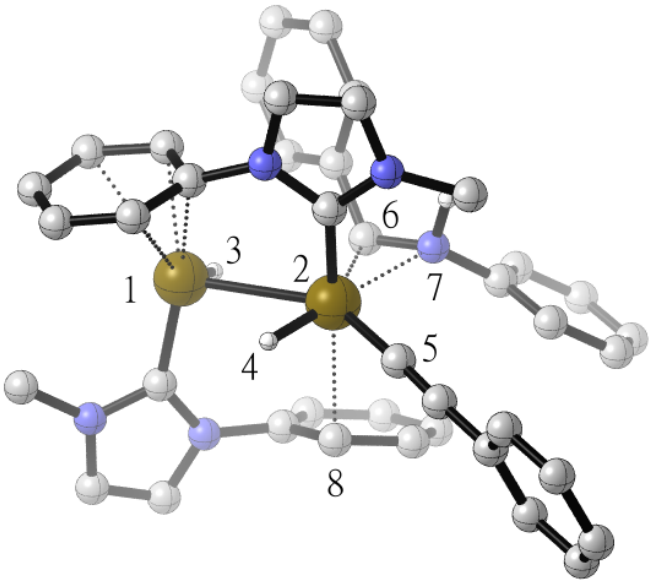


Figure S3. Complex **C**. dIr1-Ir2 2.770, dIr1-H3 1.539, dIr2-H4 1.575, aH3-Ir1-Ir2 84.1, aH4-Ir2-Ir1 61.5, dIr2-C5 1.991, dIr2-C6 2.223, dIr2-N7 2.284, dIr2-C8 2.713

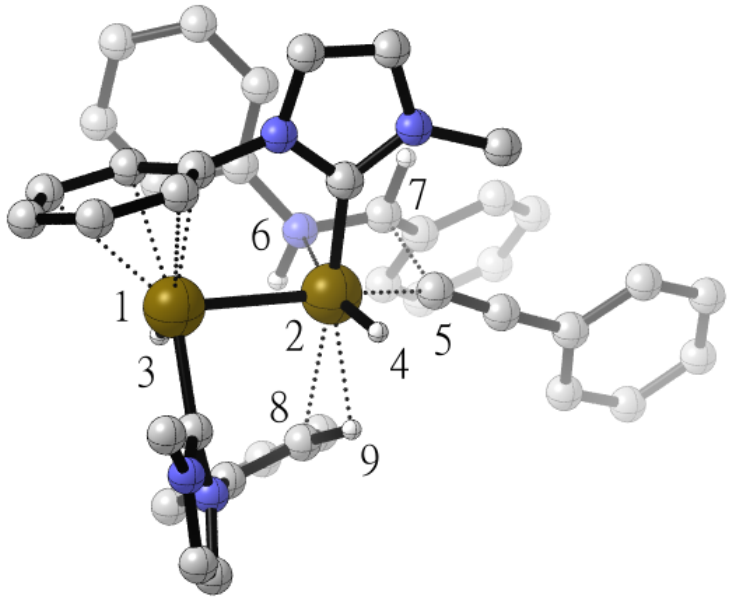


Figure S4. **TSC/D**. dIr1-Ir2 2.704, dIr1-H3 1.551, dIr2-H4 1.548, aH3-Ir1-Ir2 77.6, aH4-Ir2-Ir1 93.7, dIr2-C5 2.007, dIr 2-N6 2.688, dC5-C7 2.140, dIr2-C8 2.726, dIr2-H9 2.234.

