Supporting Information

Key factors in the synthesis of polycyclic iridaaromatics *via* the methoxyalkenylcarbene pathway

Maria Talavera,[a,†,*] Krystal M. Cid-Seara,[a] Ángeles Peña-Gallego[b,*] and Sandra Bolaño[a,*]

[a] *Universidade de Vigo, Departamento de Química Inorgánica, Campus Universitario, 36310, Vigo, Spain*

[b] *Universidade de Vigo, Departamento de Química Física, Campus Universitario, 36310, Vigo, Spain*

[†] *Current address: Humboldt-Universität zu Berlin, Department of Chemistry, Brook-Taylor-Straße 2, D-12489 Berlin, Germany.*

Corresponding authors e-mails: M.T.: talaverm@hu-berlin.de; A.P-G.: mpena@uvigo.es; S. B.: bgs@uvigo.es

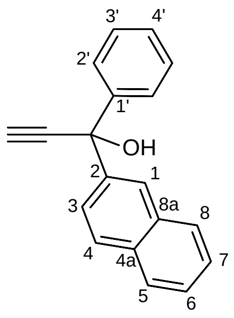
Experimental Section

General Procedures, Methods and Materials

All experiments were carried out under an atmosphere of argon by Schlenk techniques. Solvents were dried by the usual procedures[1] and, prior to use, distilled under argon. All reagents were obtained from commercial sources including the propargylic alcohol **II**. The starting material $[IrCp^*Cl(NCMe)(PMe_3)]PF_6$ was prepared as described in the literature.[2] Unless stated, NMR spectra were recorded in $(CD_3)_2CO$ (organometallic complexes) or $CDCl_3$ (organic compounds) at room temperature on Bruker ARX–400 instrument, with resonating frequencies of 400 MHz (^{1}H), 161 MHz (^{31}P{^{1}H}), and 100 MHz (^{13}C{^{1}H}) using the solvent as the internal lock. ^{1}H and ^{13}C{^{1}H} signals are referred to internal TMS and those of ^{31}P{^{1}H} to 85% H_3PO_4; downfield shifts (expressed in ppm) are considered positive. ^{1}H and ^{13}C{^{1}H} NMR (or JMOD) signal assignments were confirmed by {^{1}H, ^{1}H} COSY, {^{1}H, ^{1}H} NOESY, {^{1}H,^{13}C} HSQC, {^{1}H,^{13}C} HMBC and DEPT experiments. Coupling constants are given in hertz. Infrared spectra were run on a Jasco FT/IR–6100 spectrometer using KBr pellets. C, H, and N analyses were carried out with a Carlo Erba 1108 analyzer. Mass spectra are referred to the most abundant isotopes and they were acquired using an Apex–Qe spectrometer by high resolution electrospray technique for organometallic complexes and high and low resolution electron impact technique for organic compounds.

Synthesis of 1-(2-naphthalenyl)-1-phenyl-2-propyn-1-ol (I)

To a solution of trimethylsilylacetilene (360 µL, 2.5 mmol) in dry THF (25 mL) at around 203 K, n-buthyllithium 2.5 M in hexanes (1 mL, 2.5 mmol) was added dropwise and the reaction mixture was stirred for one hour. After that, 2-benzoylnaphthalene (527 mg, 2.27 mmol) was added and the mixture was stirred at room temperature for 3.5 hours where no ketone is presented in the solution. Then, a methanolic solution of KOH was added (6 mL, 0.5 M) at 273 K and the mixture was stirred again for 15 min. Finally, glacial acetic acid was added until pH≈7, water was added and the organic phase, which was extracted with ethylacetate, was dry with Na_2SO_4 and concentrated under vacuum. Yield: 551 mg (94%).



I

$C_{19}H_{14}O$: 258.32 g/mol. MS: Calculated *m/z*: 258.32; Experimental: 258.10 [M], 181.06 [M–Ph]. IR (cm^{-1}): ν (C≡C) 2115 (w); (H–C≡) 3288 (s) and (OH) (s). ^{1}H NMR: δ 8.25–8.19 (m, 1H, $C^{1}H$); 7.92–7.86 (m, 1H, $C^{8}H$); 7.85–7.81 (m, 1H, $C^{5}H$); 7.81–7.76 (m, 1H, $C^{4}H$); 7.71–7.64 (m, 2H, $C^{2'}H$); 7.62–7.55 (m, 1H, $C^{3}H$); 7.54–7.47 (m, 2H, $C^{6}H$ + $C^{7}H$); 7.39–7.33 (m, 2H, $C^{3'}H$); 7.33–7.27 (m, 1H, $C^{4'}H$); 3.01 (s br, 1H, O*H*); 2.95 (d, 1H, $^{5}J_{HH}$ = 0.8 Hz, *H*C≡) ppm. $^{13}C\{^{1}H\}$ NMR: δ 144.2 (s, $C^{1'}$); 141.6 (s, C^{2}); 133.0 (s, C^{4a}); 132.9 (s, C^{8a}); 128.6 (s, C^{8}); 128.5 (s, 2C $C^{3'}$); 128.4 (s, $C^{4'}$); 128.1 (s, C^{3}); 127.7 (s, C^{5}); 126.5 and 126.4 (both s, C^{6} + C^{7}); 126.2 (s, 2C $C^{2'}$); 124.53 (s, C^{3}); 124.46 (s, C^{1}); 86.3 (s, HC≡*C*); 76.0 (s, H*C*≡C); 74.5 (s, *C*–OH) ppm.

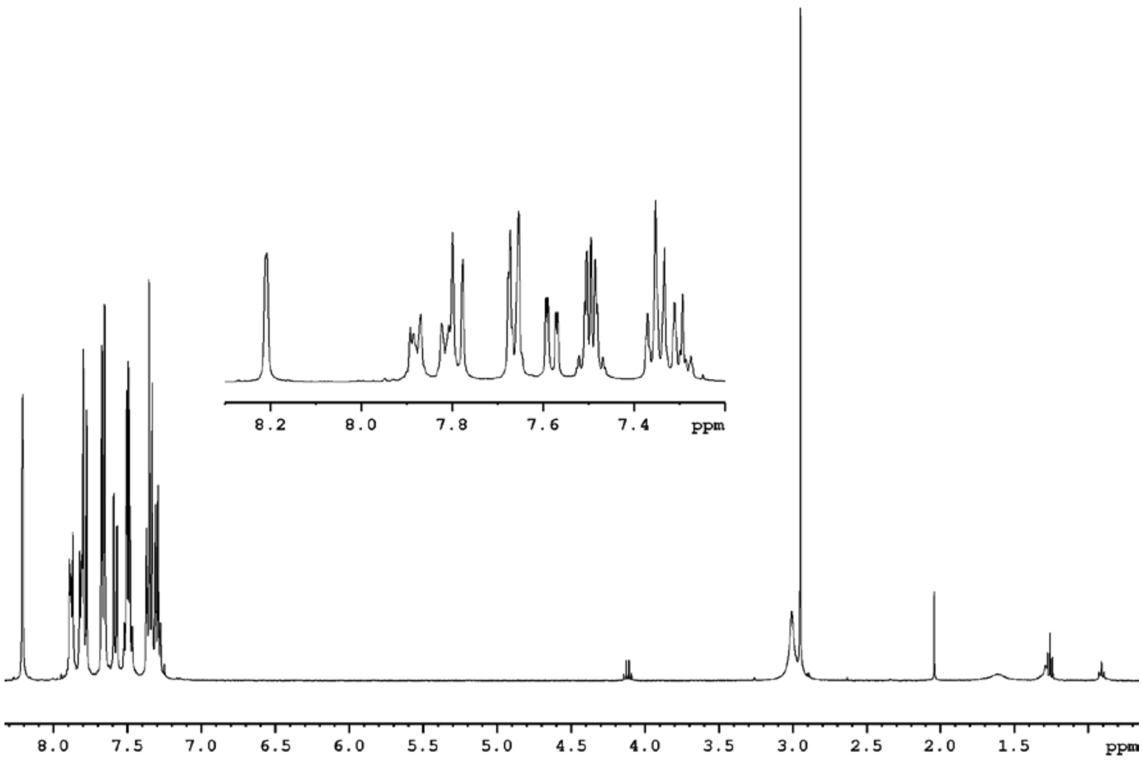


Figure S1. ^{1}H NMR spectrum of **I**.

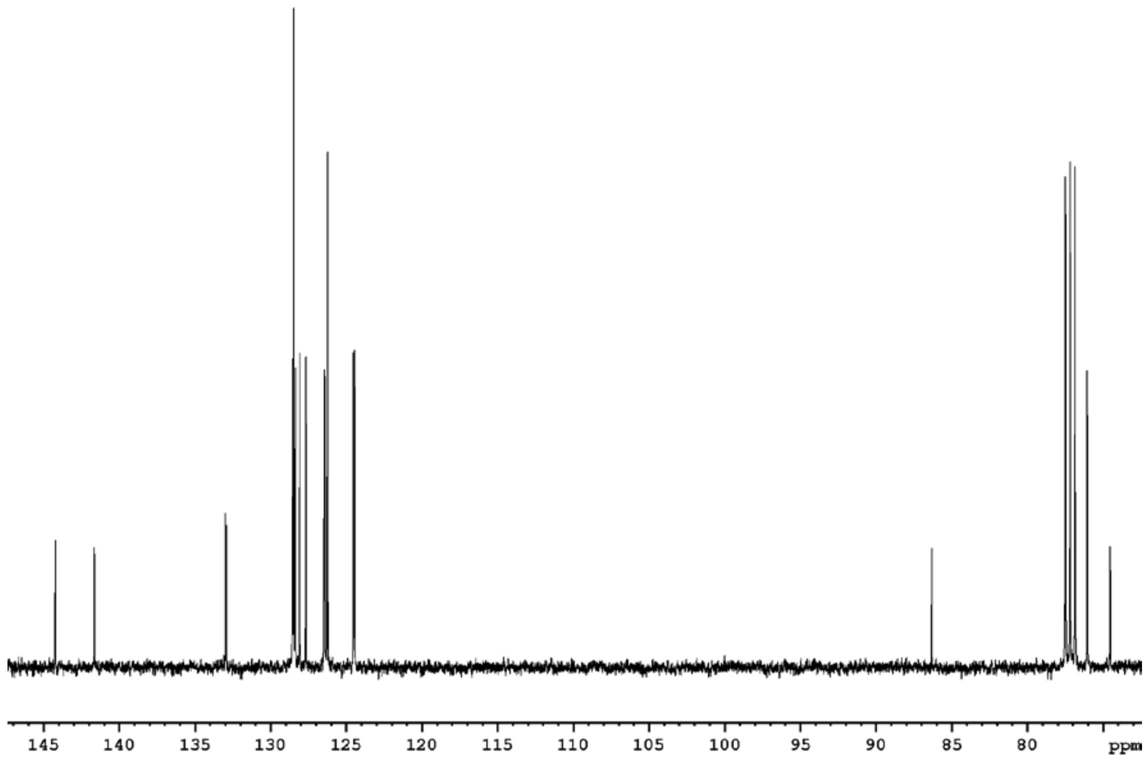


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **I**.

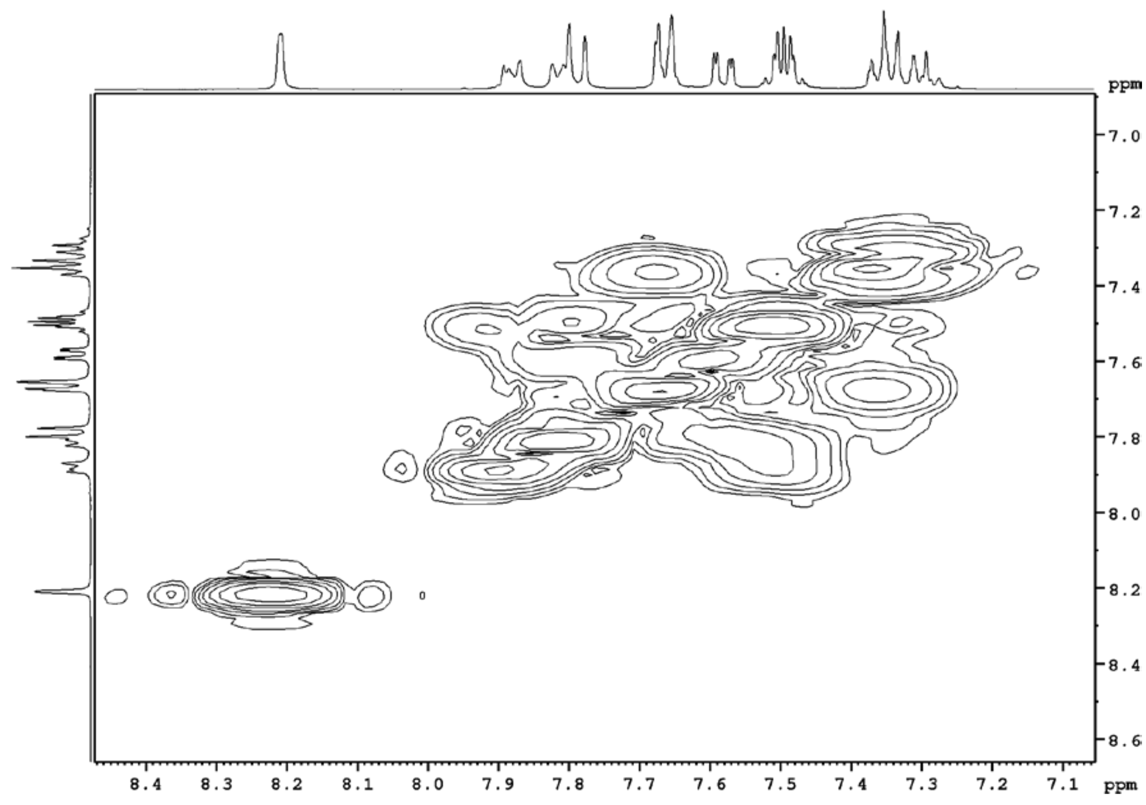


Figure S3. ^{1}H, ^{1}H COSY NMR spectrum of **I**.

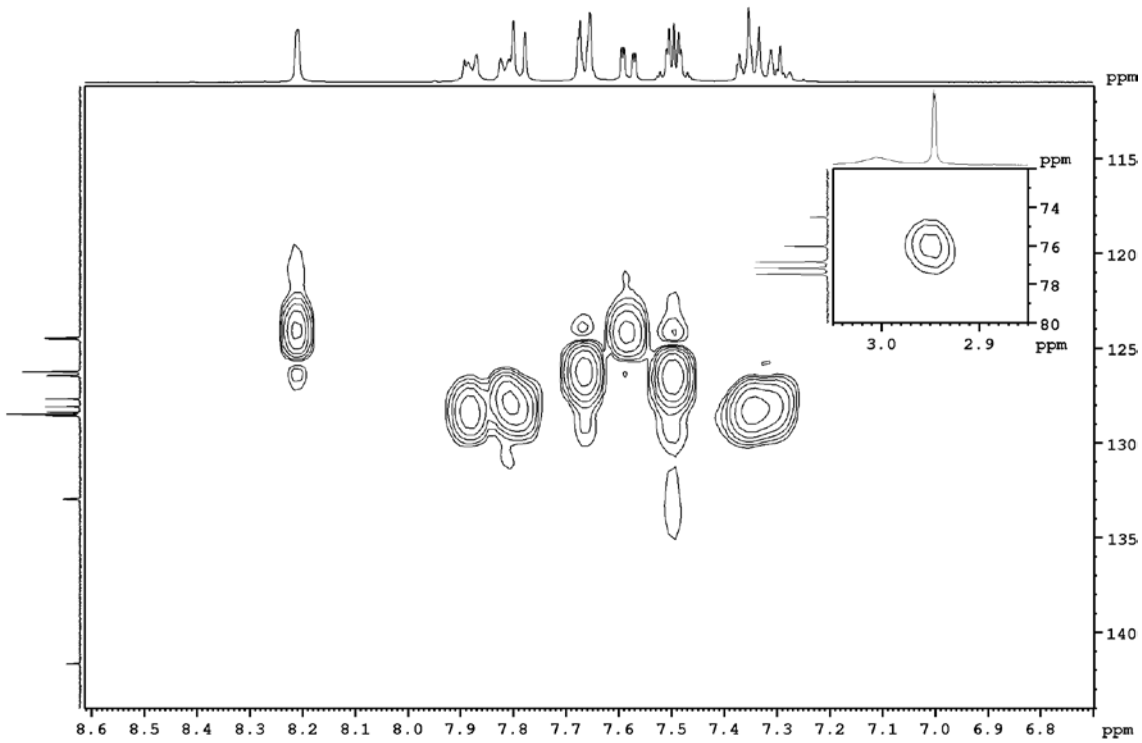


Figure S4. [1]H, [13]C HSQC NMR spectrum of **I**.

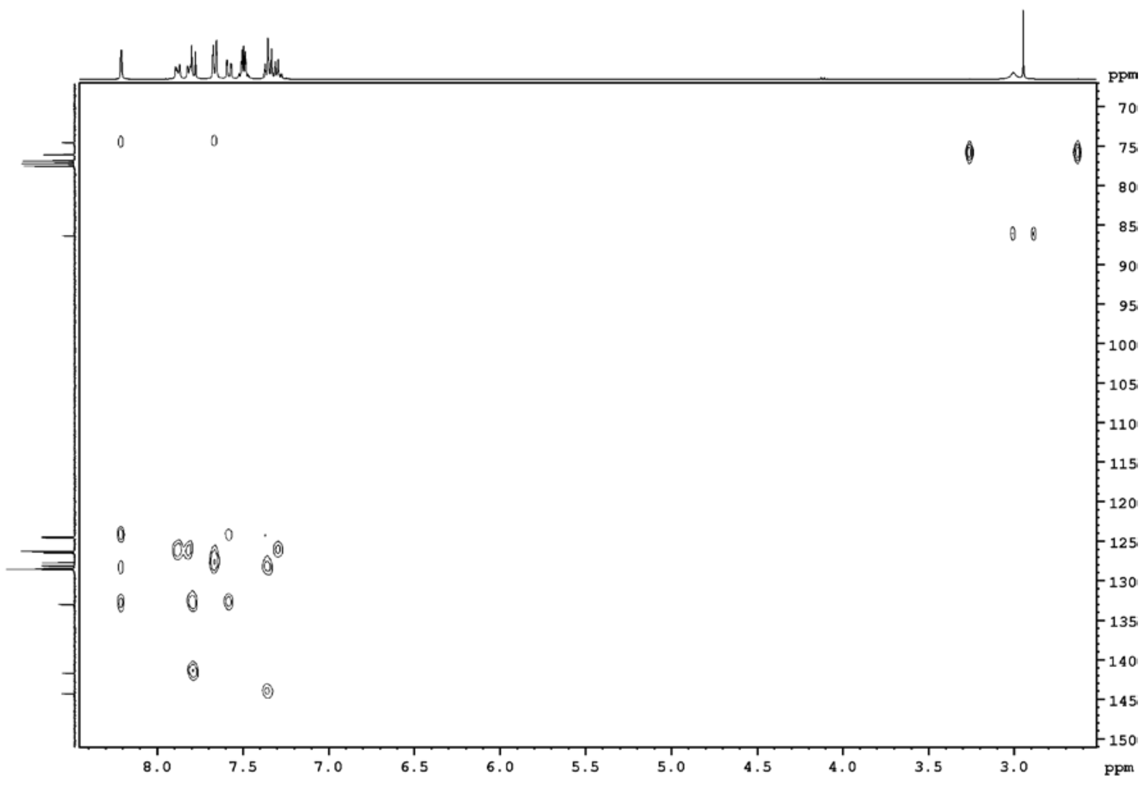


Figure S5. [1]H, [13]C HMBC NMR spectrum of **I**.

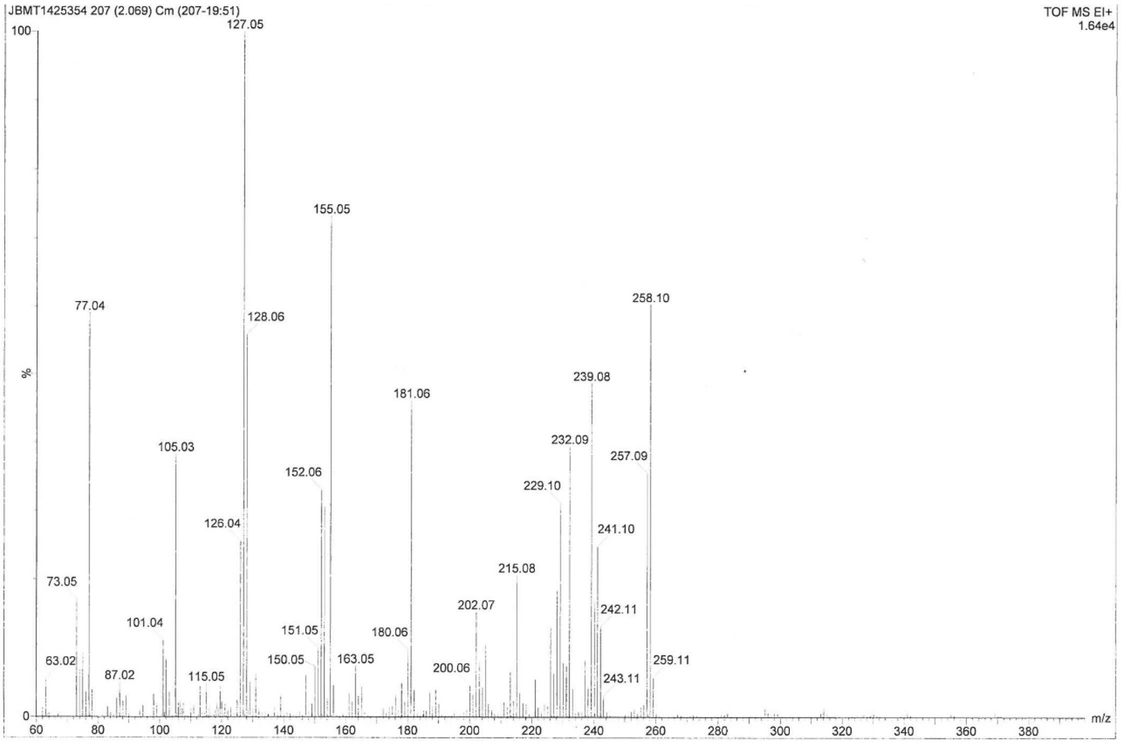
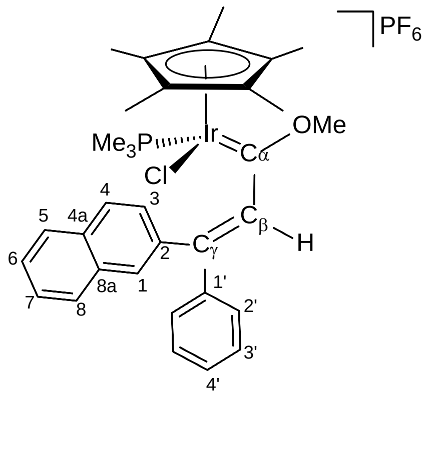


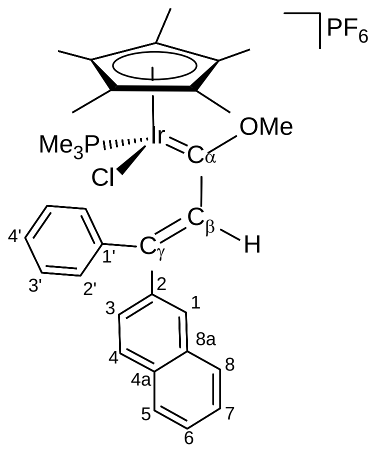
Figure S6. EI (TOF) spectrum of **I**.