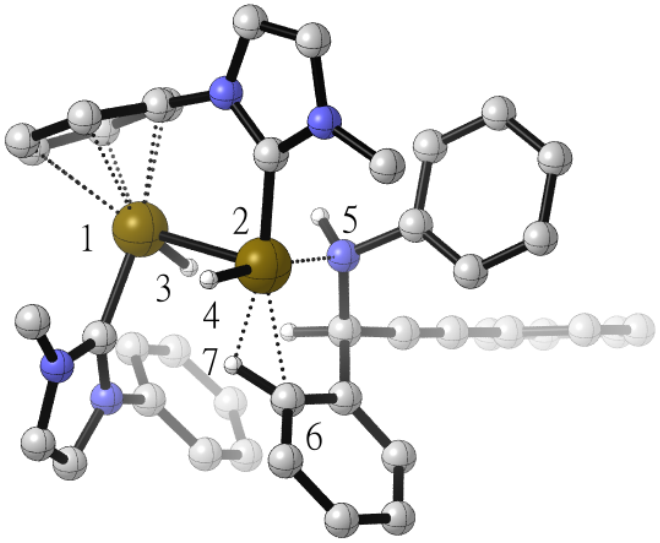


Figure S5. Complex **D**. dIr1-Ir2 2.636, dIr1-H3 1.547, dIr2-H4 1.587, aH3-Ir1-Ir2 81.5, aH4-Ir2-Ir1 89.9, dIr2 N5 2.285, dIr2-C6 2.418, dIr2-H7 1.922.

Cartesian coordinates (x, y, z in Å) of DFT optimized geometries for all calculated structures

Complex A (E = -1202.11399181 a.u.)

77 1.085668 -0.694597 -0.258210
1 0.890893 -0.102308 -1.676799
7 1.594964 2.280643 -0.051517
6 2.124969 1.018025 -0.041410
7 3.461567 1.213000 0.077975
6 3.762112 2.568165 0.147028
1 4.781865 2.930871 0.246591
6 2.588077 3.247378 0.065853
1 2.371681 4.312077 0.080087
77 -1.085637 0.694535 0.258161
1 -0.890473 0.102120 1.676627
7 -1.595029 -2.280731 0.051742
6 -2.124974 -1.018088 0.041456
7 -3.461570 -1.213000 -0.077989
6 -3.762183 -2.568158 -0.146873
1 -4.781950 -2.930824 -0.246438
6 -2.588184 -3.247429 -0.065567
1 -2.371854 -4.312144 -0.079661
6 -0.192766 -2.521730 0.135043
6 0.539812 -2.772864 -1.050799
6 1.953394 -2.956754 -0.969197
1 2.525415 -3.159041 -1.876414
6 2.594208 -2.836056 0.268604
1 3.678940 -2.937478 0.328619
6 1.838865 -2.654092 1.469508
1 2.351943 -2.620175 2.432406
6 0.452402 -2.544792 1.417418
6 -4.463826 -0.154271 -0.130310
1 -4.311971 0.541181 0.705321
1 -4.399294 0.387739 -1.084095
1 -5.460202 -0.602895 -0.042176
6 4.463921 0.154364 0.130108
1 4.400096 -0.387229 1.084183
1 4.311514 -0.541452 -0.705109
1 5.460208 0.603008 0.041055
1 0.017457 -2.851898 -2.004654
1 -0.144800 -2.415948 2.320938
6 0.192706 2.521636 -0.134893
6 -0.540004 2.772717 1.050899
6 -0.452352 2.544890 -1.417321
6 -1.953531 2.956960 0.969156
1 -0.017728 2.851647 2.004807
6 -1.838790 2.654344 -1.469529
1 0.144912 2.416100 -2.320807
6 -2.594227 2.836430 -0.268700
1 -2.525600 3.159381 1.876313
1 -2.351770 2.620541 -2.432483
1 -3.678932 2.938091 -0.328844

Complex B (E = -1510.04773042 a.u.)

77 2.243247 0.126695 -0.151643
1 2.175132 0.037566 -1.691685
7 0.775189 2.838184 -0.288669
6 1.895291 2.067608 -0.464394
7 2.801921 2.915760 -1.031926
6 2.262142 4.178604 -1.217052
1 2.831917 4.997186 -1.647562
6 0.989472 4.137219 -0.748252
1 0.233070 4.910391 -0.661593
77 -0.413463 -0.275672 0.081872
1 -0.542180 -0.840589 1.504179
7 1.133325 -2.729762 -0.202678
6 -0.049389 -2.102271 -0.507706
7 -0.754767 -3.020493 -1.220638
6 -0.027089 -4.196646 -1.352493
1 -0.422113 -5.056536 -1.885479
6 1.160338 -4.018318 -0.716777
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6 4.606319 -1.466106 0.449539
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6 3.360322 -1.519463 2.535812
1 3.342540 -1.395670 3.620210
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1 4.106863 2.055064 -2.454498
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1 3.494444 -2.121376 -1.316625
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6 -0.440254 1.916022 1.647299
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1 0.511757 1.720066 2.140665
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1 -1.665833 3.250508 -1.262998
6 -2.844864 2.217949 1.774590
1 -1.637616 1.415428 3.373612
1 -3.797259 3.008187 0.001531
1 -3.782817 2.122043 2.323320
6 -2.375901 -0.407841 0.037521
6 -3.605315 -0.378543 0.003811
6 -5.028554 -0.284944 -0.044180
6 -5.664744 0.520852 -1.014788
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6 -7.223435 -0.868135 0.841837
1 -5.352883 -1.604792 1.638964
6 -7.839583 -0.065503 -0.123688
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1 -7.831874 -1.412056 1.568297