Preparation of *cis*- and *trans*- [IrCp*Cl{=C(OMe)–CH=C(2–$C_{10}H_7$)(Ph)}(PMe_3)]PF_6 (1)

To a yellow solution of [IrCp*Cl(NCMe)(PMe_3)]PF_6 (120 mg, 0.19 mmol) in methanol (10 mL), 1-(2-naphthalenyl)-1-phenyl-2-propyn-1-ol (49 mg, 0.19 mmol) was added and the mixture was stirred for 30 min. The dark red solution obtained was vacuum-concentrated yielding a dark red solid that was washed with pentane (3 × 5 mL). Finally, the mixture of ***Z/E*-1** (~47:53 mole ratio, respectively) was dried under vacuum. Yield: 159 mg (97%).



***Z*-1**



***E*-1**

Anal. Calcd for $C_{33}H_{40}OClF_6IrP_2$ (856.29 g/mol): C 46.29, H 4.71; found: C 46.45, H 4.79. MS: Calculated *m/z* for $[M]^+$: 711.21222; Experimental: 711.21076. IR (cm^{-1}): ν (PF_6) 840 (s).

Analytical data for ***Z*-1**: ^{1}H NMR: δ 8.07–7.97 (m, 2H, C^4H + C^8H); 7.97–7.93 (m, 1H, C^5H); 7.78–7.75 (m, 1H, C^1H); 7.65–7.57 (m, 2H, C^6H + C^7H); 7.53–7.47 (m, 1H, $C^{4'}H$); 7.47–7.41 (m, 4H, $C^{2'}H$ + $C^{3'}H$); 7.35–7.32 (m, 1H, C^3H); 7.35 (s br, $C_\beta H$); 4.28 (s, 3H, OCH_3); 1.82 (d, 15H, $^4J_{HP}$ = 1.9 Hz, $C_5(CH_3)_5$); 1.81 (d, 9H, $^2J_{HP}$ = 10.7 Hz, $P(CH_3)_3$) ppm. $^{31}P\{^1H\}$ NMR: δ –29.42 (s, $P(CH_3)_3$); –143.90 (sept, $^1J_{PF}$ = 708.0 Hz, PF_6) ppm. $^{13}C\{^1H\}$ NMR: δ 263.9 (d, $^2J_{CP}$ = 10.1 Hz, C_α); 151.9 (s br, C_γ); 141.5 (s, $C^{1'}$); 139.1 (s, C_β); 137.5 (s, C^2); 134.3 (s, C^{4a}); 133.6 (s, C^{8a}); 131.6 (s, $C^{4'}$); 130.3 (s, 2C $C^{2'}$); 129.8 (s, 2C $C^{3'}$); 129.6 (s, C^8); 128.7 (s, C^4); 128.6 (s, C^5); 129.5 (s, C^1); 128.1 (s, C^6); 127.73 (s, C^3); 127.70 (s, C^7); 100.03 (d, $^2J_{CP}$ = 2.0 Hz, $C_5(CH_3)_5$); 69.2 (s, OCH_3); 14.9 (d, $^1J_{CP}$ = 40.9 Hz, $P(CH_3)_3$); 9.0 (d, $^3J_{CP}$ = 0.8 Hz, $C_5(CH_3)_5$) ppm.

Analytical data for ***E*-1**: ^{1}H NMR: δ 8.07–7.97 (m, 1H, C^4H); 7.97–7.93 (m, 1H, C^5H); 7.90–7.86 (m, 2H, C^1H + C^8H); 7.68–7.65 (m, 1H, C^3H); 7.65–7.57 (m, 1H, C^6H); 7.56 (s, 1H, $C_\beta H$); 7.56–7.53 (m, 1H, C^7H); 7.53–7.47 (m, 3H, $C^{3'}H$ + $C^{4'}H$); 7.31–7.28 (m, 2H, $C^{2'}H$); 4.33 (s, 3H, OCH_3); 1.86 (d, 15H, $^4J_{HP}$ = 2.2 Hz, $C_5(CH_3)_5$); 1.82 (d, 9H, $^2J_{HP}$ = 11.1 Hz, $P(CH_3)_3$) ppm. $^{31}P\{^1H\}$ NMR: δ –29.96 (s, $P(CH_3)_3$); –143.9 (sept, $^1J_{PF}$ = 708.0 Hz, PF_6) ppm. $^{13}C\{^1H\}$ NMR: δ 263.9 (d, $^2J_{CP}$ = 10.1 Hz, C_α); 152.1 (s br, C_γ); 141.5 (s, $C^{1'}$); 139.7 (s, C_β); 138.7 (s, C^2); 135.1 (s, C^{4a}); 133.9 (s, C^{8a}); 131.8 (s, C^1); 130.1 (s, $C^{4'}$); 129.9 (s, 2C $C^{2'}$); 129.8 (s, C^8); 129.27 (s, 2C $C^{3'}$); 129.26 (s, C^5); 128.8 (s, C^6); 128.7 (s, C^4); 127.9 (s, C^7); 126.1 (s, C^3); 99.8 (d, d, $^2J_{CP}$ = 2.2 Hz $C_5(CH_3)_5$); 69.3 (s, OCH_3); 14.9 (d, $^1J_{CP}$ = 40.8 Hz, $P(CH_3)_3$); 9.1 (d, $^3J_{CP}$ = 0.8 Hz, $C_5(CH_3)_5$) ppm.

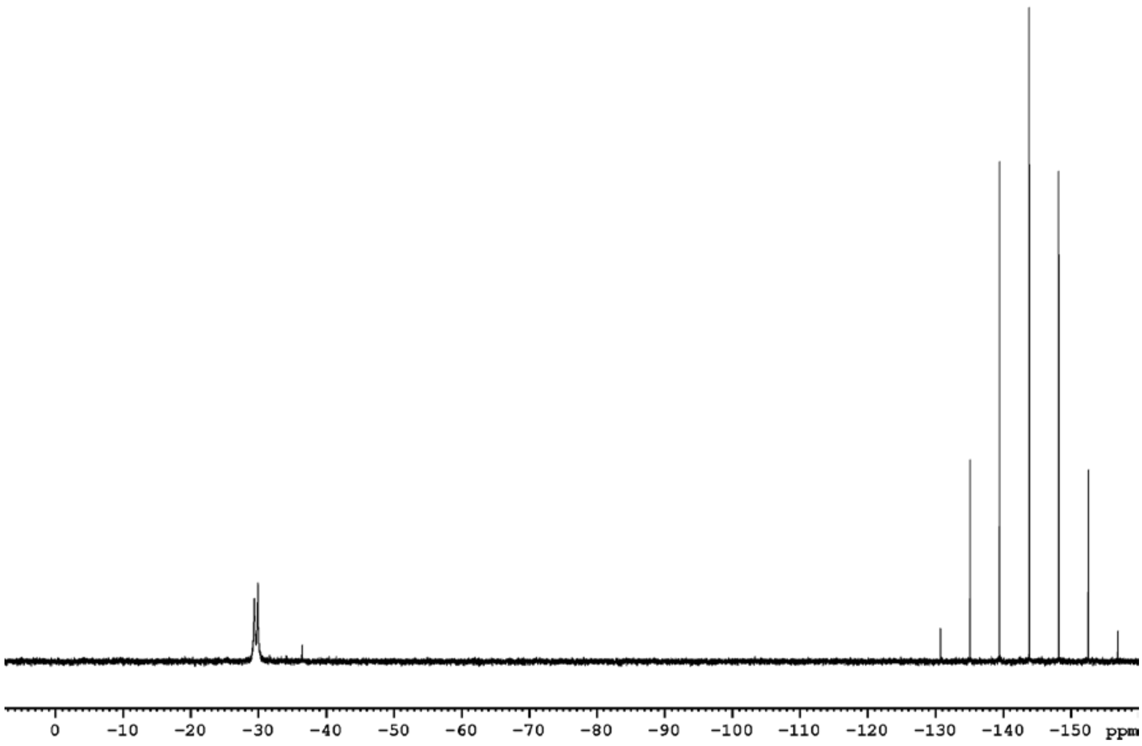


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of **1**.

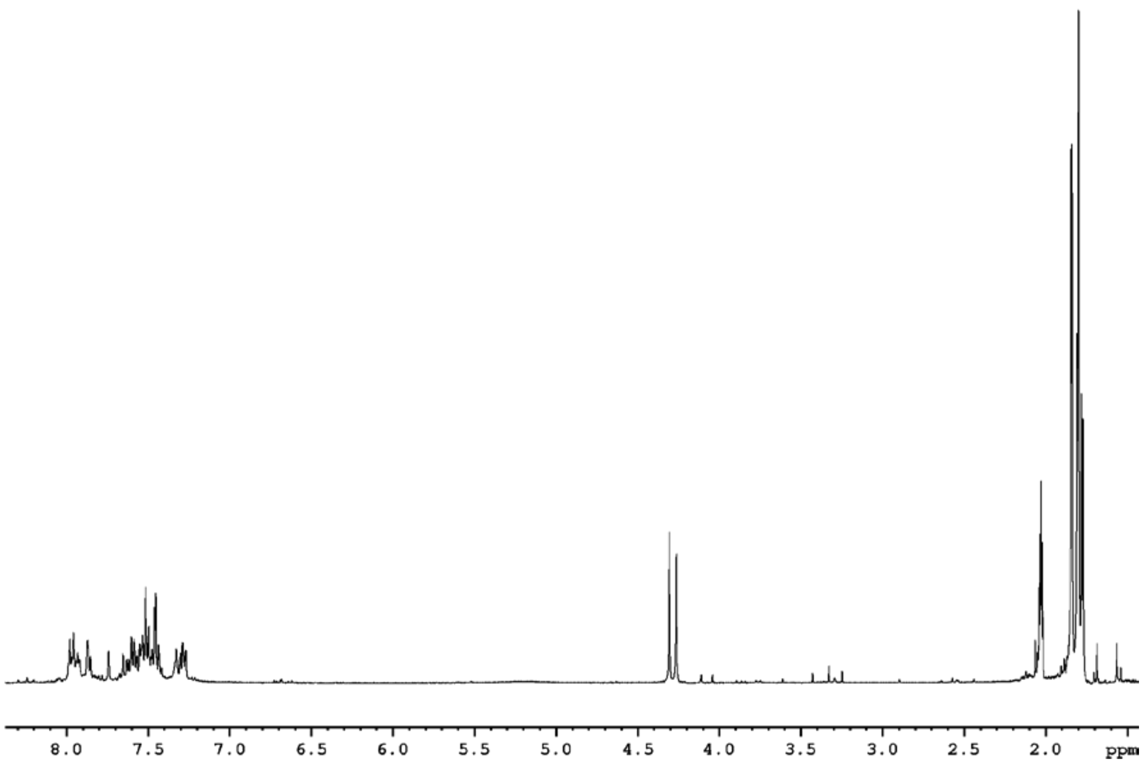


Figure S8. ^{1}H NMR spectrum of **1**.

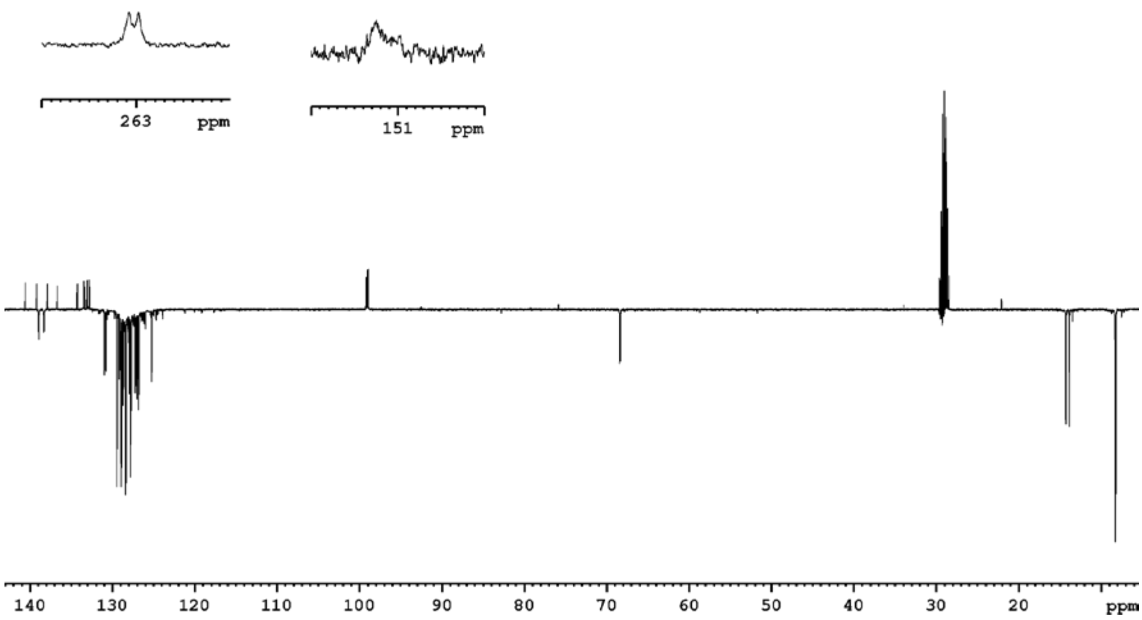


Figure S9. $^{13}C\{^{1}H\}$-JMOD NMR spectrum of **1**.

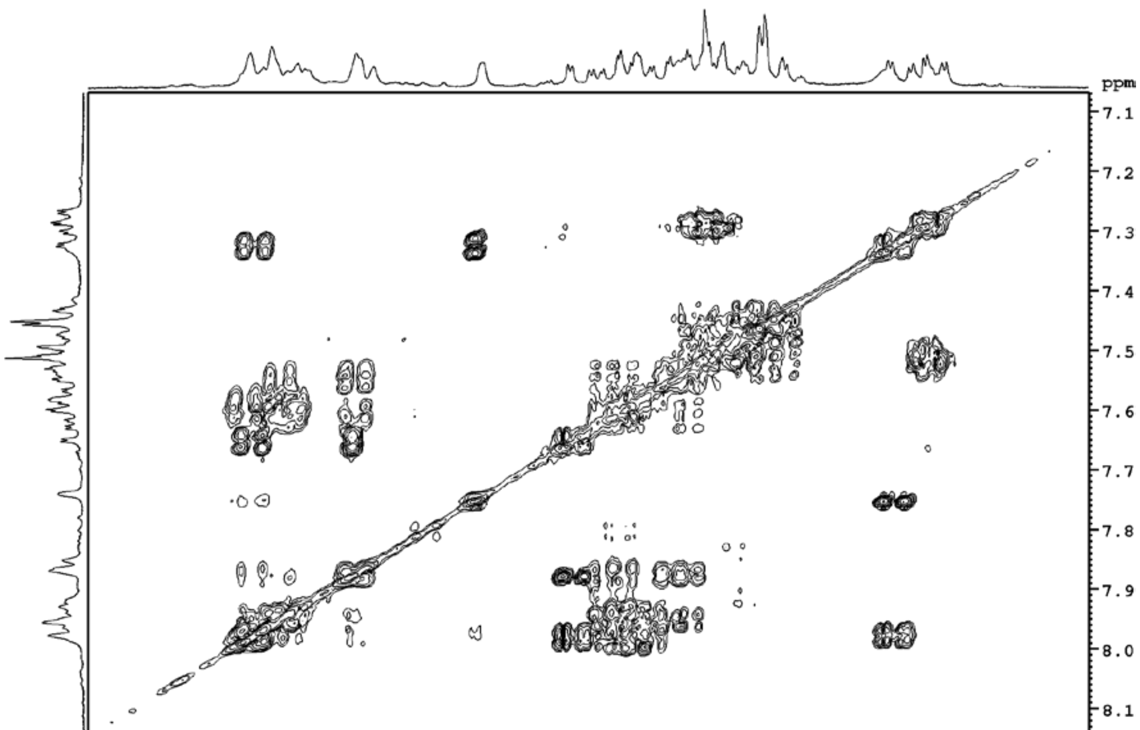


Figure S10. ^{1}H, ^{1}H COSY NMR spectrum of **1**.

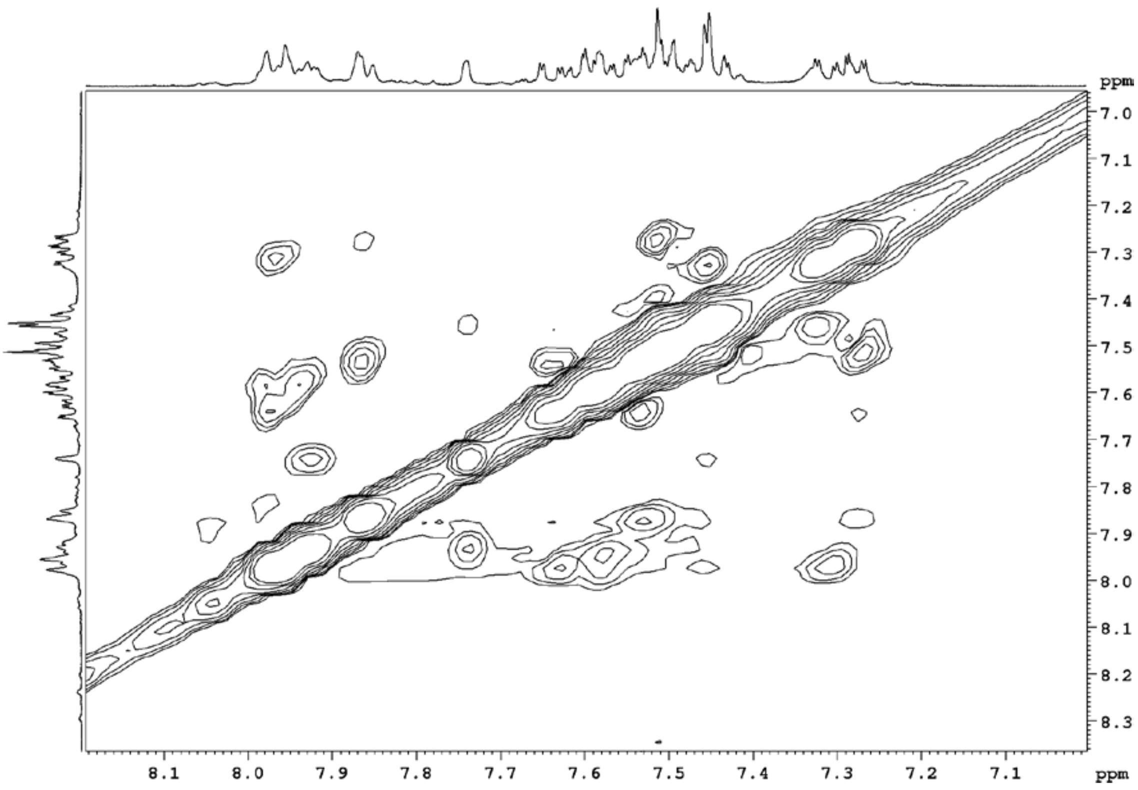


Figure S11. ^{1}H, ^{1}H NOESY NMR spectrum of **1**.

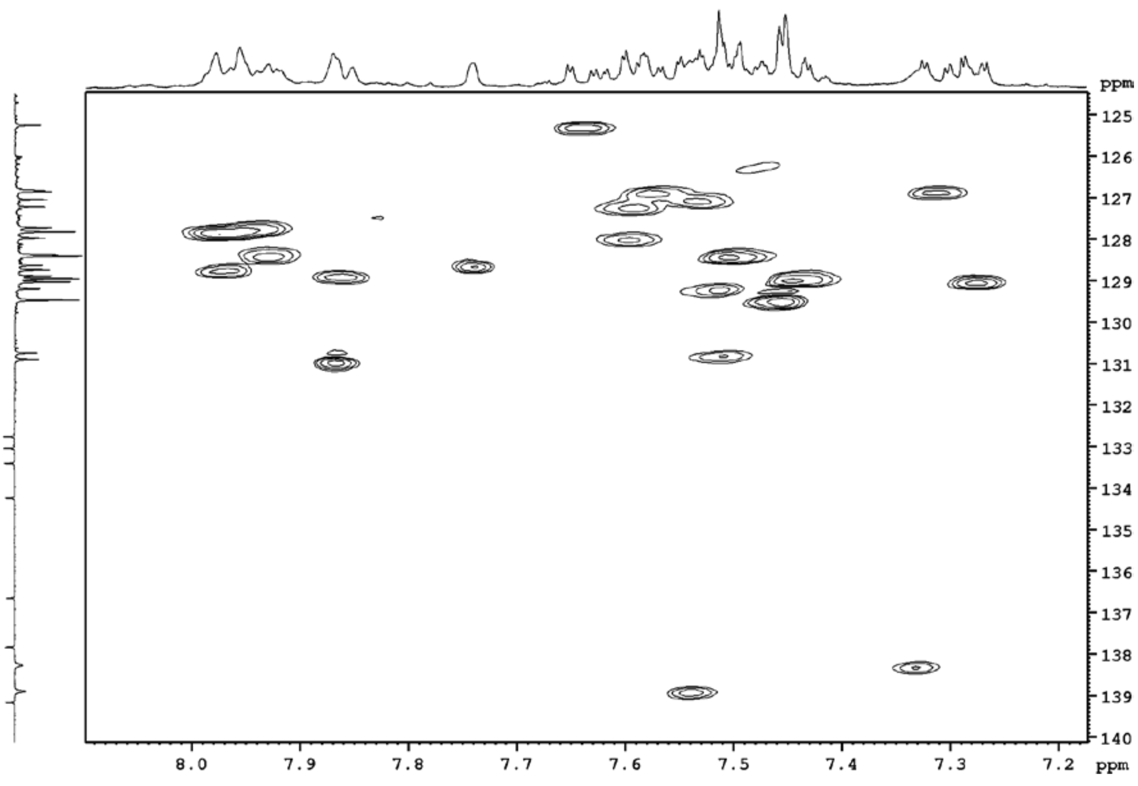


Figure S12. Section of the ^{1}H, ^{13}C HSQC NMR spectrum of **1**.

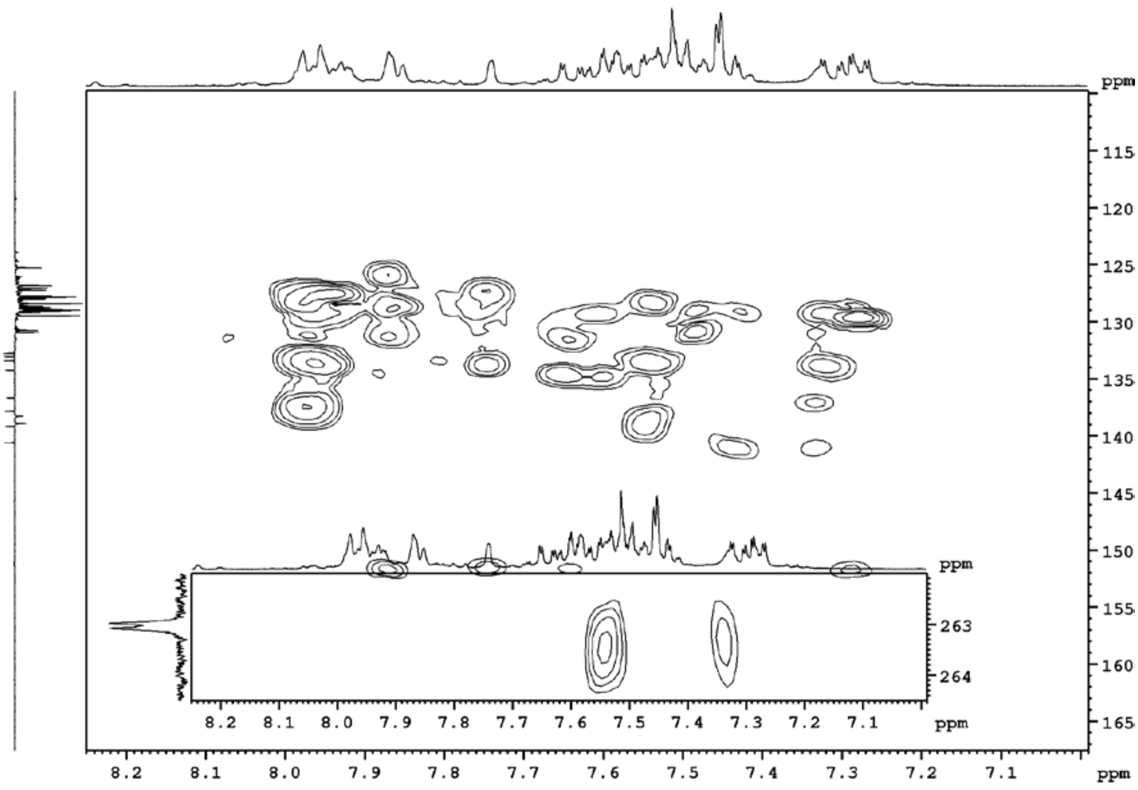


Figure S13. [1]H, [13]C HMBC NMR spectrum of **1**.

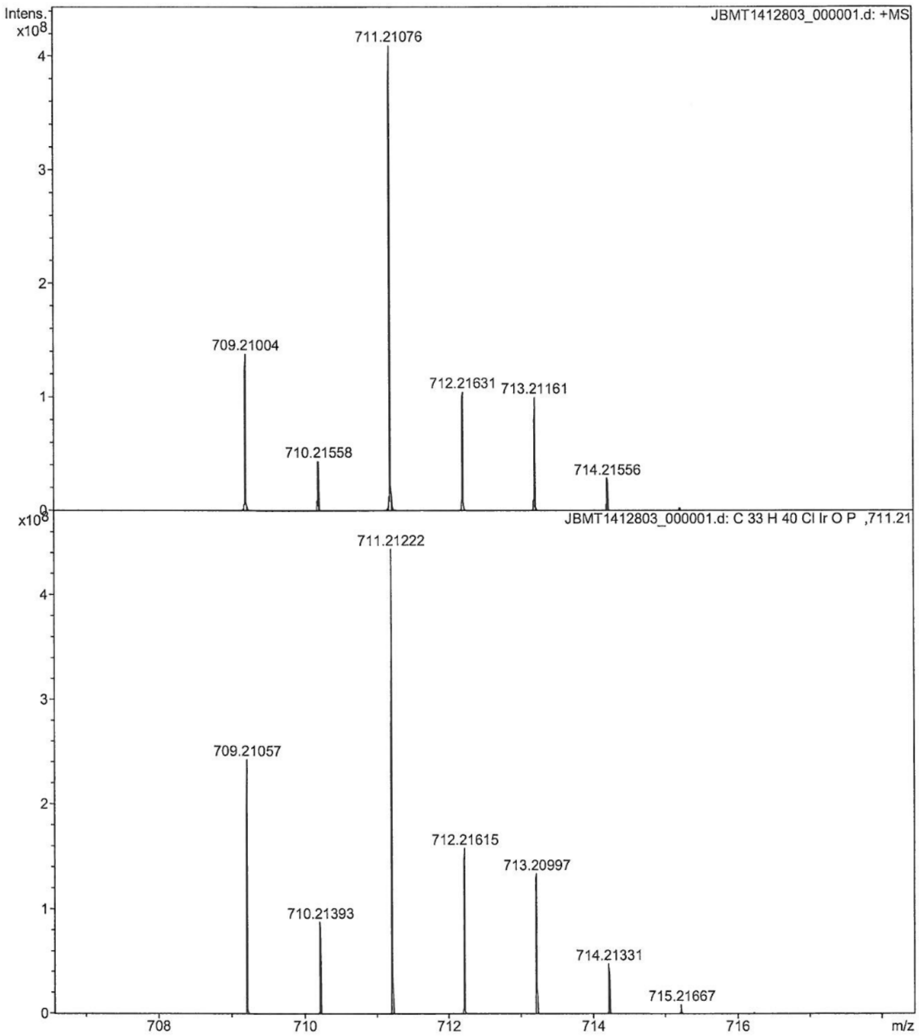
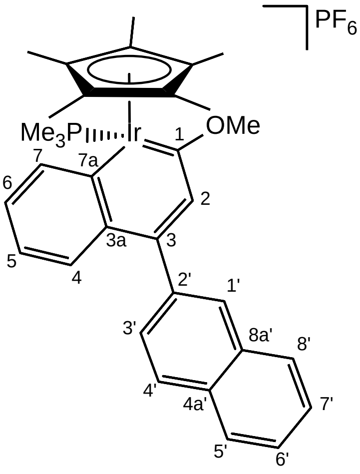


Figure S30. ESI spectrum of **1**, theoretical (down) and experimental (up).

Preparation of [IrCp*{=C(OMe)–CH=C(*o*–C$_6$H$_4$)(2–C$_{10}$H$_7$)}(PMe$_3$)]PF$_6$ (2) and [IrCp*{=C(OMe)–CH=C(*o*–C$_{10}$H$_6$)(Ph)}(PMe$_3$)]PF$_6$ (3)

A red solution of the mixture *Z/E*-[IrCp*Cl{=C(OMe)–CH=C(2–C$_{10}$H$_7$)(Ph)}(PMe$_3$)]PF$_6$ (**1**) (315 mg, 0.37 mmol) in 10 mL of dichloromethane was treated with AgPF$_6$ (106 mg, 0.40 mmol). The red solution was stirred 5 min at room temperature obtaining a brown solution of the iridabinaphthalene complex **2** while the iridantracene complex **3** was precipitated with silver salts. The solution was filtered and vacuum-concentrated giving a brown solid that was washed with pentane (3 × 5 mL) and dried under vacuum. Yield: 126 mg (~78% calculated on ***E*-1**).



2

Analytical data for **2**: Anal. Calcd for $C_{33}H_{39}OF_6IrP_2$ (819.83 g/mol): C 48.35, H 4.79; found: C 48.62, H 4.83. IR (cm^{-1}): ν (PF_6) 839 (s). MS: Calculated *m/z* for $[M]^+$: 675.23638; Experimental: 675.23505. ^{1}H NMR: δ 8.11 (s, 1H, C$^{1'}$*H*); 8.08–8.00 (m, 4H, C$^{4'}$*H* + C$^{5'}$*H* + C$^{8'}$*H* + C^7*H*); 7.68–7.62 (m, 3H, C^4*H* + C$^{6'}$*H* + C$^{7'}$*H*); 7.62–7.57 (m, 1H, C$^{3'}$*H*); 7.21–7.13 (m, 2H, C^5*H* + C^6*H*); 6.99 (d, $^4J_{HP}$ = 1.3 Hz, 1H, C^2*H*); 4.65 (s, 3H, OC*H*$_3$); 1.88 (d, $^4J_{HP}$ = 1.7 Hz, 15H, $C_5(CH_3)_5$); 1.39 (d, $^2J_{HP}$ = 11.1 Hz, 9H, P(C*H*$_3$)$_3$) ppm. ^{31}P{^{1}H} NMR: δ –34.26 (s, *P*(CH$_3$)$_3$); –143.88 (sept, $^1J_{PF}$ = 707.8 Hz, *P*F$_6$) ppm. ^{13}C{^{1}H} NMR: δ 250.0 (d, $^2J_{CP}$ = 9.7 Hz, *C^1*); 177.7 (s, *C^3*); 156.6 (d, $^2J_{CP}$ = 9.9 Hz, *C^{7a}*); 143.9 (d, $^3J_{CP}$ = 5.0 Hz, *C^7*); 140.3 (s, *C$^{2'}$*); 137.3 (s, *C^4*); 135.1 (s, *C^{3a}*); 134.4 (s, *C$^{4a'}$*); 133.9 (s, *C$^{8a'}$*); 131.6 (s, *C^6*); 129.3 and 128.7 (both s, *C$^{5'}$*+ *C$^{8'}$*); 128.9 (s, *C$^{1'}$*); 128.8 (s, *C$^{4'}$*); 128.1 and 127.9 (both s, *C$^{6'}$* + *C$^{7'}$*); 127.6 (s, *C$^{3'}$*); 123.9 (s, *C^5*); 120.7 (d, $^3J_{CP}$ = 1.7 Hz, *C^2*); 100.3 (d, $^2J_{CP}$ = 1.8 Hz, *C$_5$*(CH$_3$)$_5$); 64.6 (s, O*C*H$_3$); 14.0 (d, $^1J_{CP}$ = 41.0 Hz, P(*C*H$_3$)$_3$); 9.6 (s, C$_5$(*C*H$_3$)$_5$) ppm.

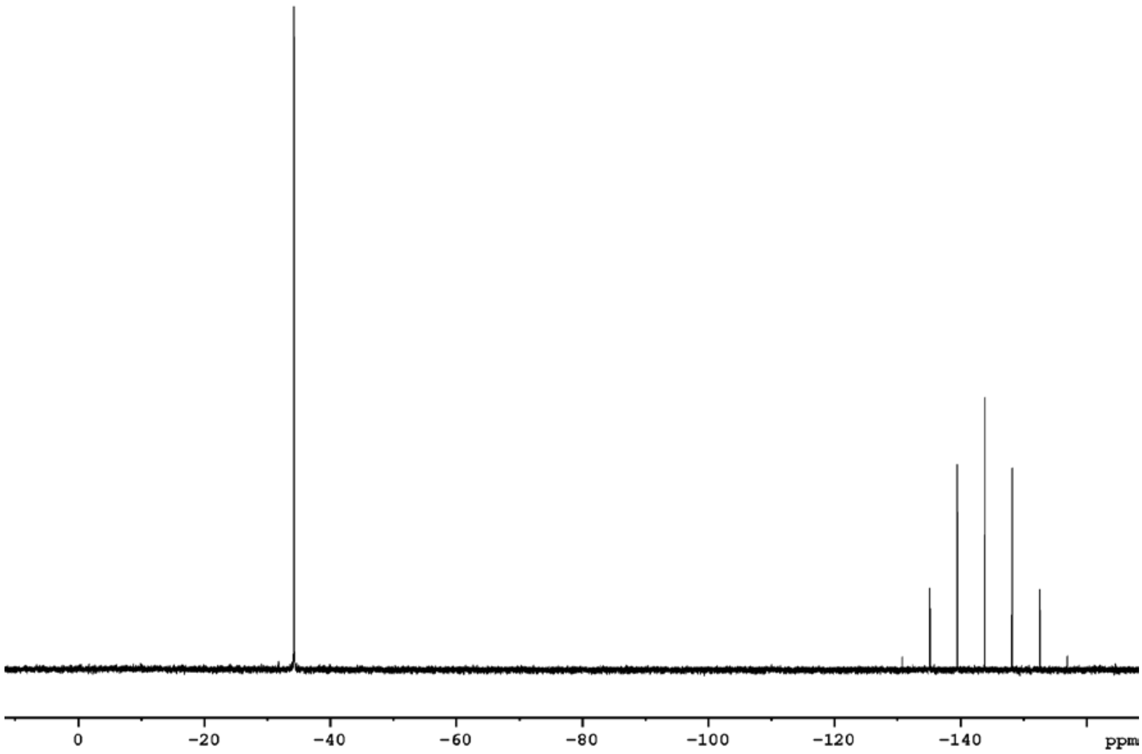


Figure S15. $^{31}P\{^1H\}$ NMR spectrum of **2**.

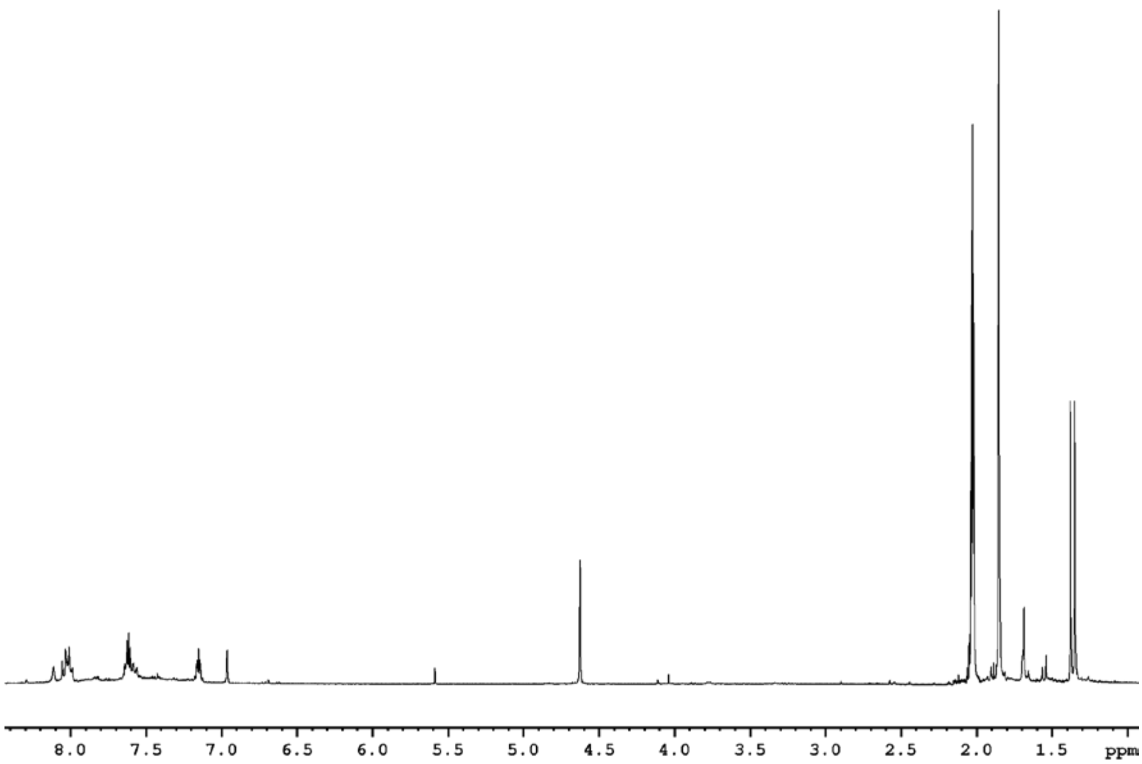


Figure S16. ^1H NMR spectrum of **2**.

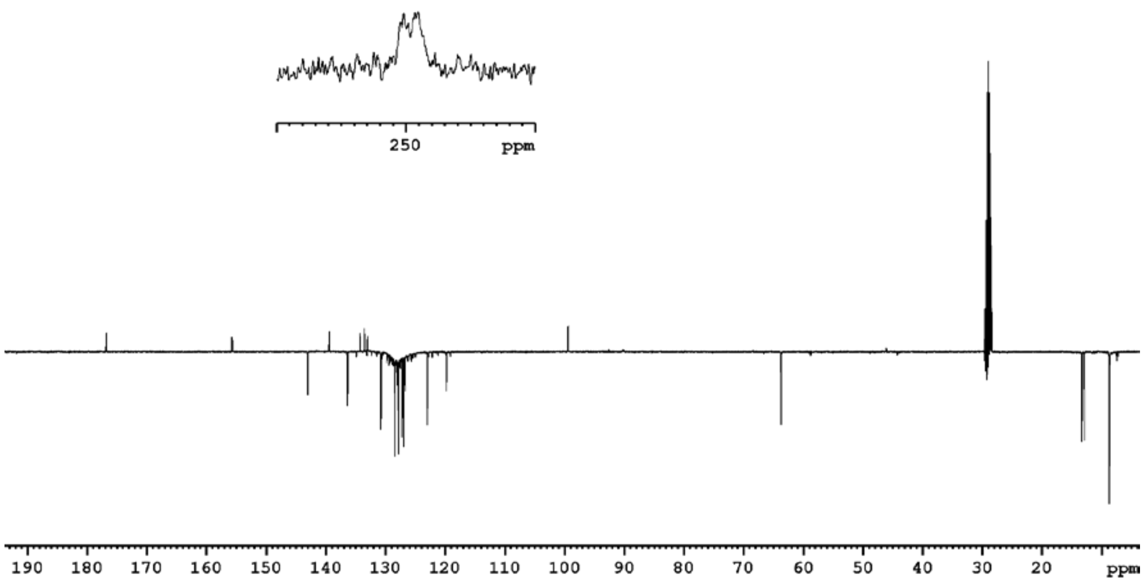


Figure S17. $^{13}C\{^1H\}$ JMOD NMR spectrum of **2**.

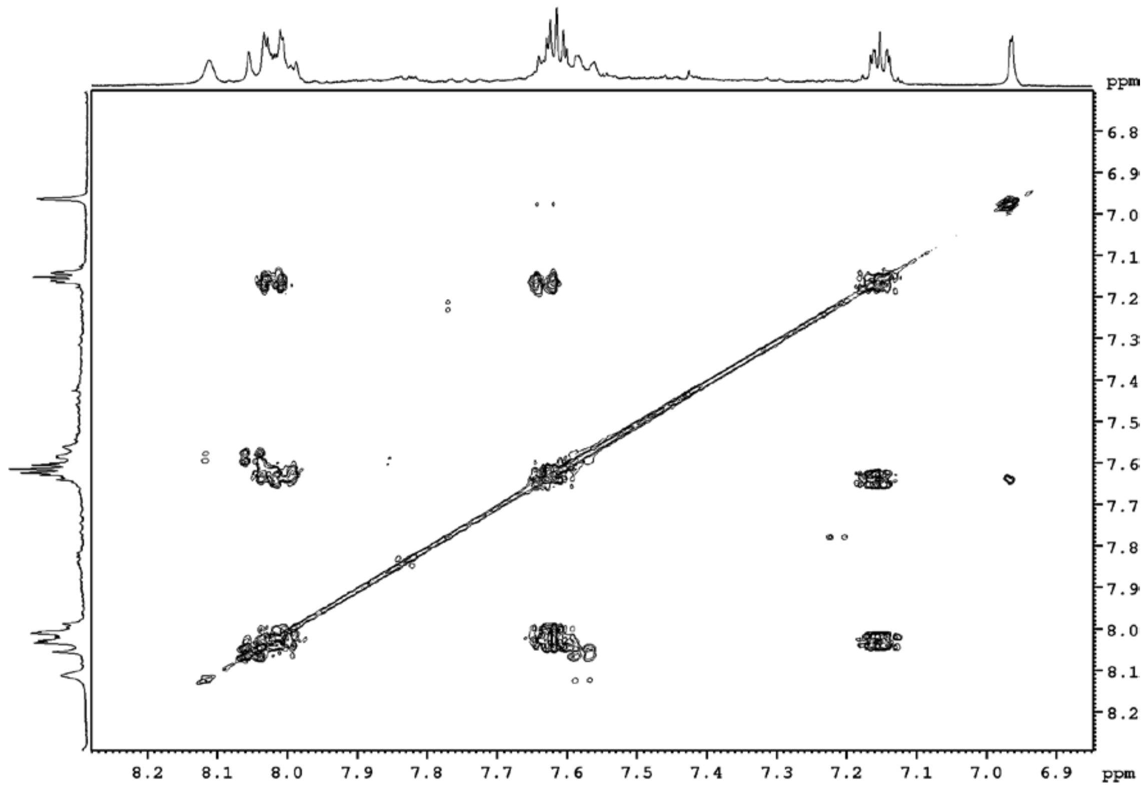


Figure S18. ^1H, ^1H COSY NMR spectrum of **2**.

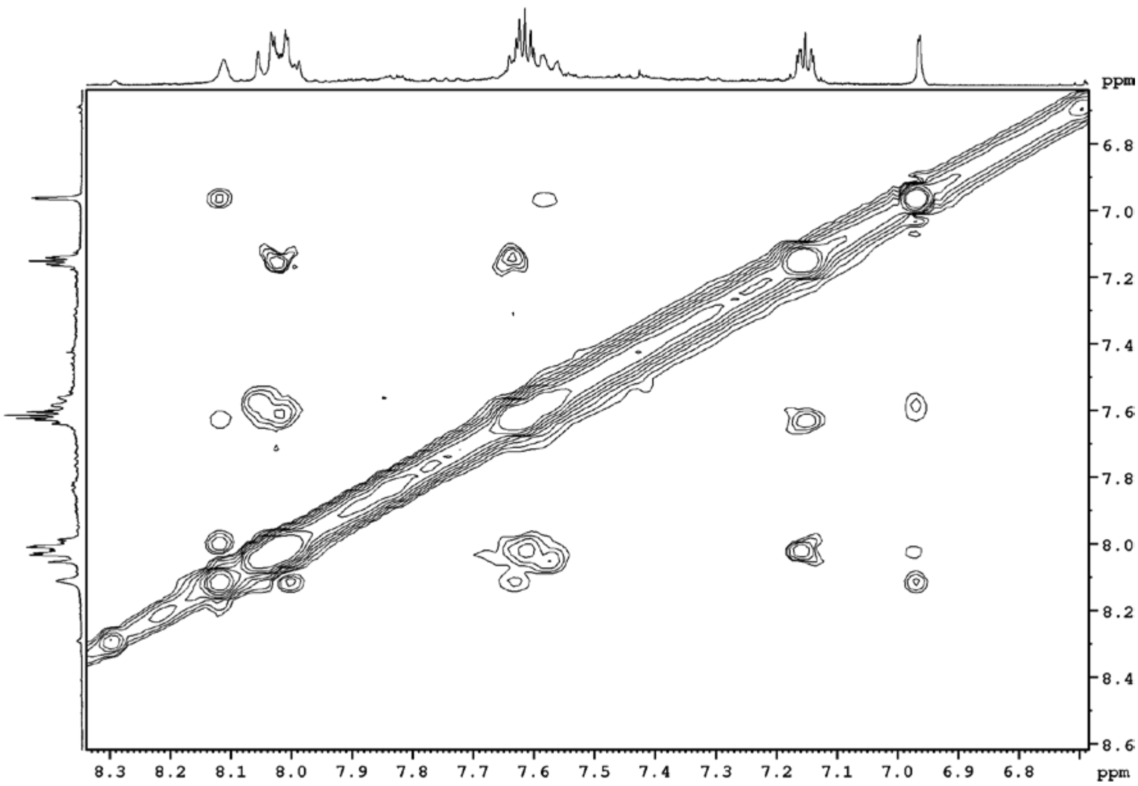


Figure S19. ^{1}H, ^{1}H NOESY NMR spectrum of **2**.