1 -8.928065 0.019096 -0.154208

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7 2.830861 -3.209204 1.573763
6 2.507415 -3.915657 2.721143
1 3.032957 -4.820417 3.014172
6 1.473646 -3.261706 3.311359
1 0.903716 -3.479690 4.209713
77 -0.433170 -0.046612 -0.231826
1 0.025518 -1.459248 -0.755458
7 1.157965 0.709396 -2.620487
6 -0.063946 0.712145 -2.018724
7 -0.874961 1.388986 -2.879305
6 -0.155100 1.808581 -3.993511
1 -0.623865 2.365099 -4.800500
6 1.121831 1.380248 -3.836700
1 2.000154 1.480724 -4.467690
6 2.333708 0.072531 -2.114775
6 3.284100 0.823127 -1.372235
6 4.558682 0.247995 -1.114474
1 5.301129 0.832126 -0.567823
6 4.854859 -1.037117 -1.554191
1 5.834595 -1.472093 -1.349213
6 3.900950 -1.774580 -2.309202
1 4.156759 -2.769342 -2.679864
6 2.667022 -1.224291 -2.623542
6 -2.298032 1.699589 -2.736656
1 -2.744272 1.014927 -2.011247
1 -2.435195 2.748967 -2.431653
1 -2.790089 1.551860 -3.706252
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1 4.672443 -2.803243 0.633445
1 4.366474 -4.515700 1.038508
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1 1.944126 -1.756923 -3.243240
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6 2.087832 4.365554 -1.103686
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6 3.211784 4.478693 -0.277843
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7 -3.510054 2.888316 -1.080764
6 -3.296820 4.258897 -1.058187
1 -3.906117 4.950960 -1.632881
6 -2.244521 4.484775 -0.230751
1 -1.739848 5.402639 0.055515
77 -0.045348 0.134680 -0.748502
1 -0.369513 0.763921 -2.125725
7 -1.563412 -2.342820 -1.263498
6 -0.431216 -1.619494 -1.530854
7 0.289236 -2.418526 -2.371594
6 -0.371765 -3.622868 -2.589383
1 0.042879 -4.398116 -3.227634
6 -1.537473 -3.577442 -1.897330
1 -2.347882 -4.294188 -1.801864
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1 -4.235339 -1.593958 2.454331
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6 -5.032641 -1.066649 -0.832234
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6 1.528352 -2.084402 -3.068131

1 1.595138 -2.710536 -3.966299
1 1.517890 -1.029713 -3.356364
1 2.403753 -2.268956 -2.432315
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1 -4.989189 2.969263 -2.550712
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6 0.454973 2.479998 0.547473
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6 1.590901 2.350833 1.353107
1 0.507982 2.289048 -0.540943
6 0.379221 3.312779 3.216829
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6 3.083514 0.490311 -1.392546
1 2.366340 -2.041608 -0.023408
1 1.336001 -0.136035 1.983819
6 2.423549 -1.152700 0.602772
7 1.267550 -0.924631 1.344796
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6 5.227734 0.056989 -2.505326
6 5.057360 1.809575 -0.807738
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6 7.191595 1.278911 -1.808104
1 7.196829 -0.276955 -3.313892
1 6.899681 2.803205 -0.299612
1 8.265328 1.462386 -1.890151
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6 3.967618 -0.045018 2.258238
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1 3.127952 0.368760 2.817725
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1 7.009715 -1.606804 0.399948
1 7.371535 -0.163080 2.401345
6 0.494858 -1.994046 1.895265
6 0.421575 -3.256496 1.294410
6 -0.202147 -1.745298 3.084953
6 -0.331340 -4.266461 1.899234
1 0.949203 -3.471629 0.365337
6 -0.948920 -2.761671 3.682909
1 -0.150052 -0.756552 3.547880
6 -1.015806 -4.029037 3.094739
1 -0.373916 -5.252026 1.431111
1 -1.473273 -2.562141 4.619788
1 -1.590351 -4.826995 3.568175