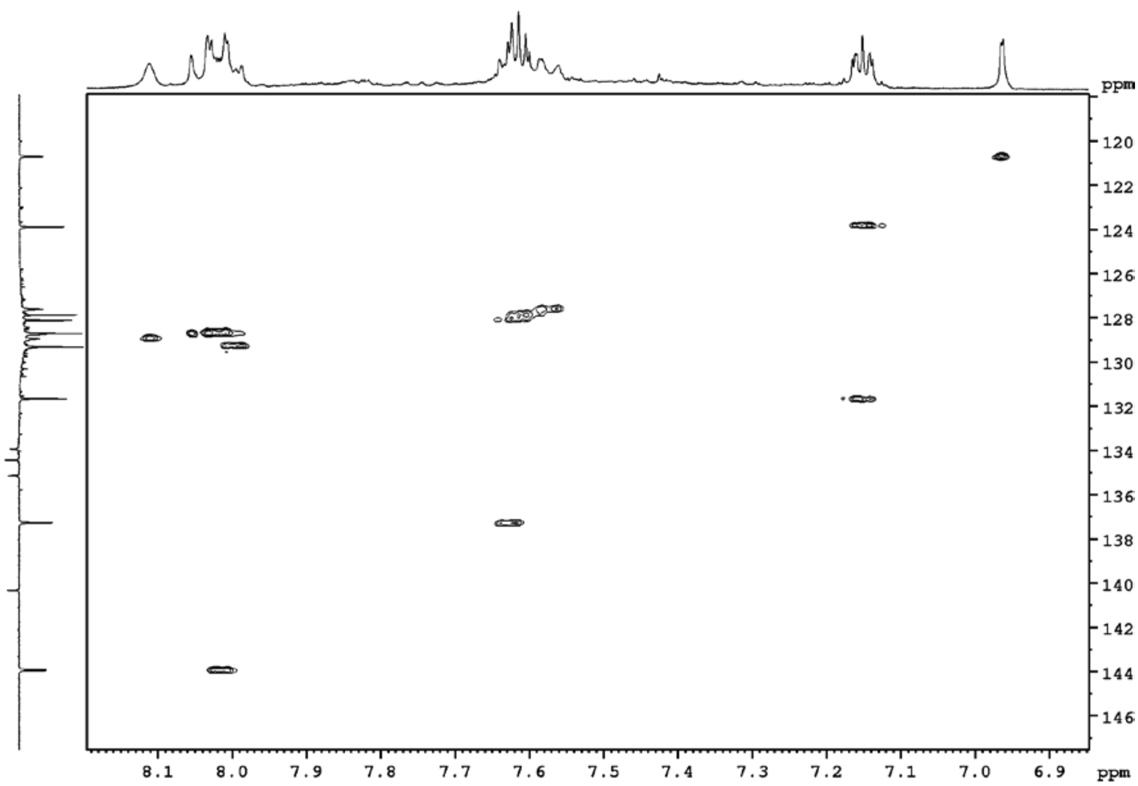


Figure S20. ^{1}H, ^{13}C HSQC NMR spectrum of **2**.

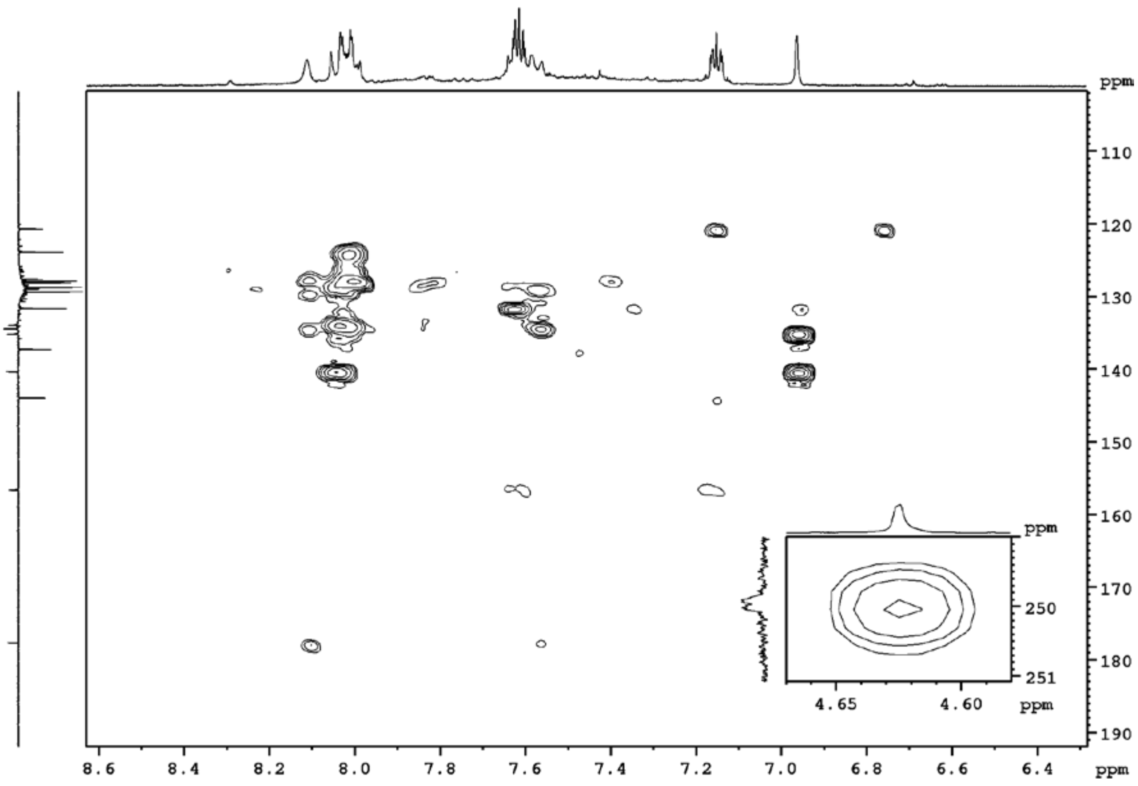


Figure S21. ^{1}H, ^{13}C HMBC NMR spectrum of **2**.

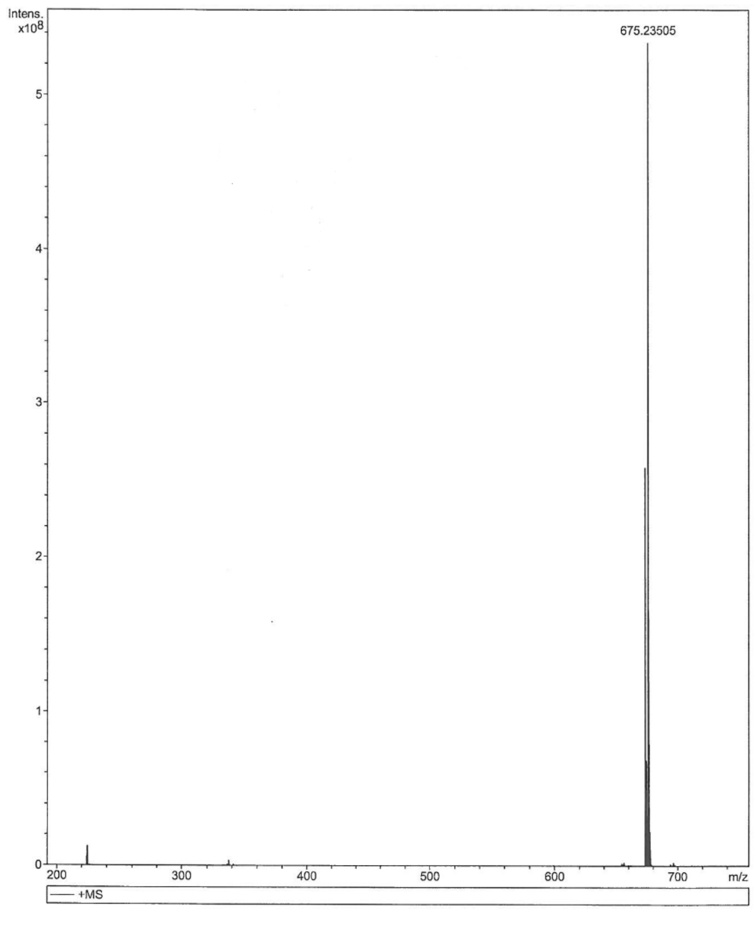
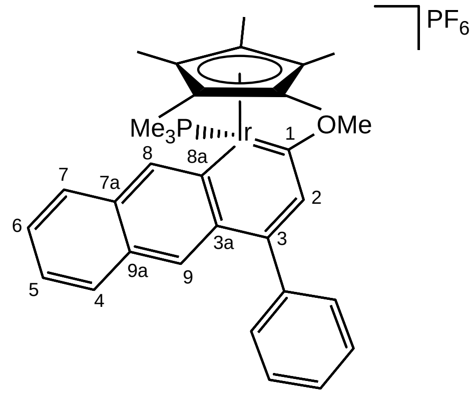


Figure S22. ESI spectrum of **2**.

On the other hand, the iridantracene complex **3** was separated from the silver salts using acetone (5 mL) as extracting solvent. The dark solution was filtered and vacuum-concentrated giving a brown solid that was washed with pentane (3 × 5 mL) and dried under vacuum. Yield: 64 mg (~45% calculated on ***Z*-1**).



3

Analytical data for **3**: Anal. Calcd for $C_{33}H_{39}OF_6IrP_2$ (819.83 g/mol): C 48.35, H 4.79; found: C 48.70, H 4.86. IR (cm^{-1}): ν (PF_6) 839 (s). MS: Calculated *m/z* for $[M]^+$: 675.23638; Experimental: 675.23571. ^{1}H NMR: δ 8.31 (s, 1H, C^8H); 8.22 (s, 1H, C^9H); 7.88 (d, $^3J_{HH}$ = 8.3 Hz, 1H, C^4H); 7.71 (d, $^3J_{HH}$ = 8.2 Hz, 1H, C^7H); 7.67–7.54 (m, 6H, *Ph* + C^5H); 7.41–7.34 (m, 1H, C^6H); 6.96 (d, $^4J_{HP}$ = 1.2 Hz, 1H, C^2H); 4.68 (s, 3H, OCH_3); 1.87 (d, $^4J_{HP}$ = 1.8 Hz, 15H, $C_5(CH_3)_5$); 1.42 (d, $^2J_{HP}$ = 11.0 Hz, 9H, $P(CH_3)_3$) ppm. $^{31}P\{^1H\}$ NMR: δ –34.05 (s, $P(CH_3)_3$); –143.98 (sept, $^1J_{PF}$ = 707.9 Hz, PF_6) ppm. $^{13}C\{^1H\}$ NMR (253 K): δ 251.3 (d, $^2J_{CP}$ = 11.2 Hz, C^1); 176.1 (s, C^3); 142.6 (s, C_{ipso}); 141.9 (d, $^2J_{CP}$ = 10.2 Hz, C^{8a}); 141.1 (d, $^3J_{CP}$ = 5.7 Hz, C^8); 137.8 (s, C^9); 135.5 (s, C^{7a}); 133.9 (d, $^3J_{CP}$ = 0.5 Hz, C^{3a}); 130.4 (s, C^{9a}); 130.1 (s, C^7); 129.8 (s, 130.5–128.5 (all s, *Ph* + C^5); 126.2 (s, C^4); 125.4 (s, C^6); 123.3 (d, $^3J_{CP}$ = 1.7 Hz, C^2); 99.4 (d, $^2J_{CP}$ = 2.3 Hz, $C_5(CH_3)_5$); 65.0 (s, OCH_3); 13.5 (d, $^1J_{CP}$ = 40.9 Hz, $P(CH_3)_3$); 9.4 (d, $^3J_{CP}$ = 0.8 Hz, $C_5(CH_3)_5$) ppm.

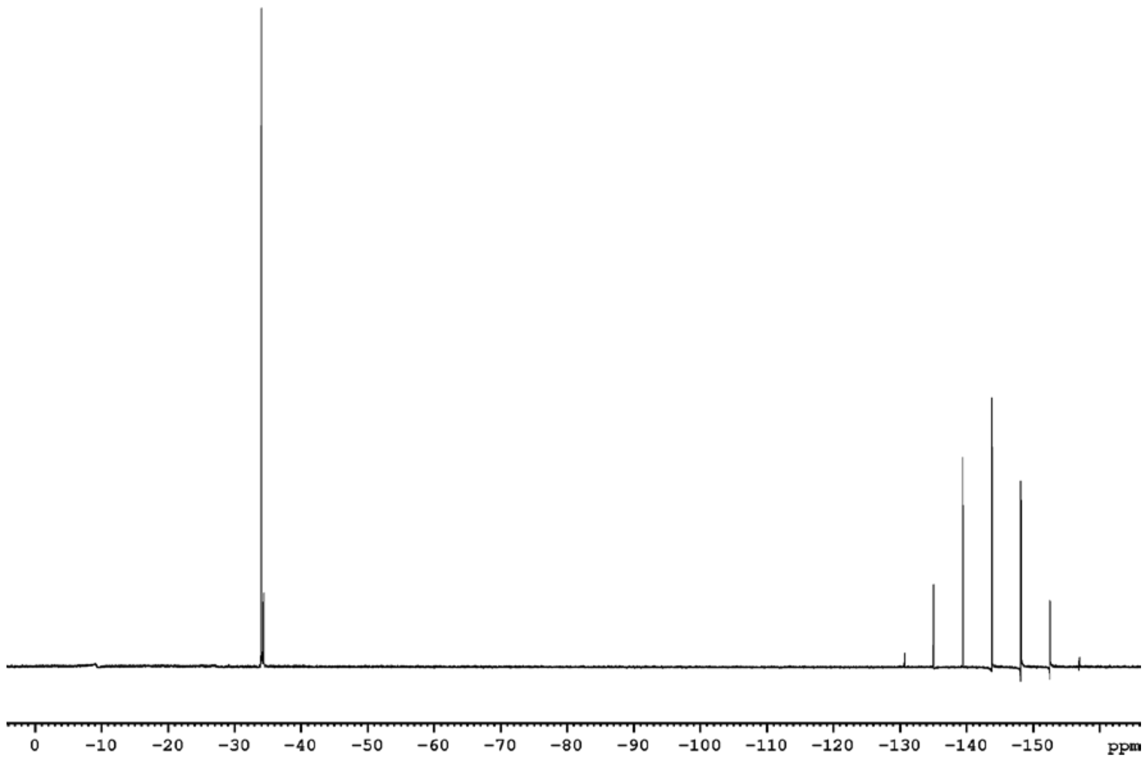


Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum of **3**.

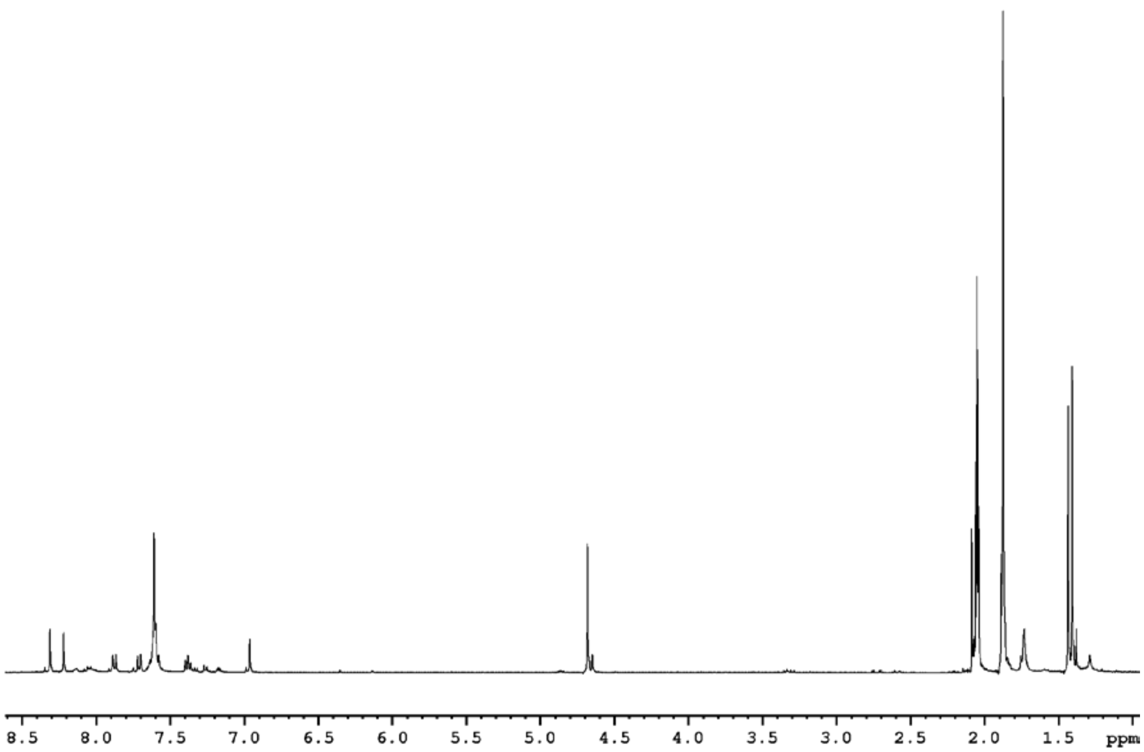


Figure S24. ^{1}H NMR spectrum of **3**.

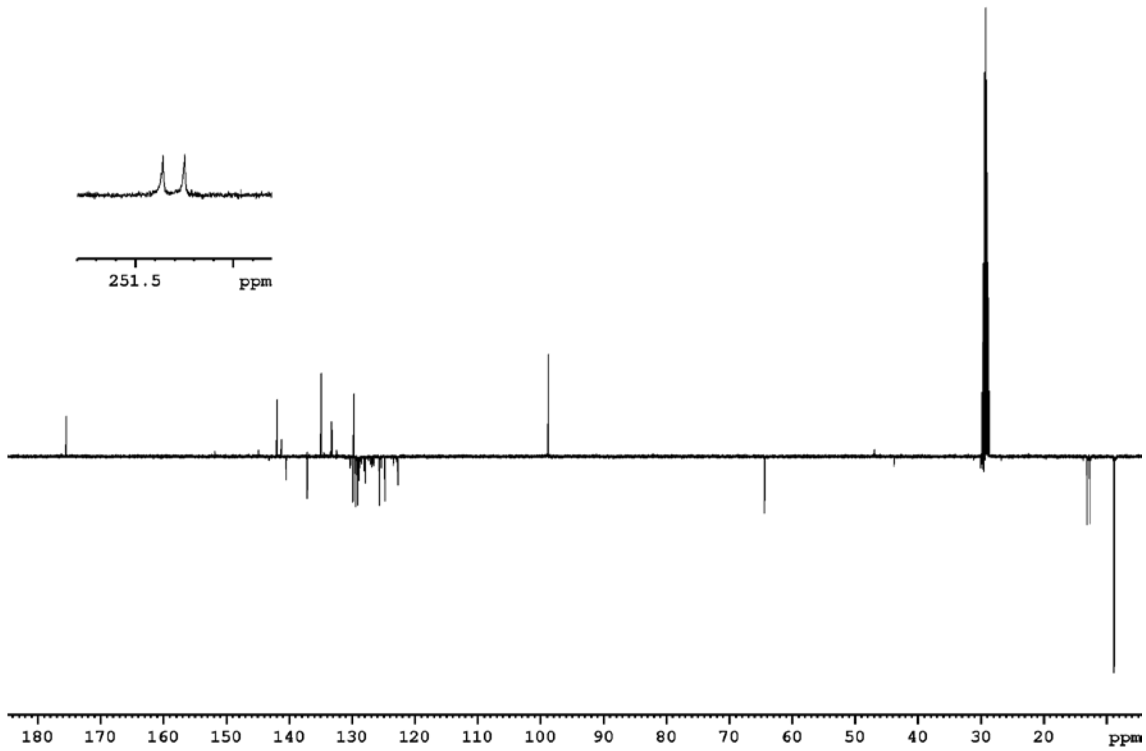


Figure S25. $^{13}C\{^{1}H\}$ JMOD NMR spectrum of **3**.

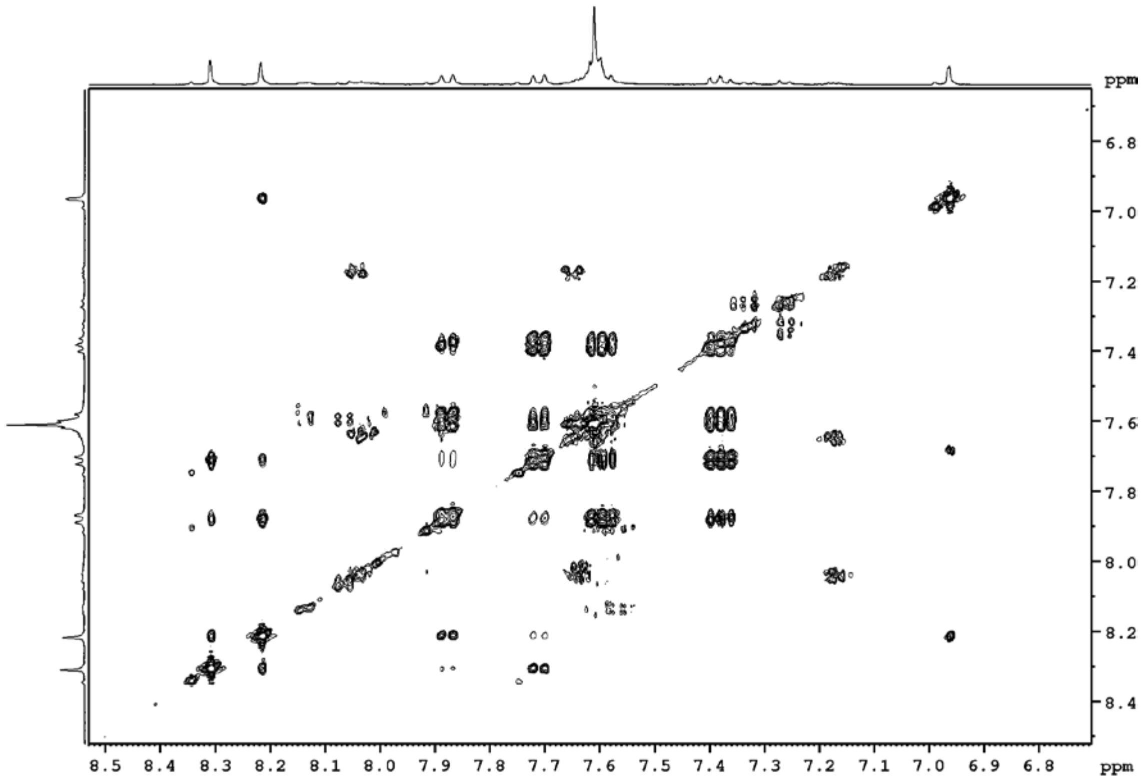


Figure S26. ^{1}H, ^{1}H COSY NMR spectrum of **3**.

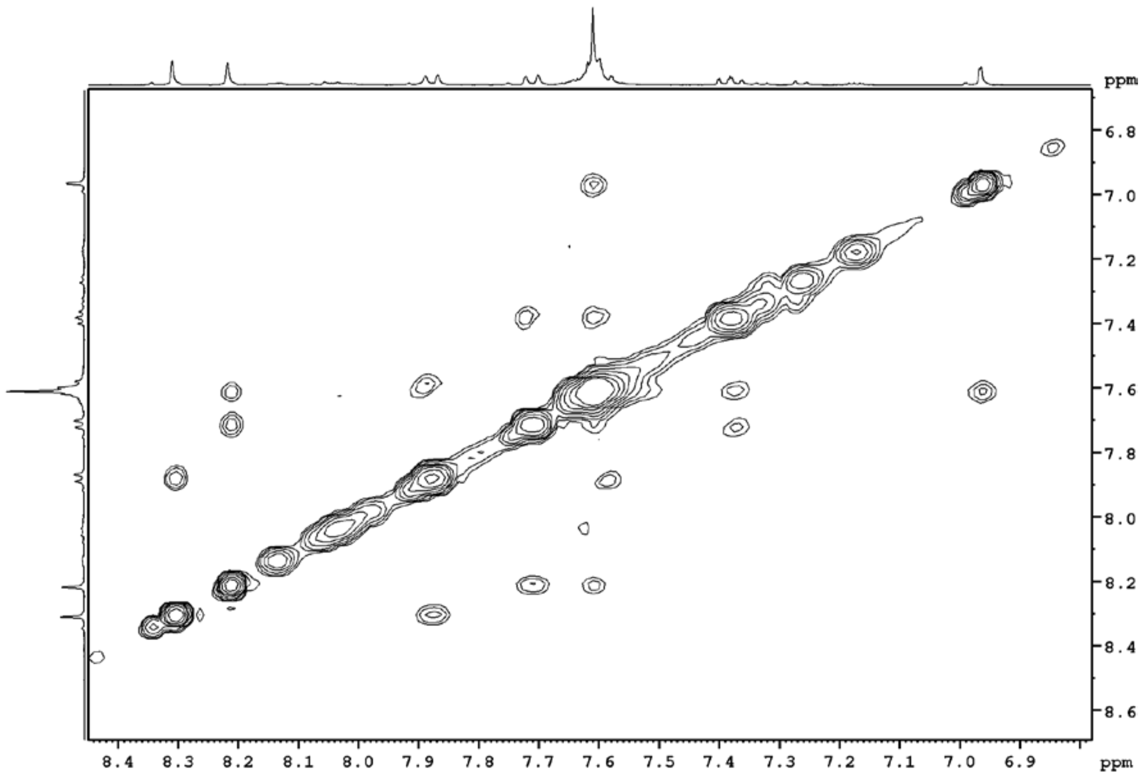


Figure S27. ^1H, ^1H NOESY NMR spectrum of **3**.

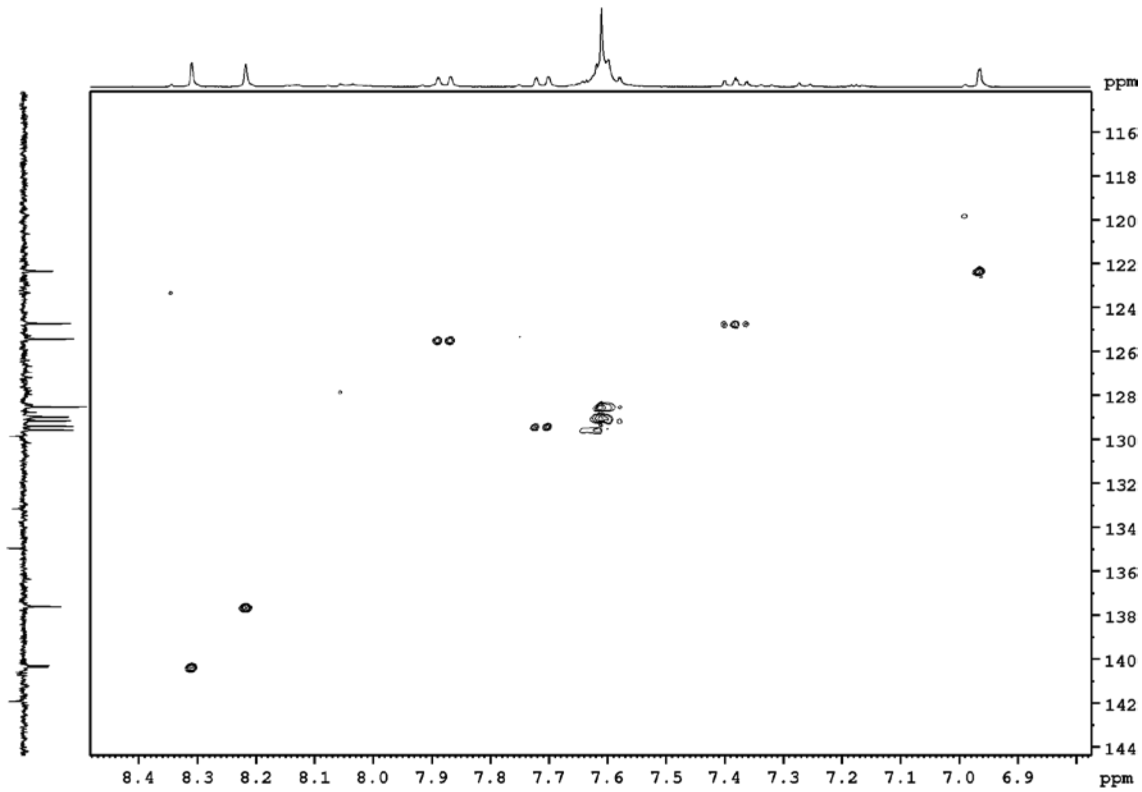


Figure S28. ^1H, ^{13}C HSQC NMR spectrum of **3**.

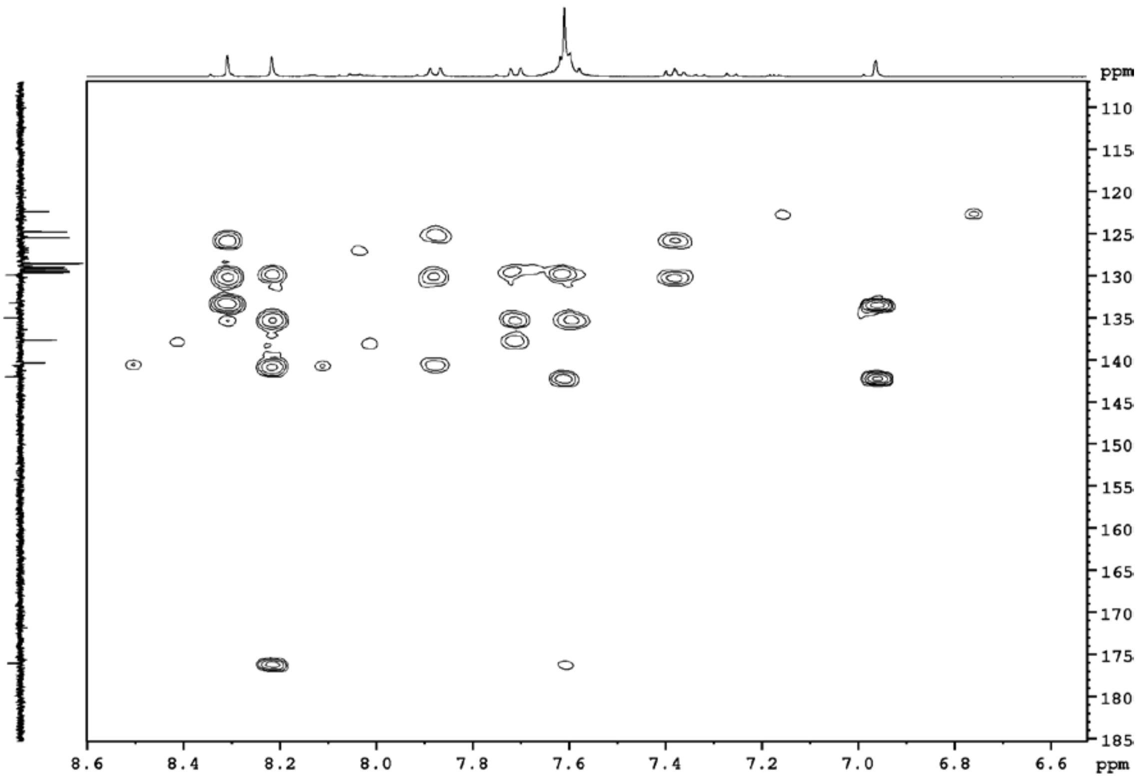


Figure S29. ^{1}H, ^{13}C HMBC NMR spectrum of **3**.

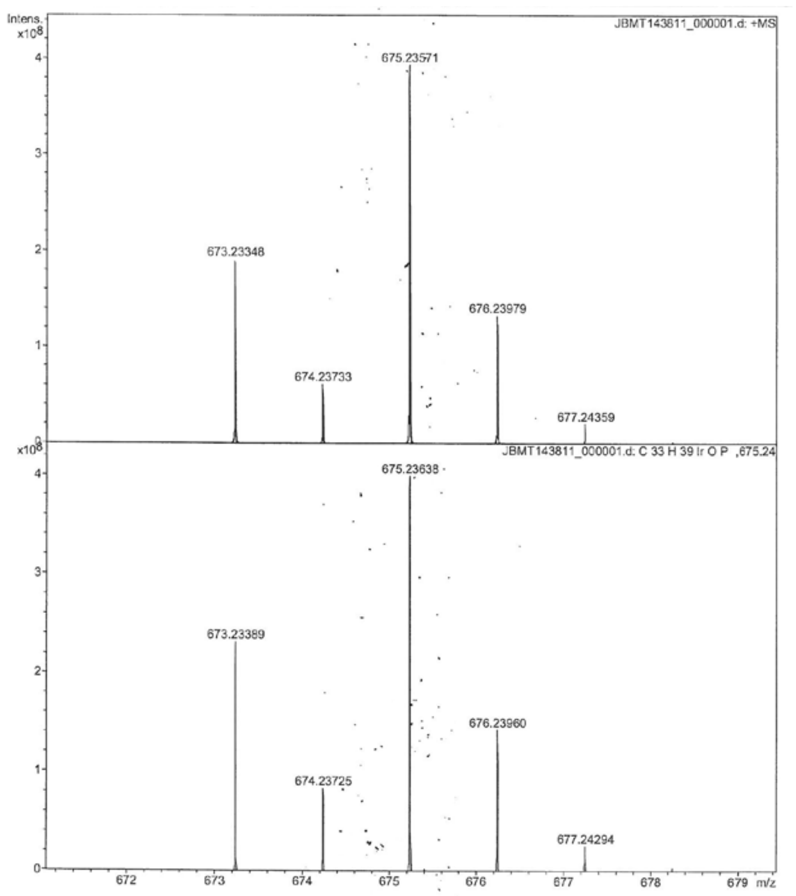
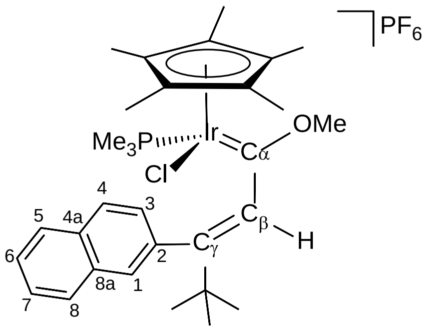


Figure S30. ESI spectrum of **3**, theoretical (down) and experimental (up).

Preparation of $[IrCp^*Cl\{=C(OMe)–CH=C(2–C_{10}H_7)(\textit{t}Bu)\}(PMe_3)]PF_6$ (*E*-4)

To a yellow solution of $[IrCp^*Cl(NCMe)(PMe_3)]PF_6$ (100 mg, 0.16 mmol) in methanol (10 mL), 4,4-dimethyl-3-(1-naphthalenyl)-1-pentyn-3-ol (42 mg, 0.18 mmol) was added and the mixture was stirred for 3h 30 min. The brown solution obtained was vacuum-concentrated yielding a brown solid that was washed with pentane (3 × 3 mL) and dried under vacuum. The product obtained has a 20% of impurities based on $^{31}P\{^1H\}$ NMR spectrum. Yield: 123 mg (92%).



***E*-4**

Analytical data for ***E*-4**: $C_{31}H_{44}OClF_6IrP_2$ (836.29 g/mol). MS: Calculated *m/z* for $[M]^+$: 691.24350; Experimental: 691.24313. IR (cm^{-1}): ν (PF_6) 841 (s). ^1H NMR: δ 7.98–7.88 (m, 3H, $C^4H + C^5H + C^8H$); 7.61 (s br, 1H, C^1H); 7.57–7.51 (m, 2H, C^6H + C^7H); 7.36–7.28 (m, 2H, $C_\beta H + C^3H$); 4.14 (s, 3H, OCH_3); 1.80 (d, 15H, $^4J_{HP}$ = 2.1 Hz, $C_5(CH_3)_5$); 1.76 (d, 9H, $^2J_{HP}$ = 11.2 Hz, $P(CH_3)_3$); 1.26 (s, 9H, $C(CH_3)_3$) ppm. $^{31}P\{^1H\}$ NMR: δ –31.42 (s, $P(CH_3)_3$); –143.89 (sept, $^1J_{PF}$ = 708.0 Hz, PF_6) ppm. $^{13}C\{^1H\}$ NMR: δ 268.9 (s br, C_α); 164.6 (observed by HMBC correlations, C_γ); 140.4 (s, C_β); 126.1 (s, C^1); 133.3 and 133.2 (both s, $C^{4a} + C^{8a}$); 127.6 (s, C^4); 128.5 (s, C^5); 137.6 (s, C^2); 127.1 (s, C^7); 127.3 (s, C^6); 128.7 (s, C^8); 127.1 (s, C^3); 99.1 (d, $^2J_{CP}$ = 2.3 Hz, $C_5(CH_3)_5$); 69.6 (s, OCH_3); 39.8 (s, $C(CH_3)_3$) 29.6 (s, $C(CH_3)_3$); 14.9 (d, $^1J_{CP}$ = 40.7 Hz, $P(CH_3)_3$); 9.0 (d, $^3J_{CP}$ = 0.9 Hz, $C_5(CH_3)_5$) ppm.

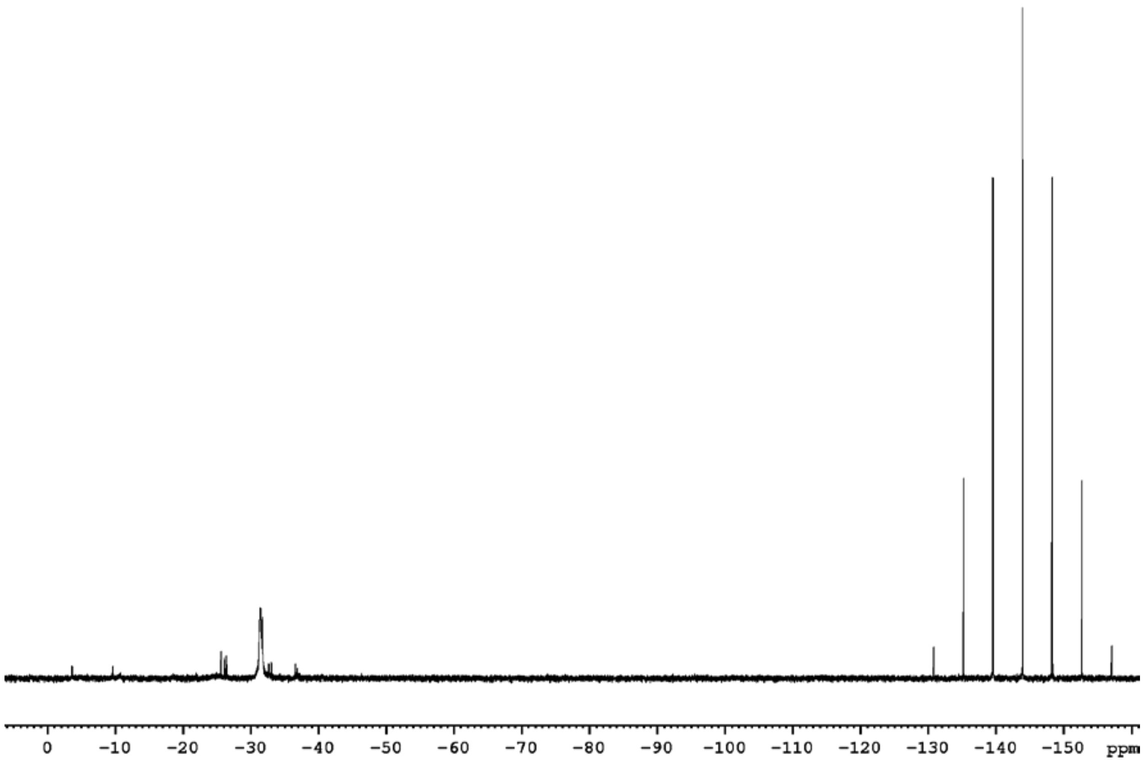


Figure S31. $^{31}P\{^{1}H\}$ NMR spectrum of ***E*-4**.

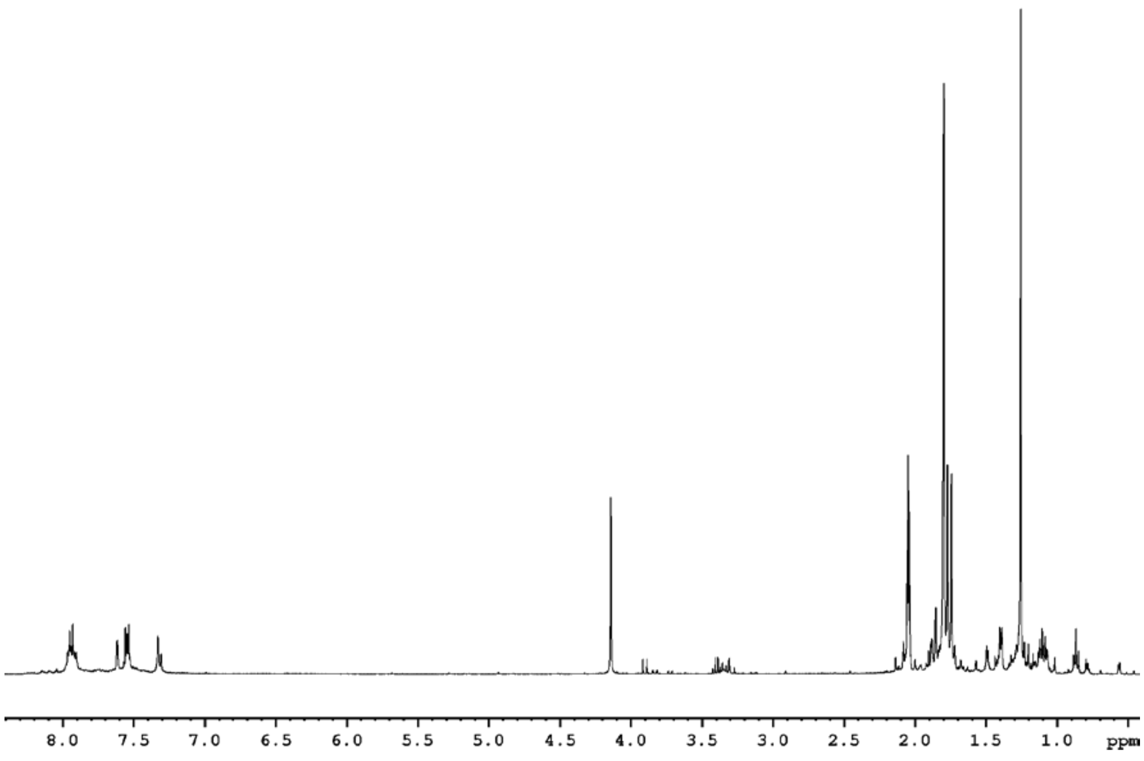


Figure S32. ^{1}H NMR spectrum of ***E*-4**.

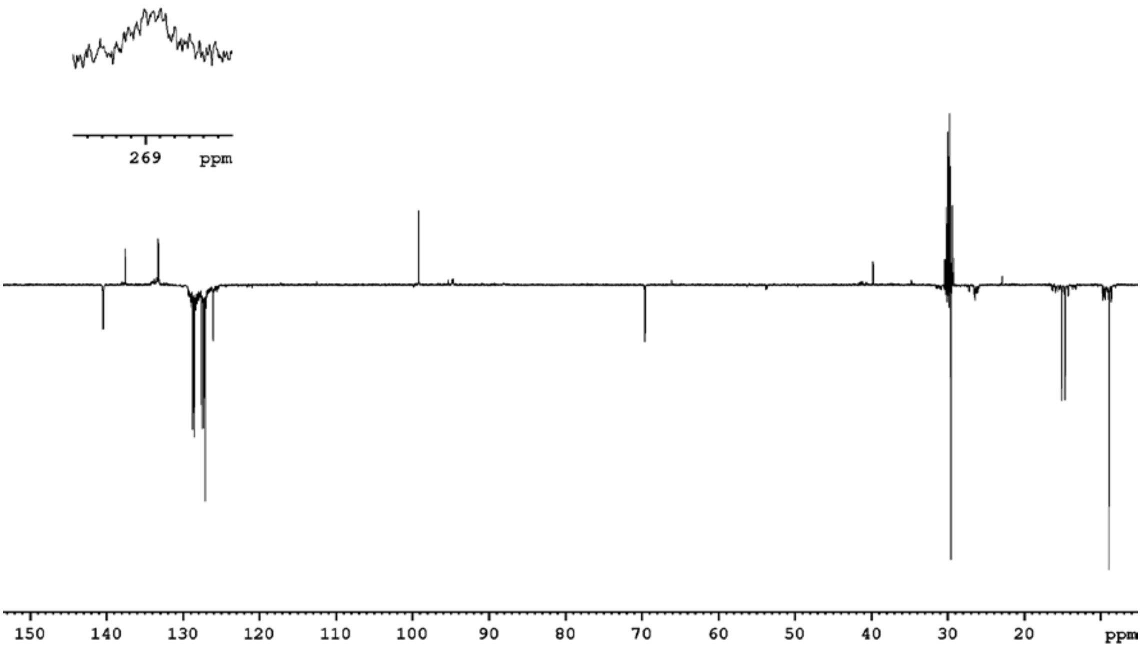


Figure S33. $^{13}C\{^{1}H\}$ JMOD NMR spectrum of ***E*-4**.

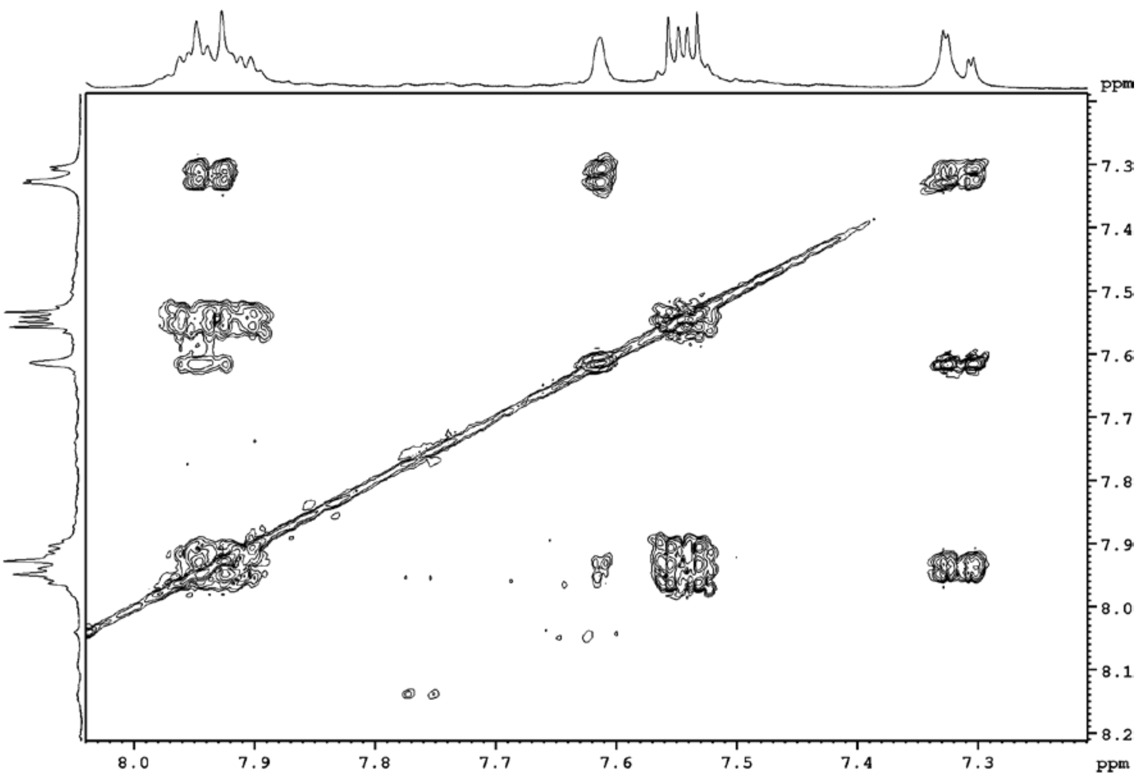


Figure S34. ^{1}H, ^{1}H COSY NMR spectrum of ***E*-4**.