Complex D (E = -2066.82265287 a.u.)
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1 -2.187584 -0.988190 1.750200
7 -1.598414 3.142366 0.602193
6 -2.348012 2.013179 0.402320
7 -3.350489 2.092918 1.320257
6 -3.234345 3.247110 2.079732
1 -3.948048 3.503519 2.857806
6 -2.133327 3.904932 1.633633
1 -1.693092 4.851103 1.933469
77 -0.849057 -0.912205 0.901597
1 -0.692506 1.161138 -1.051243
7 -2.149189 -2.652239 -1.194930
6 -1.451424 -2.546326 -0.016936
7 -1.240536 -3.828806 0.365853
6 -1.784845 -4.720934 -0.550955
1 -1.708437 -5.797472 -0.423199
6 -2.369179 -3.988794 -1.533856
1 -2.909451 -4.285275 -2.428444
6 -2.687408 -1.505433 -1.837298
6 -4.010298 -1.074388 -1.483977
6 -4.462048 0.155560 -1.964386
1 -5.445432 0.528158 -1.671122
6 -3.641264 0.947027 -2.824836
1 -3.994356 1.918695 -3.172358
6 -2.399384 0.447896 -3.269039
1 -1.797381 1.024936 -3.972583
6 -1.922773 -0.814814 -2.805430
6 -0.521546 -4.224749 1.571491
1 0.516486 -4.489538 1.331691
1 -0.530095 -3.386078 2.280740
1 -1.029699 -5.080754 2.034352
6 -4.417344 1.117172 1.501344
1 -5.215554 1.272336 0.761653
1 -4.003663 0.105932 1.406129
1 -4.839366 1.236703 2.506389
1 -4.604094 -1.679780 -0.798865
1 -0.971154 -1.222634 -3.144586
6 -0.379207 3.504761 -0.061725
6 -0.340317 3.639622 -1.453492
6 0.761334 3.737961 0.713454
6 0.866839 3.966943 -2.074687
1 -1.251234 3.502240 -2.036319
6 1.961405 4.075015 0.083540
1 0.715820 3.632934 1.797987
6 2.018687 4.177235 -1.309096
1 0.903817 4.078326 -3.160222
1 2.856453 4.245646 0.684280
1 2.959662 4.435798 -1.798304
6 1.864111 0.533378 0.276938
1 1.311163 1.327615 -0.250974
7 1.168126 -0.736561 -0.156592
1 0.987485 -0.641700 -1.154972
6 3.252308 0.581676 -0.152733
6 4.406224 0.587802 -0.535633
6 5.766536 0.589322 -0.970566
6 6.676609 -0.351532 -0.445845
6 6.211993 1.528183 -1.923373
6 8.004290 -0.347981 -0.868145
1 6.330333 -1.080110 0.289609

6	7.542125	1.524311	-2.337940
1	5.507342	2.255687	-2.330695
6	8.439136	0.588289	-1.812260
1	8.706051	-1.077906	-0.459287
1	7.883722	2.254225	-3.074785
1	9.481035	0.588706	-2.139544
6	1.856752	-1.987471	0.048189
6	2.488007	-2.292326	1.260924
6	1.837077	-2.934711	-0.982887
6	3.108065	-3.534527	1.423400
1	2.513405	-1.567447	2.071474
6	2.445999	-4.177886	-0.808578
1	1.352434	-2.692724	-1.933043
6	3.088887	-4.481890	0.396452
1	3.612020	-3.759839	2.365632
1	2.434117	-4.904428	-1.623693
1	3.579954	-5.447766	0.528866
6	1.634234	0.763365	1.766146
6	0.312890	0.720302	2.254308
6	2.672179	0.986534	2.668430
6	0.033977	0.888889	3.615729
1	-0.550689	0.873255	1.547761
6	2.398352	1.153098	4.032992
1	3.699635	1.017950	2.301707
6	1.086469	1.093767	4.511963
1	-1.000686	0.872412	3.962376
1	3.222365	1.327143	4.728372
1	0.883868	1.220863	5.577098

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