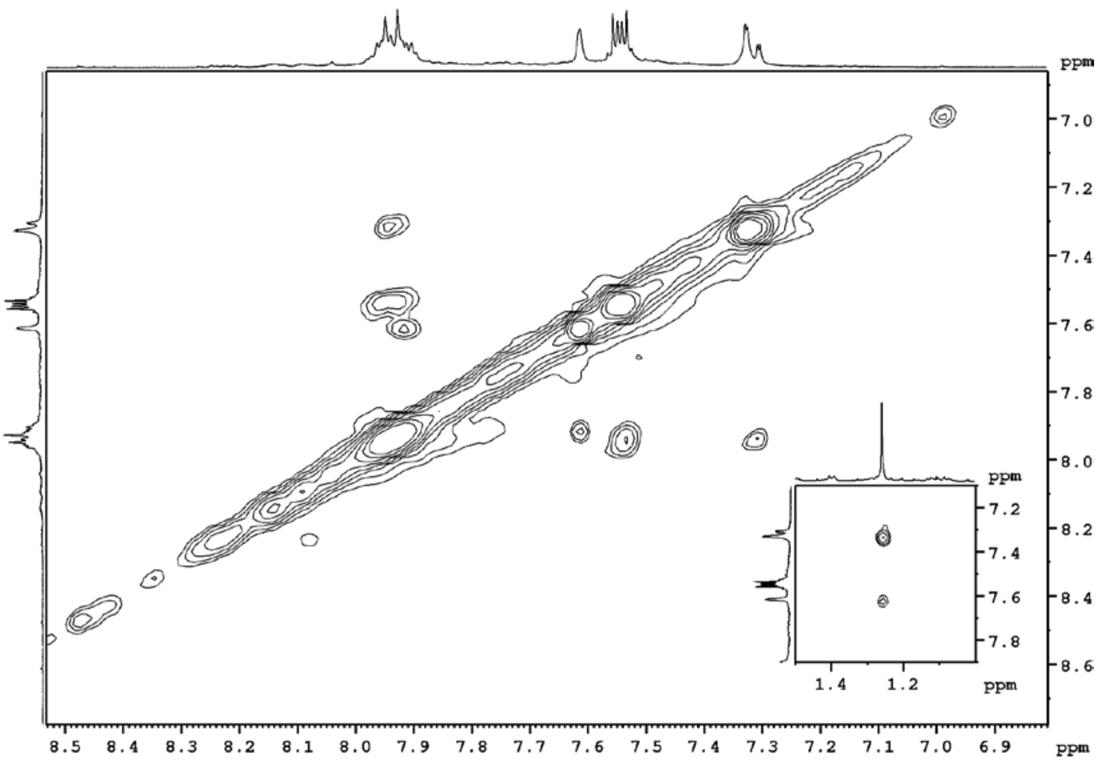


Figure S35. ^{1}H, ^{1}H NOESY NMR spectrum of ***E*-4**.

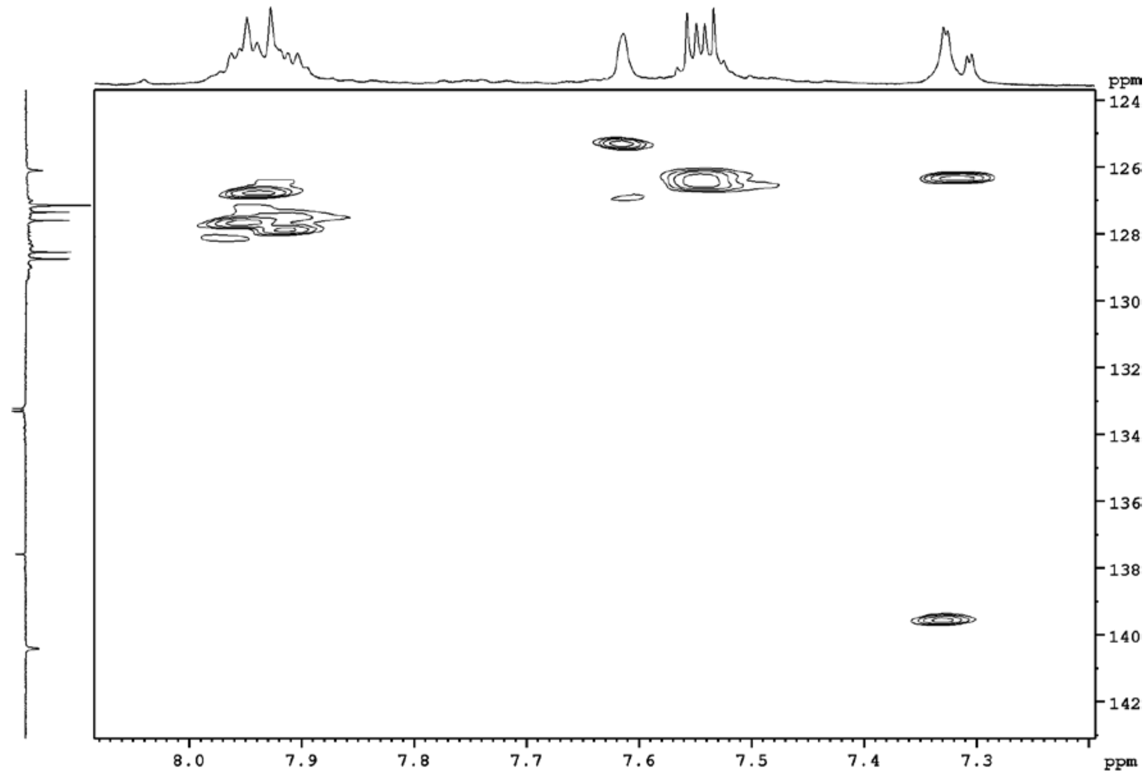


Figure S36. ^{1}H, ^{13}C HSQC NMR spectrum of ***E*-4**.

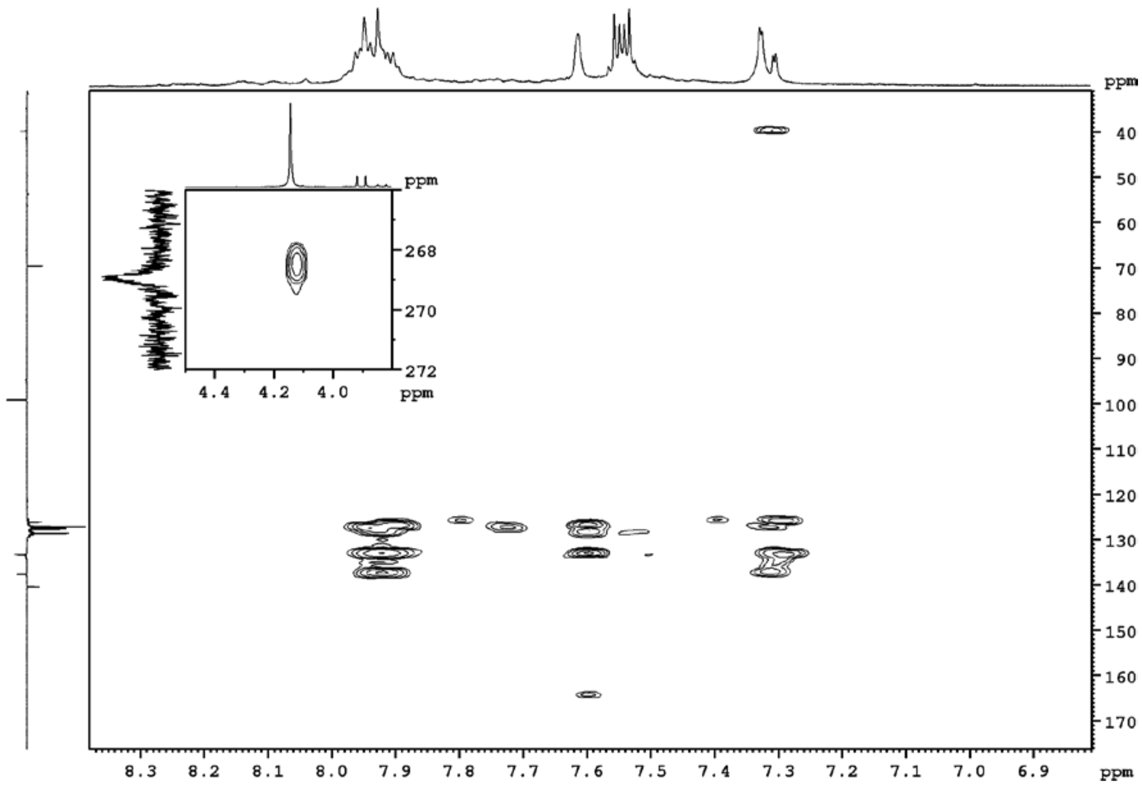


Figure S37. [1]H, [13]C HMBC NMR spectrum of ***E*-4**.

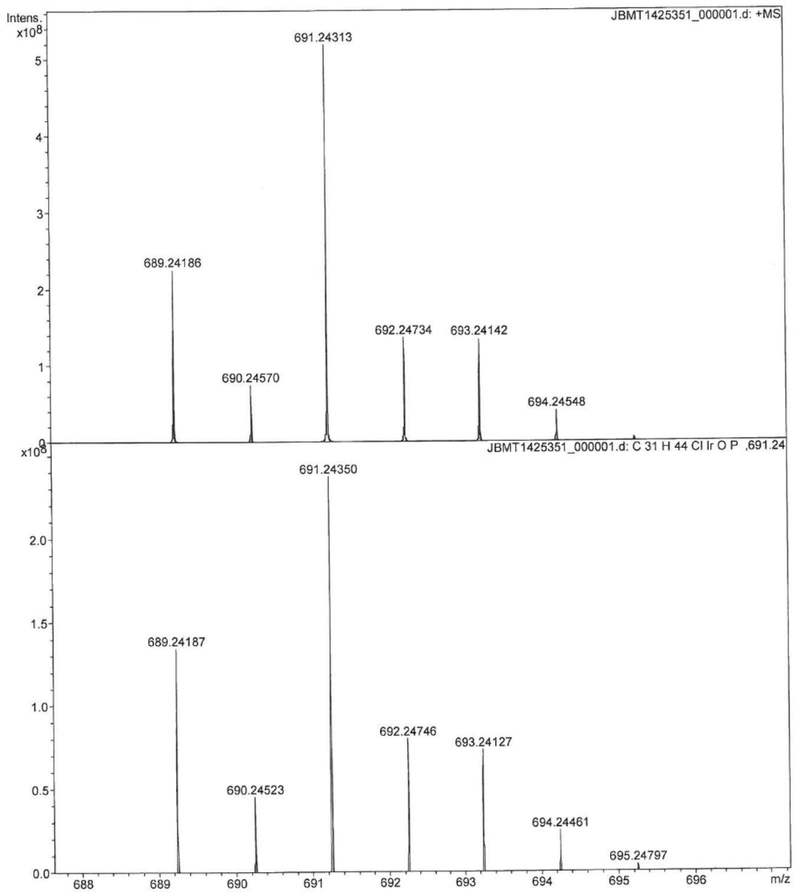
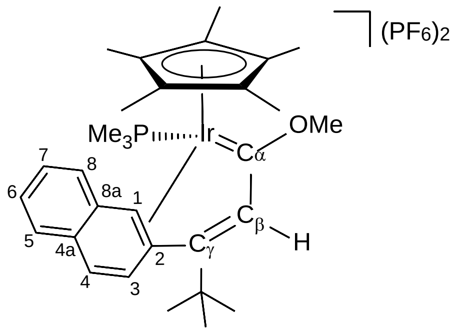


Figure S38. ESI spectrum of ***E*-4**, theoretical (down) and experimental (up).

Preparation of [IrCp*{=C(OMe)–CH=C(η^2-2-$C_{10}H_7$)(*t*Bu)}(PMe_3)]$(PF_6)_2$ (5)

To a brown solution of [IrCp*Cl{=C(OMe)–CH=C(2–$C_{10}H_7$)(*t*Bu)}(PMe_3)]PF_6 (***E*-4**) (100 mg, 0.12 mmol) in dichloromethane (10 mL), silver hexafluorophosphate (34 mg, 0.13 mmol) was added and the mixture was stirred for 5 min. The dark brown solution obtained was vacuum-concentrated yielding a dark brown solid. Then, the final product was extracted with acetone (6 mL) and filtered. The dark brown solution was vacuum-concentrated and the dark brown solid obtained was washed with pentane (3 × 5 mL) and dried under vacuum. Yield: 99 mg (87%). Due to the instability of complex **5**, it was only characterized in solution by NMR spectroscopy, which supports the formulation proposed.



5

Analytical data for **5**: $C_{31}H_{44}OF_{12}IrP_3$ (945.80 g/mol). IR (cm^{-1}): ν (PF_6) 840 (s). ^{1}H NMR: δ 8.24–8.19 (m, 1H, C^8H); 8.11–8.06 (m, 1H, C^5H); 8.02 (s, 1H, $C_\beta H$); 7.94 (d, $^3J_{HH}$ = 8.8 Hz, 1H, C^4H); 7.74–7.68 (m, 2H, C^6H + C^7H); 7.16 (dd, $^3J_{HH}$ = 8.8, $^4J_{HH}$ = 1.1 Hz, 1H, C^3H); 6.68 (d br, $^2J_{HP}$ = 10.6 Hz, 1H, C^1H); 5.07 (d, 3H, $^5J_{HP}$ = 0.7 Hz, OCH_3); 2.07 (d, 9H, $^2J_{HP}$ = 10.2 Hz, $P(CH_3)_3$); 1.29 (d, 15H, $^4J_{HP}$ = 2.0 Hz, $C_5(CH_3)_5$); 1.15 (s, 9H, $C(CH_3)_3$) ppm. ^{31}P{^{1}H} NMR: δ –29.35 (s, $P(CH_3)_3$); –143.93 (sept, $^1J_{PF}$ = 708.0 Hz, PF_6) ppm. ^{13}C{^{1}H} NMR: δ 248.7 (d, $^2J_{CP}$ = 12.9 Hz, C_α); 203.8 (s, C_γ); 144.1 (s, C_β); 135.0 (s, C^{8a}); 132.0 (s, C^8); 131.8 (s, C^{4a}); 130.5 (s, C^5); 130.6 and 130.1 (s, C^7 + C^6); 127.8 (s, 2C C^4 + C^3); 107.5 (s br, $C_5(CH_3)_5$); 104.9 (s, C^2); 74.2 (s, C^1); 70.2 (s, OCH_3); 41.9 (s, $C(CH_3)_3$) 29.8 (s, $C(CH_3)_3$); 15.8 (d, $^1J_{CP}$ = 42.3 Hz, $P(CH_3)_3$); 8.2 (s, $C_5(CH_3)_5$) ppm.

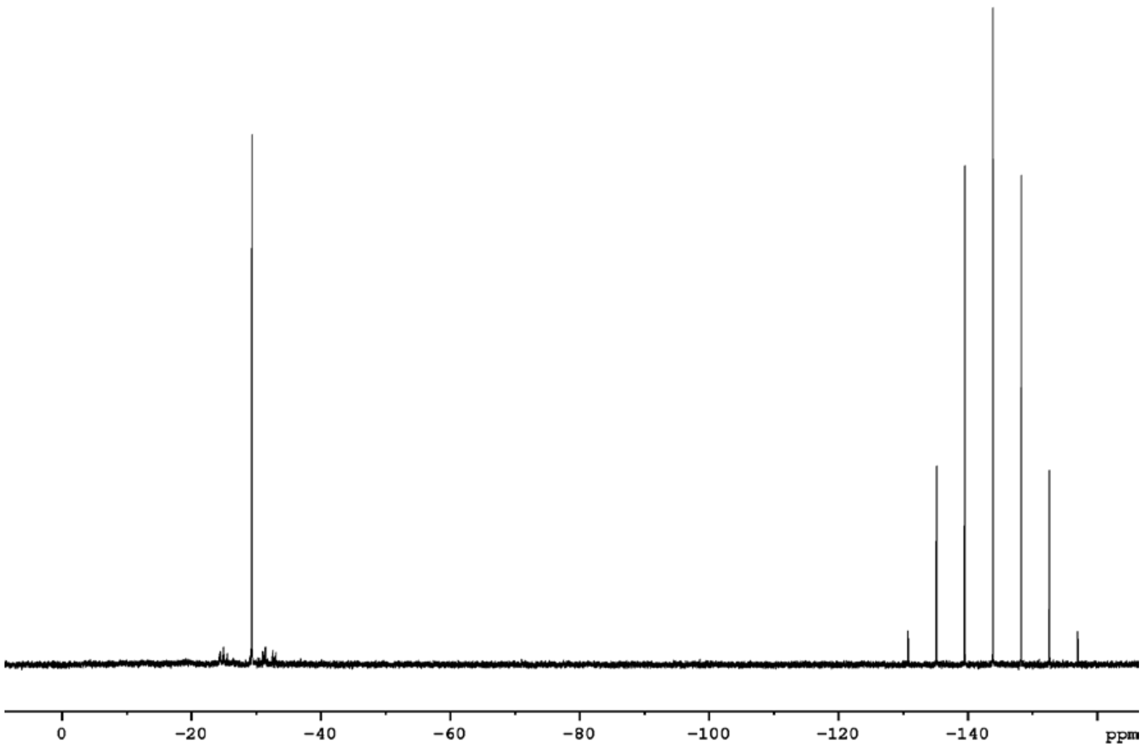


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum of **5**.

Figure S40. ^{1}H NMR spectrum of **5**.

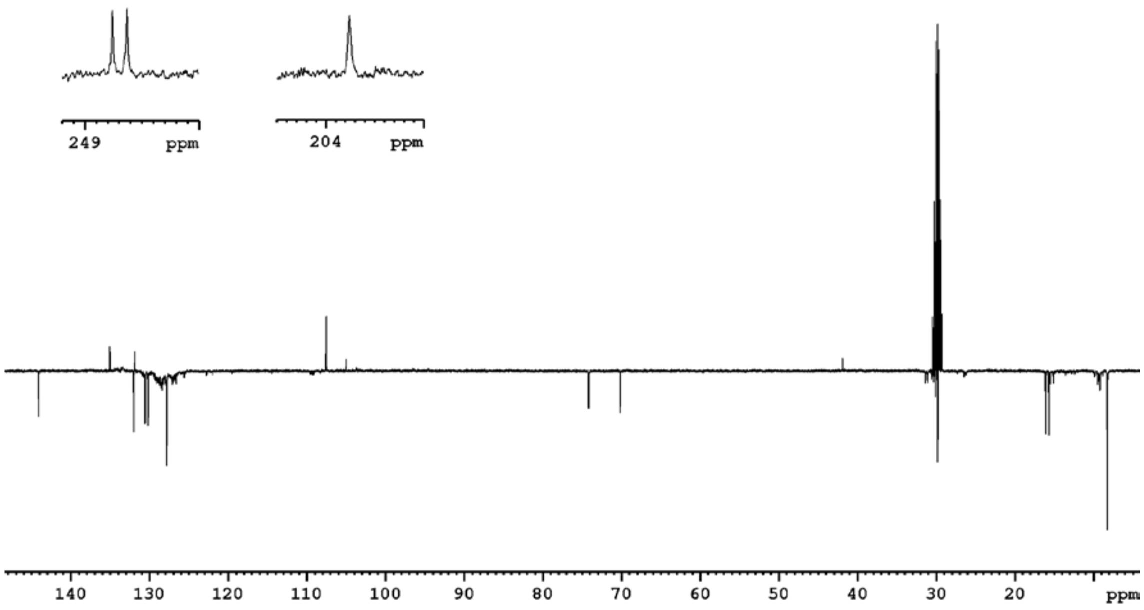


Figure S41. $^{13}C\{^{1}H\}$ JMOD NMR spectrum of **5**.

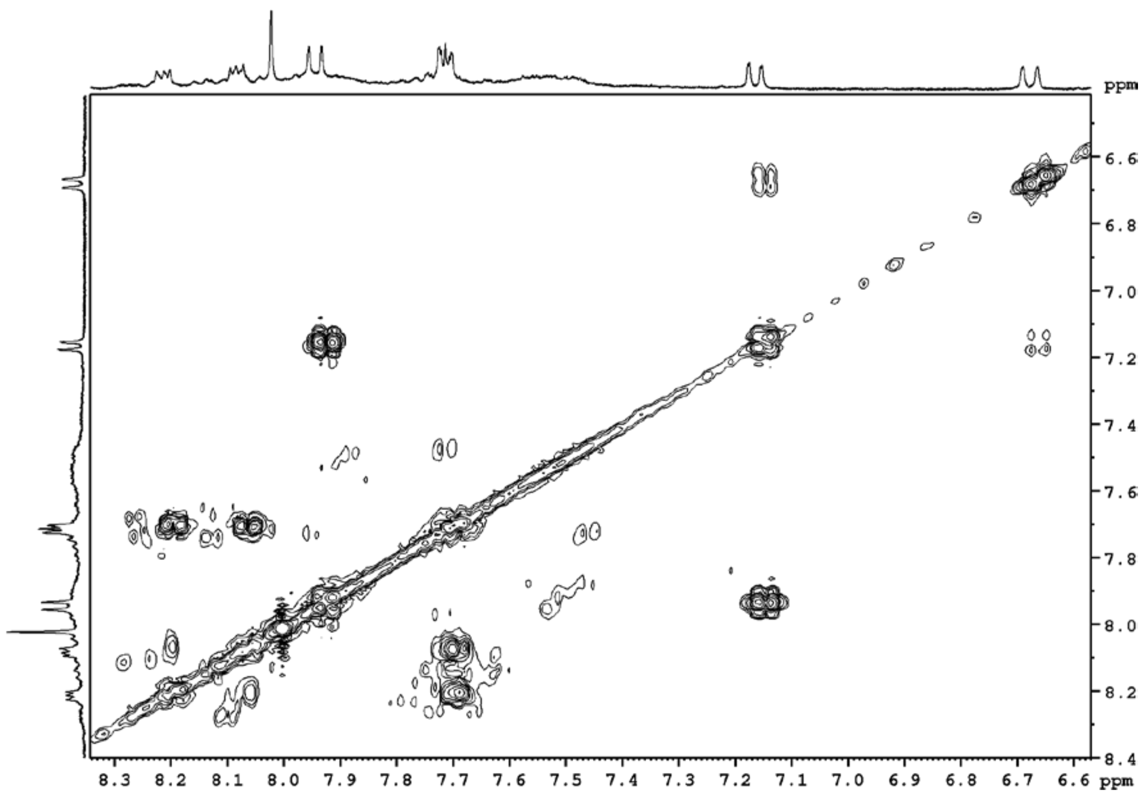


Figure S42. ^{1}H, ^{1}H COSY NMR spectrum of **5**.

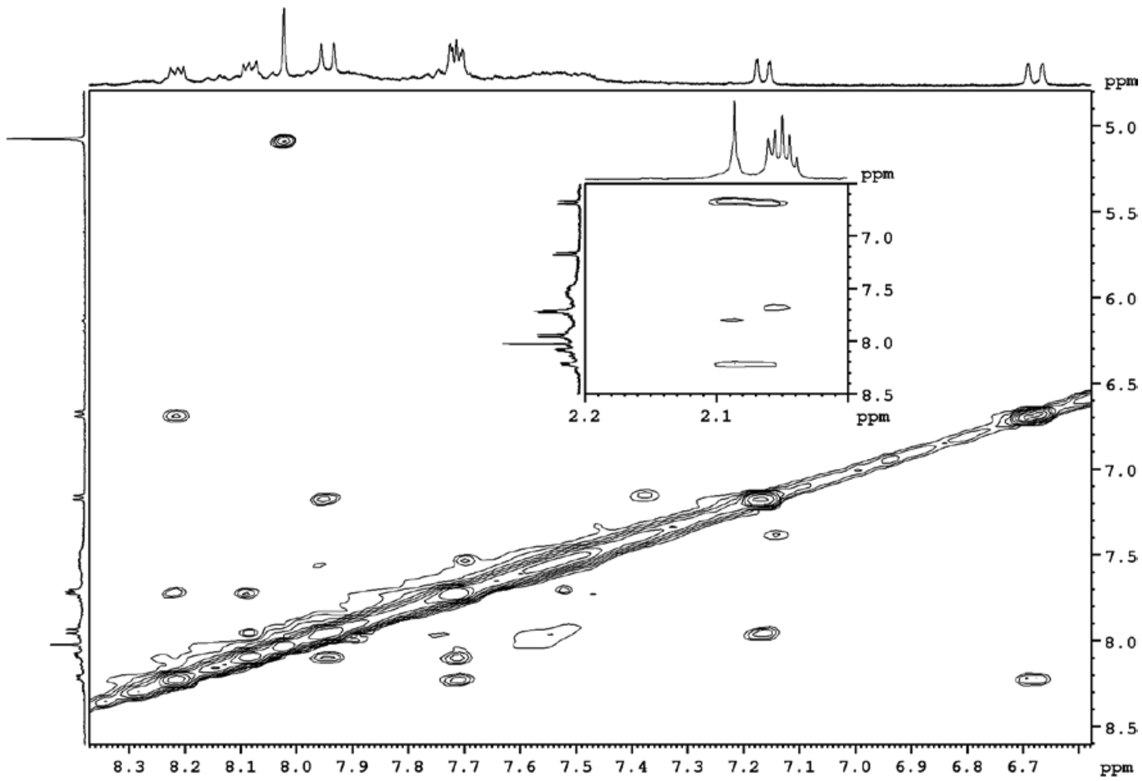


Figure S43. ^{1}H, ^{1}H NOESY NMR spectrum of **5**.

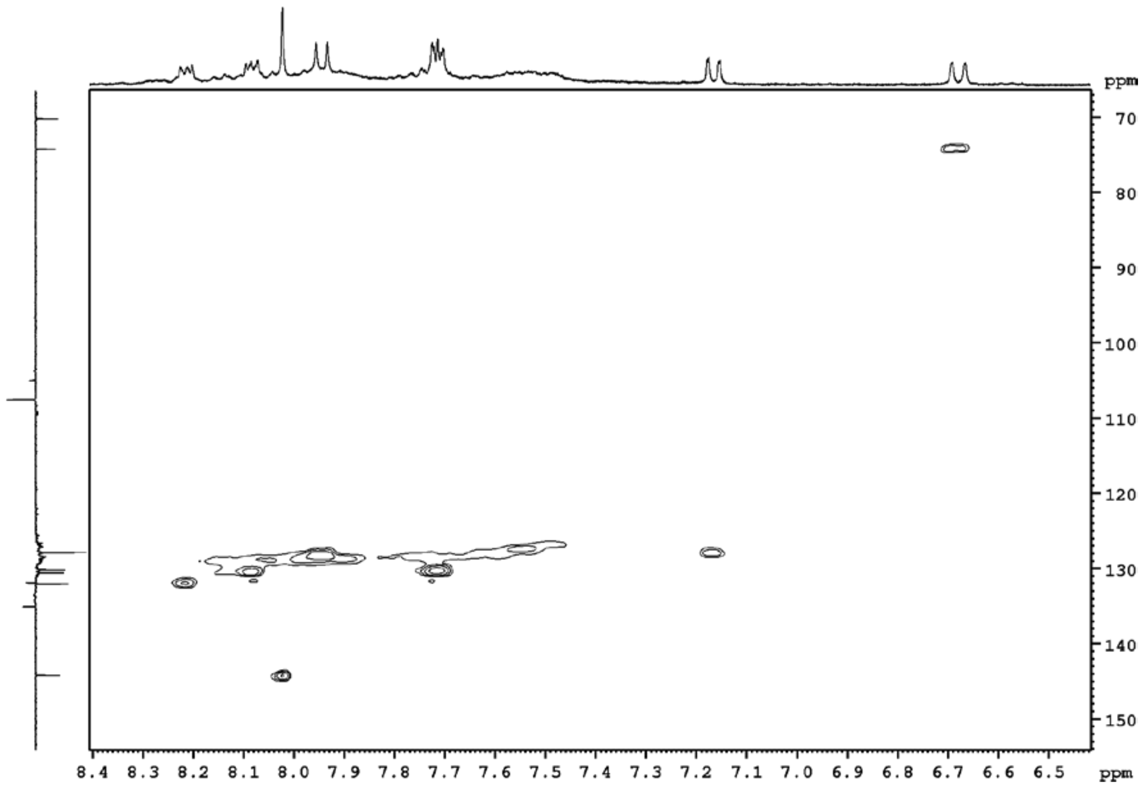


Figure S44. ^{1}H, ^{13}C HSQC NMR spectrum of **5**.

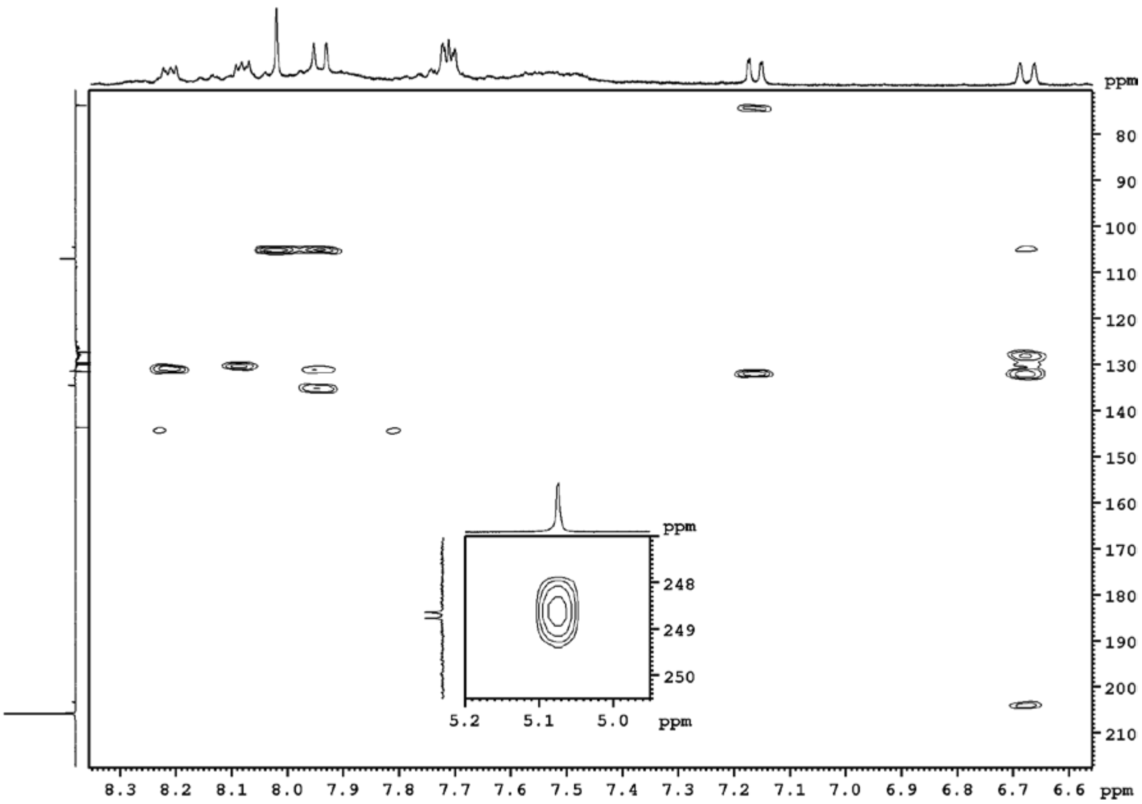


Figure S45. ^{1}H, ^{13}C HMBC NMR spectrum of **5**.

Computational details

General procedure and Analysis of Data

All calculations were carried out with the GAUSSIAN 09 program package.[3] Structures were optimized at the B3LYP level employing a combination of double zeta basis set and pseudopotential for the valence and core electrons (LANL2DZ), respectively, for the iridium atom and 6-31G(d,p) basis set for the rest of the elements in gas phase. Harmonic frequency calculations were performed at the same level to confirm them as local minimums and to obtain energy corrections. Molecular Orbitals were obtained at the same theoretical level.

Calculated Anisotropy of the Current-Induced Density (ACID)

The ACID[4] plots of the most representative structures are present in Figure S15. The isosurface value is 0.05.

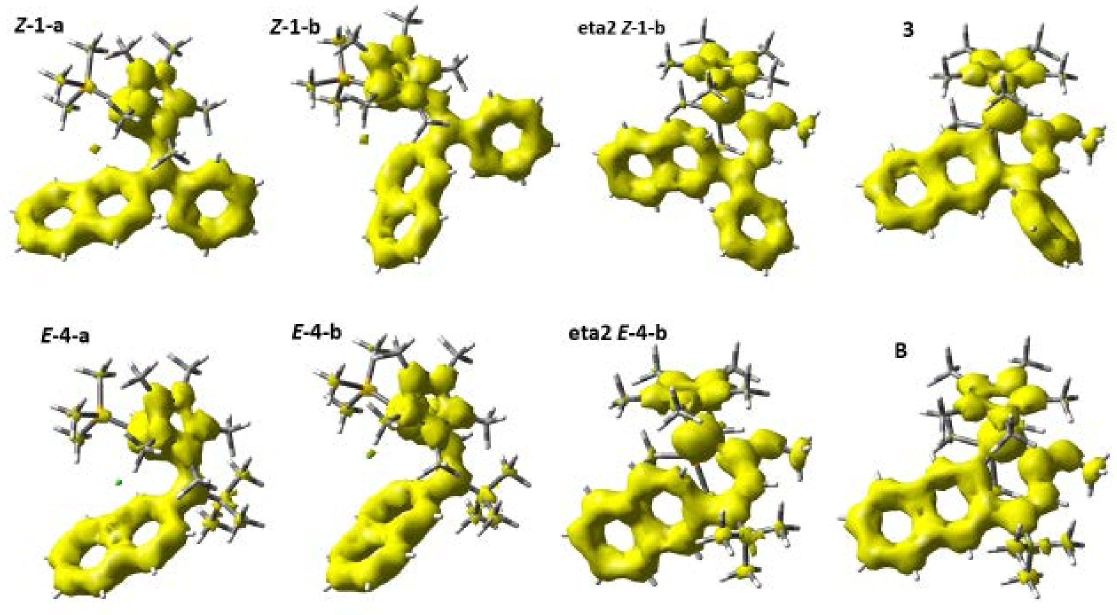


Figure S46. ACID figures of some of the complexes under study.

Fukui Indices

The Fukui indices of the naphtalenyl group of complexes ***Z*-1** and ***E*-4** were calculated. In Table S1, the most important results are shown.

Table S1. Fukui indices

Complex	C1 atom	C4 atom
***Z*-1a**	0.138	0.148
***Z*-1b**	0.140	0.146
***E*-4a**	0.148	0.146
***E*-4b**	0.149	0.144

Frontier Orbitals

The HOMO and LUMO orbitals of reactants with isosurface value=0.02 electrons/Bohr^3 are depicted in Figure S16. The energy gaps in eV are also shown.

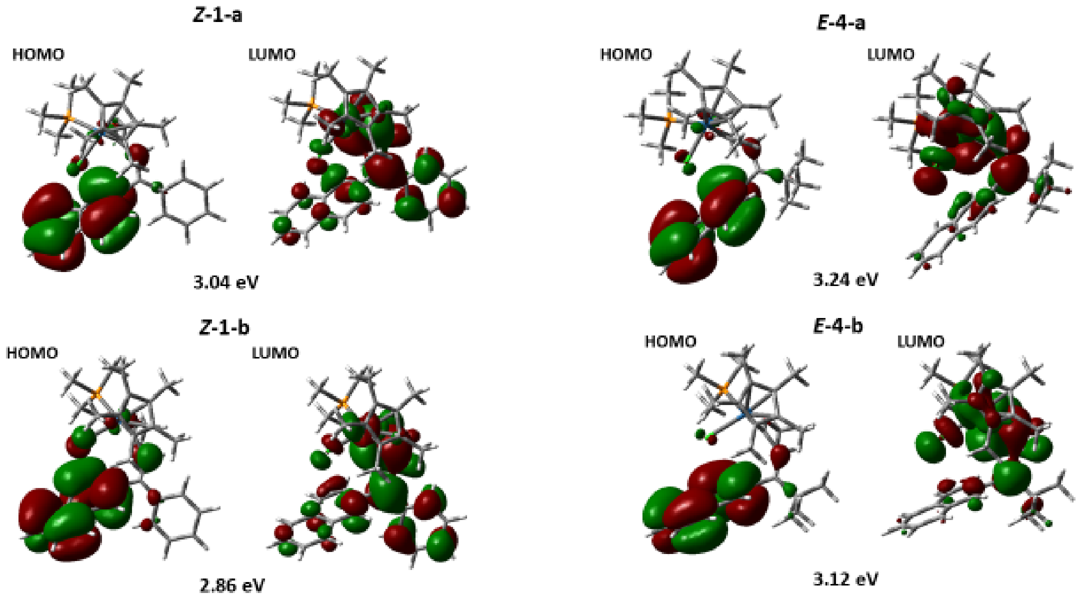


Figure S42. HOMO/LUMO orbitals and energy gaps of the methoxy(alkenyl)carbeneiridium complexes.

Table S2. HOMO-LUMO gap (eV) of reactants and intermediates

Complex	Gap	Complex	Gap
***Z*-1a**	3.04	***Z*-1a- η^2**	3.04
***Z*-1b**	2.86	***Z*-1b- η^2**	3.15
***E*-4a**	3.24	**5**	3.31
***E*-4b**	3.12	***E*-4b- η^2**	3.29

Relevant Ir-C distances, Cartesian coordinates and Energy of all the calculated compounds

Table S3. Energy of the optimized structures.

Complex	B3LYP Energy (H)	Complex	B3LYP Energy (H)	Complex	B3LYP Energy (H)
***E*-1**	-2263.00601284	**A**	-1802.19731409	**C**	-1728.38001296
***Z*-1a**	-2263.00432940	***Z*-4**	-2189.20117841	**D-a**	-2380.95137168
***Z*-1b**	-2263.00542343	***E*-4a**	-2189.20351991	**D-b**	-2380.94970945
***Z*-1a- η^2**	-1802.48628907	***E*-4b**	-2189.20351991	**E**	-1920.15253890
***Z*-1b- η^2**	-1802.48628907	**5**	-1728.67811173	**F**	-1920.1439109
2	-1802.19828623	***E*-4b- η^2**	-1728.67968467		
3	-1802.19731409	**B**	-1728.38868246		

Table S4. Cartesian coordinates of all optimized structures.

Complex *E*-1

C	-1.6736410	-2.3092740	-0.9323450
C	-2.9063830	-1.7497520	-1.4836860
C	-2.5659430	-0.6380420	-2.2831300
C	-1.1018300	-0.5416490	-2.3336590
C	-0.5648820	-1.6191710	-1.5848560
C	-1.5728550	-3.6245770	-0.2141580
H	-0.6644860	-3.6841780	0.3896760
H	-1.5515570	-4.4559850	-0.9301890
H	-2.4237480	-3.7858220	0.4515000
C	-4.2670160	-2.3527560	-1.3082790
H	-4.3630120	-3.2237150	-1.9684830
H	-5.0645740	-1.6565950	-1.5726990
H	-4.4382190	-2.7073890	-0.2893510
C	-3.4846630	0.2597010	-3.0517120
H	-3.2612390	1.3100070	-2.8440660
H	-4.5327960	0.0804810	-2.8047860
H	-3.3616580	0.0933290	-4.1285190
C	-0.3643770	0.4499800	-3.1771810
H	0.7121760	0.4038690	-3.0078160
H	-0.6985620	1.4676770	-2.9576540
H	-0.5484170	0.2531170	-4.2403580
C	0.8592730	-2.0748260	-1.5661250
H	1.0098640	-2.8063300	-2.3702320
H	1.1149660	-2.5677840	-0.6260920
H	1.5600690	-1.2552590	-1.7268300
C	1.1721010	-0.1497480	1.1086470
Ir	-1.7008880	-0.2513230	-0.0811820
C	-0.2673230	-0.2398030	1.2796860
P	-3.3379040	-0.0366920	1.6008680
C	-3.7093130	-1.5367670	2.6006760
H	-4.4748710	-1.3100280	3.3490230
H	-2.8005900	-1.8755090	3.0995730
H	-4.0786320	-2.3390850	1.9577380
C	-4.9678890	0.4411880	0.8977110
H	-5.6899010	0.6059610	1.7031850
H	-5.3482150	-0.3398390	0.2384260
H	-4.8392960	1.3623760	0.3259040
C	-3.0583460	1.2863540	2.8456340
H	-3.9400600	1.3770190	3.4868620
H	-2.8909910	2.2252450	2.3151050
H	-2.1877380	1.0583120	3.4593840
H	1.7026020	-0.9347360	1.6450460
O	-0.6334860	-0.6179040	2.5184470
C	0.2872840	-0.6628540	3.6362760
H	-0.3430410	-0.6640060	4.5257720
H	0.9484480	0.2057550	3.6355710
H	0.8767580	-1.5832560	3.6089660
C	1.9847210	0.7497040	0.4588770
C	1.5484590	2.0881490	0.0049690
C	0.8084430	2.9242520	0.8574730
C	1.9850160	2.6032450	-1.2327350
C	0.5176120	4.2375030	0.4893140
H	0.5013370	2.5556380	1.8307020
C	1.6614790	3.9013210	-1.6130180
H	2.5827790	1.9802920	-1.8910120
C	0.9361900	4.7263980	-0.7465450
H	-0.0385560	4.8755670	1.1685830
Cl	-2.1201010	2.1412490	-0.4013390
H	1.9910210	4.2791340	-2.5760900
C	3.4343410	0.4472160	0.3496530
C	4.3981380	1.5008170	0.4324290
C	3.8964050	-0.8568690	0.2003110
C	5.7437290	1.2345290	0.3734470
H	4.0579660	2.5204620	0.5687730
C	5.2763260	-1.1599910	0.1211900
H	3.1905200	-1.6770370	0.1141290
C	6.2283210	-0.0915220	0.2119960
H	6.4602530	2.0471480	0.4554660
H	0.7069280	5.7478940	-1.0340700
C	7.6123570	-0.3951330	0.1380130
C	5.7481200	-2.4919070	-0.0470560
C	7.0969660	-2.7534590	-0.1144220
C	8.0367250	-1.6959080	-0.0208710
H	5.0259630	-3.3011280	-0.1186490
H	8.3327250	0.4150150	0.2082540
H	9.0980220	-1.9177920	-0.0765500
H	7.4490730	-3.7726500	-0.2401570

Complex *Z*-1a

C	-2.7156930	-1.4684920	-1.2546730
C	-3.2442290	-0.1875360	-1.7216410
C	-2.1987670	0.5130640	-2.3592680
C	-1.0148120	-0.3555260	-2.3902670
C	-1.3687360	-1.5962710	-1.8028010
C	-3.5441350	-2.6039750	-0.7243230
H	-2.9436720	-3.2901400	-0.1225040
H	-3.9840840	-3.1804680	-1.5478970
H	-4.3646080	-2.2470590	-0.0974180
C	-4.6807160	0.2300140	-1.6275350
H	-5.2511960	-0.2481570	-2.4334950
H	-4.8040200	1.3084910	-1.7387250
H	-5.1429400	-0.0781140	-0.6867920
C	-2.2540770	1.8644990	-2.9992760
H	-1.4347380	2.4955370	-2.6435140
H	-3.1941220	2.3780450	-2.7892440
H	-2.1615620	1.7688580	-4.0877230
C	0.2640340	0.0076450	-3.0787990
H	1.0396390	-0.7423870	-2.9141110
H	0.6358000	0.9698920	-2.7155810
H	0.1033230	0.0922830	-4.1603820
C	-0.5730890	-2.8619830	-1.8397330
H	-0.8774080	-3.4491060	-2.7154290
H	-0.7474100	-3.4820270	-0.9578440
H	0.4966460	-2.6700030	-1.9244540
C	0.7839350	-1.7730020	0.9874000
Ir	-1.4935820	0.0097330	-0.1227890
C	-0.4725580	-1.0703730	1.1816450
P	-2.7518910	0.9617220	1.6158330
C	-4.0677080	-0.0853920	2.3631350
H	-4.5561620	0.4510600	3.1822410
H	-3.6261820	-1.0077190	2.7414800
H	-4.8219330	-0.3370990	1.6138840
C	-3.6485540	2.4745170	1.0804470
H	-4.1407250	2.9397370	1.9399600
H	-4.4055540	2.2304660	0.3334840
H	-2.9274490	3.1700120	0.6471550
C	-1.7780700	1.5665290	3.0513300
H	-2.4333910	2.1037940	3.7430500
H	-1.0015220	2.2376410	2.6802490
H	-1.3130850	0.7298680	3.5726140
H	0.7195560	-2.8277130	1.2516890
O	-1.1353910	-1.4384040	2.2923400
C	-0.5381230	-2.2579900	3.3277400
H	-1.1578060	-2.1009650	4.2106210
H	0.4926520	-1.9552340	3.5216320
H	-0.5712120	-3.3132950	3.0438790
C	2.0248170	-1.3442990	0.5796780
C	3.0744990	-2.3573050	0.2970390
C	2.7487800	-3.6353510	-0.2032530
C	4.4311020	-2.0772620	0.5603380
C	3.7356120	-4.5872260	-0.4391010
H	1.7170880	-3.8781020	-0.4318030
C	5.4170640	-3.0348890	0.3318170
H	4.7088820	-1.1121790	0.9671100
C	5.0752260	-4.2908720	-0.1713240
H	3.4624990	-5.5590820	-0.8387710
Cl	-0.3273680	2.1631210	-0.0984400
H	6.4536370	-2.7999820	0.5526600
C	2.4372600	0.0756820	0.5783390
C	2.1894730	0.8890900	1.7230150
C	3.1770630	0.6048730	-0.4719870
C	2.6787090	2.1705580	1.7954420
H	1.6489050	0.4655030	2.5631580
C	3.6534270	1.9368820	-0.4449860
H	3.3986530	-0.0090180	-1.3405520
C	3.4112020	2.7378760	0.7199540
H	2.5085890	2.7694060	2.6859660
H	5.8449360	-5.0343830	-0.3541290
C	3.9185890	4.0632420	0.7595920
C	4.3901510	2.4959870	-1.5263500
C	4.8647180	3.7851420	-1.4575870
C	4.6263930	4.5754470	-0.3044810
H	4.5750060	1.8862580	-2.4068490
H	3.7365930	4.6692300	1.6428750
H	5.0073180	5.5914140	-0.2649500
H	5.4268700	4.2038450	-2.2866570

Complex *Z*-1b

C	-2.9092450	-1.7735950	-0.2445000
C	-3.4755200	-0.7630450	-1.1389700
C	-2.5488270	-0.5270250	-2.1767070
C	-1.4194180	-1.4511920	-2.0061830
C	-1.6995540	-2.2755600	-0.8855640
C	-3.6548980	-2.4692820	0.8584320
H	-2.9727550	-2.8661480	1.6141090
H	-4.2409860	-3.3084440	0.4628730
H	-4.3484190	-1.7927220	1.3631160
C	-4.8504260	-0.1802200	-1.0099940
H	-5.5878380	-0.8968360	-1.3922890
H	-4.9617050	0.7392780	-1.5871080
H	-5.1185130	0.0275030	0.0287280
C	-2.6776640	0.4245660	-3.3244620
H	-1.7791270	1.0408850	-3.4185800
H	-3.5339190	1.0914520	-3.2080380
H	-2.8097510	-0.1311430	-4.2604780
C	-0.2792240	-1.5613530	-2.9708100
H	0.5025580	-2.2251570	-2.5972180
H	0.1660830	-0.5788900	-3.1500820
H	-0.6257420	-1.9581320	-3.9327220
C	-0.9688740	-3.5160910	-0.4804000
H	-1.4809160	-4.3864060	-0.9097220
H	-0.9541840	-3.6516470	0.6033520
H	0.0569930	-3.5219950	-0.8486590
C	1.0468700	-1.4237740	1.1908150
Ir	-1.4444850	-0.1057500	-0.0948110
C	-0.1727520	-0.6439890	1.3212820
P	-2.3147490	1.5820280	1.2935830
C	-3.4716590	1.0625190	2.6290760
H	-3.7848040	1.9338000	3.2126320
H	-2.9748440	0.3449310	3.2833730
H	-4.3615630	0.5929910	2.2032440
C	-3.2701360	2.8298040	0.3415780
H	-3.6180560	3.6264460	1.0060410
H	-4.1335580	2.3641590	-0.1358580
H	-2.6181710	3.2469480	-0.4283370
C	-1.0616020	2.6066450	2.1616110
H	-1.5527800	3.4415400	2.6697980
H	-0.3544790	2.9876220	1.4223220
H	-0.5300100	2.0017880	2.8968340
H	1.0473250	-2.3161420	1.8161550
O	-0.6266970	-0.5413340	2.5813270
C	0.1537390	-0.9554540	3.7307470
H	-0.3051610	-0.4566500	4.5843110
H	1.1982470	-0.6559660	3.6244780
H	0.0875140	-2.0385380	3.8639350
C	2.1966840	-1.2057370	0.4703750
C	3.2100140	-2.2876870	0.3802840
C	2.8372710	-3.6469520	0.3787260
C	4.5841450	-1.9779030	0.3300180
C	3.7958940	-4.6541140	0.3205180
H	1.7873980	-3.9170130	0.4044020
C	5.5430110	-2.9872190	0.2797640
H	4.9007020	-0.9413550	0.3513920
C	5.1539180	-4.3277500	0.2713010
H	3.4849970	-5.6943080	0.3066570
Cl	-0.2650100	1.7426680	-1.1792640
H	6.5961690	-2.7254550	0.2518590
C	2.5629340	0.1142230	-0.0772200
C	3.1441950	0.2362580	-1.3766260
C	2.4600560	1.2456870	0.7192970
C	3.5632180	1.4560930	-1.8436900
H	3.2399080	-0.6476350	-1.9987500
C	2.9194650	2.5114800	0.2781330
H	2.0750960	1.1573230	1.7310680
C	3.4754540	2.6252430	-1.0366580
H	3.9833430	1.5409880	-2.8421250
H	5.9018680	-5.1133660	0.2263630
C	3.9331710	3.8917050	-1.4807380
C	2.8567910	3.6661710	1.1035410
C	3.3093550	4.8828530	0.6435260
C	3.8501080	4.9963010	-0.6602370
H	2.4490330	3.5747100	2.1071850
H	4.3531140	3.9785800	-2.4789760
H	4.2049500	5.9607940	-1.0103360
H	3.2583120	5.7602310	1.2810420

Complex *Z*-1a- η²

C	-3.1481190	-1.2754700	-0.1815120
C	-3.4590180	0.1449190	-0.3812860
C	-2.8390920	0.5694220	-1.5775510
C	-2.1786270	-0.5942610	-2.1829180
C	-2.4328370	-1.7308660	-1.3671660
C	-3.8125250	-2.1812600	0.8099050
H	-3.1273220	-2.9507380	1.1680060
H	-4.6656400	-2.6827300	0.3361690
H	-4.1962520	-1.6350070	1.6723140
C	-4.4336770	0.9438730	0.4282760
H	-5.4482650	0.7296580	0.0686670
H	-4.2763110	2.0188150	0.3215230
H	-4.4169910	0.6896600	1.4892220
C	-3.0382940	1.8985710	-2.2454530
H	-2.2786600	2.1026070	-3.0028160
H	-3.0484260	2.7241740	-1.5305140
H	-4.0049830	1.9053260	-2.7644630
C	-1.5447810	-0.6041880	-3.5408350
H	-0.8800500	-1.4594390	-3.6784340
H	-0.9796700	0.3090740	-3.7455180
H	-2.3256360	-0.6718040	-4.3083520
C	-2.1318650	-3.1586830	-1.7020380
H	-2.9953340	-3.5963970	-2.2177990
H	-1.9524940	-3.7529180	-0.8052660
H	-1.2703400	-3.2556350	-2.3658910
C	2.0180400	0.3372450	-0.3895920
C	2.4061900	-1.0579790	-0.1441870
C	0.8357590	0.6219310	-1.1713310
C	1.4529110	-1.9981190	0.2241540
C	3.8194750	-1.4319720	-0.2359550
Ir	-1.1541840	-0.2857440	-0.0916030
C	0.0726250	-1.7743350	0.4991020
C	4.3610350	-2.4830520	0.5412700
C	4.6681070	-0.7673650	-1.1532540
C	5.6911610	-2.8554050	0.4006510
C	5.9940130	-1.1585680	-1.3040350
C	6.5094400	-2.2001570	-0.5276970
P	-0.9926770	0.6867790	2.0658330
C	-2.0390450	-0.1918100	3.2948330
H	-1.8943580	0.2427480	4.2882880
H	-1.7605060	-1.2476320	3.3173860
H	-3.0941390	-0.1162880	3.0306250
C	-1.5211270	2.4431520	2.1654380
H	-1.4665900	2.7920840	3.2010550
H	-2.5478960	2.5482350	1.8115420
H	-0.8694780	3.0614660	1.5442650
C	0.6498110	0.6823080	2.8908240
H	0.5382020	1.0348370	3.9203360
H	1.3432670	1.3384040	2.3648980
H	1.0620990	-0.3291930	2.9055810
C	0.4141990	1.9511430	-1.3030060
H	1.8228290	-3.0063620	0.3697150
O	-0.5816430	-2.7399800	1.1447520
C	0.0386060	-3.9725200	1.6088980
H	-0.7473160	-4.4901310	2.1562590
H	0.8765140	-3.7544080	2.2743560
H	0.3647870	-4.5824220	0.7631770
H	6.0986920	-3.6485930	1.0188150
C	1.0889690	3.0208560	-0.6609720
C	2.2968730	2.7308470	0.0606330
C	2.7320560	1.3776680	0.1690780
H	6.6255220	-0.6560670	-2.0293130
H	3.6314050	1.1674940	0.7400190
H	-0.3896940	2.1914810	-1.9883810
H	4.2714270	0.0266770	-1.7761860
H	3.7507710	-2.9738060	1.2922810
H	7.5470800	-2.4983960	-0.6399220
C	0.6582290	4.3676960	-0.7831350
C	3.0200240	3.7980990	0.6447840
C	2.5720600	5.0991180	0.5132020
H	3.1372470	5.9122770	0.9574660
C	1.3867750	5.3868600	-0.2040600
H	1.0585950	6.4162500	-0.3046430
H	3.9351350	3.5857410	1.1896270
H	-0.2421660	4.5891590	-1.3491230
H	0.5863520	-0.0839700	-1.9574600

Complex *Z*-1b- η²

C	-1.1634760	-1.4327060	-2.1603910
C	-2.3856870	-1.4554520	-1.3629600
C	-2.9125290	-0.0787520	-1.3367650
C	-1.9600760	0.7623550	-1.9448100
C	-0.8825450	-0.0810960	-2.4819520
C	-0.4359590	-2.6462780	-2.6526460
H	0.6160700	-2.4413600	-2.8594600
H	-0.8948210	-2.9901980	-3.5877560
H	-0.4986160	-3.4706480	-1.9395740
C	-3.1639750	-2.7032560	-1.0723400
H	-3.5501450	-3.1192550	-2.0111670
H	-4.0223040	-2.5163670	-0.4265870
H	-2.5392730	-3.4660530	-0.6023880
C	-4.2894850	0.3072460	-0.8933850
H	-4.3550800	1.3604260	-0.6153380
H	-4.6525200	-0.3008860	-0.0624820
H	-4.9842760	0.1473370	-1.7277360
C	-2.0870130	2.2328420	-2.1984370
H	-1.1314360	2.7479630	-2.0806660
H	-2.8095220	2.7014810	-1.5283580
H	-2.4289600	2.4057540	-3.2264740
C	0.1609040	0.3941730	-3.4381170
H	-0.2808570	0.4346820	-4.4425490
H	1.0190140	-0.2785960	-3.4867210
H	0.5139160	1.3974460	-3.2003930
C	1.7153540	-1.7575350	0.6393550
Ir	-0.9242380	-0.4221990	-0.1077250
C	0.3000710	-1.8416200	0.5806150
P	-1.9728690	-0.3439990	2.0295490
C	-3.0908730	-1.7681710	2.3463340
H	-3.4812500	-1.7046360	3.3661780
H	-2.5446740	-2.7040980	2.2228690

Complex 2

C	-3.3616210	-1.0533260	-1.3541470
C	-3.7249610	0.3410590	-1.1129610
C	-2.7548410	1.1725510	-1.7313220
C	-1.7374290	0.3137220	-2.3171070
C	-2.1720970	-1.0572270	-2.1351370
C	-4.2230920	-2.2490570	-1.0636150
H	-3.6239940	-3.1414090	-0.8680620
H	-4.8755490	-2.4706450	-1.9178340
H	-4.8728050	-2.0859440	-0.2007420
C	-5.0154470	0.7933840	-0.4928520
H	-5.8118090	0.8062150	-1.2475410
H	-4.9420140	1.8026320	-0.0817260
H	-5.3454070	0.1224380	0.3045580
C	-2.8172770	2.6620530	-1.8926350
H	-1.8310920	3.1231190	-1.8072380
H	-3.4703050	3.1288250	-1.1516240
H	-3.2165510	2.9122500	-2.8835070
C	-0.6245400	0.7762110	-3.2132450
H	0.2104630	0.0717160	-3.2165830
H	-0.2377720	1.7478490	-2.8976060
H	-0.9762850	0.8788330	-4.2475530
C	-1.5245180	-2.2664280	-2.7405850
H	-1.9941550	-2.4947420	-3.7051480
H	-1.6330190	-3.1448230	-2.1013130
H	-0.4602250	-2.1055570	-2.9266120
C	1.0915590	1.4064080	0.4920210
C	1.8387030	0.1962360	0.1765840
C	-0.3371320	1.4483180	0.4880210
C	1.2721590	-1.0696870	0.1190400
C	3.2999860	0.2651900	-0.0798500
Ir	-1.5886300	-0.0841090	-0.0809520
C	-0.1073870	-1.3561140	0.1919490

Complex 3

C	-3.3533090	-0.6196930	-0.9877350
C	-3.1946440	0.8267500	-1.0675570
C	-2.0862350	1.1158180	-1.9087890
C	-1.5063600	-0.1479270	-2.3321360
C	-2.3432900	-1.2054840	-1.8082040
C	-4.5103030	-1.3507880	-0.3683120
H	-4.2052350	-2.3233300	0.0251780
H	-5.3027630	-1.5254730	-1.1072240
H	-4.9574280	-0.7851110	0.4523090
C	-4.1647780	1.8282930	-0.5108980
H	-4.9968520	1.9710560	-1.2117480
H	-3.7028880	2.8057320	-0.3539590
H	-4.6010930	1.4990460	0.4357440
C	-1.6790580	2.4633210	-2.4263290
H	-0.5978300	2.5405480	-2.5560320
H	-1.9974580	3.2726700	-1.7647300
H	-2.1425620	2.6419710	-3.4048310
C	-0.4262830	-0.2995380	-3.3646900
H	0.0742710	-1.2674160	-3.2864340
H	0.3343330	0.4779180	-3.2621040
H	-0.8447560	-0.2240780	-4.3762370
C	-2.2304280	-2.6620910	-2.1464240
H	-2.8691680	-2.8919900	-3.0079440
H	-2.5537250	-3.2931260	-1.3162780
H	-1.2087660	-2.9415340	-2.4141990
C	1.9070210	0.1967950	0.0792470
C	2.0576530	-1.2482220	0.1563270
C	0.6114020	0.8452320	0.0363130
C	1.0205280	-2.1275970	0.4301690
C	3.3934340	-1.8771670	-0.0359570
Ir	-1.2144210	-0.1228510	-0.0673250
C	-0.3484860	-1.7914320	0.5200820

Complex A

C	-2.5868340	-1.6730350	-1.2061920
C	-2.7348460	-0.2722300	-1.5998480
C	-1.5550810	0.1192500	-2.2826500
C	-0.6307600	-1.0026590	-2.2716680
C	-1.3286970	-2.1307000	-1.6780650
C	-3.6851830	-2.5260390	-0.6383930
H	-3.2927640	-3.3829150	-0.0859770
H	-4.3184340	-2.9178940	-1.4445890
H	-4.3383050	-1.9600740	0.0312750
C	-4.0186780	0.5016780	-1.5128430
H	-4.6908100	0.2047090	-2.3278770
H	-3.8589120	1.5778550	-1.6040800
H	-4.5534070	0.3153970	-0.5774740
C	-1.3155100	1.4044570	-3.0166140
H	-0.2824570	1.7440520	-2.9134070
H	-1.9653640	2.2084790	-2.6700280
H	-1.5089160	1.2544230	-4.0862690
C	0.6545320	-1.0660820	-3.0460680
H	1.3316990	-1.8226460	-2.6435780
H	1.1775830	-0.1073810	-3.0199040
H	0.4653930	-1.3139230	-4.0980830
C	-0.8394260	-3.5478400	-1.6598210
H	-1.1890820	-4.0699550	-2.5589750
H	-1.2084150	-4.0948340	-0.7903610
H	0.2517050	-3.6006520	-1.6581780
C	1.8133720	1.0859500	0.2113570
C	2.5272830	-0.1774640	0.2872790
C	0.3967040	1.1813540	0.1374270
C	1.9413440	-1.3973990	0.5988510
Ir	-0.8410670	-0.4706210	-0.0750120
C	0.5593590	-1.6179560	0.7065040
P	-1.7554760	-0.1863380	2.0897080

H -3.9313900 -1.7558940 1.6515990
C -3.0426910 1.1159040 2.3579240
H -3.4072730 1.0753090 3.3888870
H -3.9016770 1.1112950 1.6862740
H -2.4879090 2.0425130 2.2068860
C -0.8649810 -0.4010510 3.5039440
H -1.4764750 -0.5172100 4.4033860
H -0.2820290 0.5157620 3.6111910
H -0.1804320 -1.2495980 3.4365100
H 2.2742060 -2.6116210 1.0031870
O -0.2904750 -2.9720230 0.9532700
C 0.4429560 -4.1513760 1.3971280
H -0.3241570 -4.8948370 1.6055260
H 1.0084060 -3.9327140 2.3056210
H 1.1046870 -4.5088410 0.6055230
C 2.4483280 -0.6452180 0.2596110
C 1.8078960 0.6565580 -0.0517610
C 2.2901840 1.4236880 -1.1510440
C 0.9005050 1.2521940 0.8536860
C 1.8990330 2.7311760 -1.3210460
H 2.9906660 0.9717320 -1.8438690
C 0.5595280 2.6439340 0.7357130
H 0.7666890 0.7816970 1.8192220
C 1.0407180 3.3848650 -0.3922310
H 2.2915150 3.3037250 -2.1576730
C 0.7260490 4.7633170 -0.5107350
C -0.1525180 3.3380350 1.7445700
C -0.4310480 4.6844020 1.6136070
C -0.0054580 5.3995700 0.4698630
H -0.4505860 2.8116820 2.6458780
H 1.0913090 5.3158760 -1.3715170
H -0.2328400 6.4568830 0.3818500
H -0.9655410 5.2059260 2.4014100
C 3.9090490 -0.7244370 0.1974220
C 4.7117090 0.4047190 0.4887720
C 4.5531730 -1.9461860 -0.1153090
C 6.0981990 0.3056220 0.4899620
H 4.2460920 1.3469960 0.7553830
C 5.9386330 -2.0316190 -0.1367800
H 3.9629240 -2.8140250 -0.3910210
C 6.7151080 -0.9086980 0.1736590
H 6.7005000 1.1727970 0.7398960
H 6.4185690 -2.9678110 -0.4023490
H 7.7981910 -0.9800210 0.1635320

C 4.1786640 -0.6031050 0.5525100
C 3.8172510 1.1904340 -1.0386660
C 5.5700280 -0.5817660 0.2830830
C 5.1569130 1.2127310 -1.3399670
C 6.0738400 0.3411590 -0.6913450
P -2.2219290 -0.3668930 2.1598570
C -3.1421350 -1.9242610 2.5032240
H -3.3064290 -2.0465180 3.5782300
H -2.5689550 -2.7715100 2.1211550
H -4.1103410 -1.9062640 1.9980770
C -3.3046240 0.9325550 2.8888390
H -3.5822850 0.6600840 3.9115730
H -4.2124720 1.0492720 2.2929750
H -2.7710920 1.8849430 2.9074150
C -0.8197800 -0.4369730 3.3483340
H -1.1892880 -0.5338290 4.3731710
H -0.2251410 0.4746080 3.2608030
H -0.1815880 -1.2928010 3.1170610
C -0.9303400 2.6755700 0.8500520
H 1.9626280 -1.8876020 -0.0568840
O -0.4921860 -2.6398200 0.2966900
C 0.4571080 -3.7246940 0.4076990
H -0.1453970 -4.6150960 0.5835480
H 1.1398020 -3.5637940 1.2462550
H 1.0232960 -3.8417040 -0.5204300
C -0.1918060 3.8002330 1.2117790
C 1.2049090 3.7391420 1.2437660
C 1.8287910 2.5570590 0.8884690
H 5.5329230 1.9058860 -2.0874510
H 2.9092140 2.4987110 0.9379900
H -2.0126230 2.7556860 0.8429470
H -0.7055890 4.7196160 1.4802050
H 1.7920850 4.5982100 1.5513970
H 3.1346360 1.8613010 -1.5495970
H 3.8080130 -1.2968780 1.3025890
C 6.4801740 -1.4501110 0.9458500
C 7.4648340 0.3548350 -0.9715520
C 8.3202280 -0.5024810 -0.3152770
C 7.8241440 -1.4118970 0.6518710
H 6.0980060 -2.1457970 1.6881770
H 8.5121290 -2.0791310 1.1617930
H 9.3830450 -0.4836040 -0.5359970
H 7.8452680 1.0534460 -1.7115220

C 3.8956540 -2.7961240 0.9025510
C 4.1458440 -1.6195600 -1.1975100
C 5.1202290 -3.4280920 0.6935400
C 5.3587230 -2.2708670 -1.4139980
C 5.8521410 -3.1718640 -0.4677450
P -1.5726380 0.4510060 2.1742710
C -2.9583150 -0.4561040 2.9781480
H -3.0169530 -0.2092540 4.0426370
H -2.8005940 -1.5301460 2.8592120
H -3.9043960 -0.1916850 2.5005730
C -1.9622620 2.2172140 2.5186530
H -2.1555770 2.3577120 3.5864820
H -2.8426930 2.5301080 1.9542130
H -1.1146540 2.8397580 2.2253910
C -0.1554320 0.1313990 3.3035060
H -0.4083410 0.4299070 4.3249040
H 0.7150570 0.6977480 2.9663990
H 0.0965910 -0.9313460 3.2942700
C 0.6123060 2.2320620 0.0141320
H 1.3020140 -3.1715930 0.5145510
O -1.2119390 -2.7441010 0.9127530
C -0.7875720 -4.0738950 1.2905110
H -1.6915910 -4.5733020 1.6370800
H -0.0507790 -4.0360120 2.0971130
H -0.3772330 -4.6109720 0.4310040
H 5.5036410 -4.1186880 1.4383430
C 1.7852540 3.0336910 0.0359350
C 3.0560220 2.3808770 0.1084800
C 3.0746220 0.9761700 0.1311410
H 5.9187280 -2.0744310 -2.3231120
H 4.0372650 0.4861360 0.2185140
H -0.3351050 2.7611960 -0.0266530
H 3.7651640 -0.9247940 -1.9394680
H 3.3371930 -2.9899190 1.8136330
H 6.8021180 -3.6702970 -0.6339190
C 1.7488550 4.4526930 0.0065460
C 4.2459310 3.1628040 0.1606390
C 4.1770920 4.5350950 0.1305660
H 5.0839010 5.1303030 0.1669920
C 2.9163070 5.1829330 0.0517770
H 2.8765300 6.2679440 0.0287950
H 5.2057670 2.6568230 0.2195260
H 0.7877900 4.9569510 -0.0519540

C -2.3996580 -1.7444230 2.8332490
H -2.7255660 -1.5657840 3.8623320
H -1.6216410 -2.5071260 2.8176810
H -3.2494460 -2.1079070 2.2508740
C -3.1850650 0.9529020 2.3441240
H -3.5421440 0.8552650 3.3738390
H -4.0025040 0.7000090 1.6644970
H -2.8869900 1.9864800 2.1649570
C -0.5419290 0.4135760 3.3356710
H -0.9961630 0.4531830 4.3298460
H -0.1974760 1.4109890 3.0545100
H 0.3219280 -0.2547070 3.3595480
C -0.1636470 2.5198530 0.1297340
H 2.6195650 -2.2348120 0.7219990
O 0.1293910 -2.7889310 1.2078380
C 1.0415410 -3.7867290 1.7173030
H 0.4086980 -4.5562320 2.1583120
H 1.7011630 -3.3625660 2.4789170
H 1.6336600 -4.2203530 0.9065510
C 0.6764590 3.6837730 0.2265660
C 2.0826350 3.5202140 0.3299160
C 2.6244710 2.2725640 0.3144350
H 3.6957350 2.1636610 0.4190860
C 0.1061770 4.9820980 0.2292410
C -1.5640660 2.7668310 0.0289950
C -1.2552040 5.1651880 0.1374680
C -2.0991400 4.0378860 0.0363950
H -3.1740080 4.1739170 -0.0427000
H -1.6775020 6.1653100 0.1389130
H -2.2254710 1.9182810 -0.0664670
H 0.7720970 5.8372670 0.3044920
H 2.7140260 4.3980040 0.4305320
C 4.0013880 -0.2236810 0.0769370
C 4.5698160 0.3092820 -1.0953520
C 4.8432190 -0.8681290 1.0006710
C 5.9358550 0.1859650 -1.3397340
H 3.9333660 0.8051700 -1.8215550
C 6.2133430 -0.9683650 0.7644920
H 4.4254510 -1.2627770 1.9222220
C 6.7623520 -0.4483530 -0.4091110
H 6.3557490 0.5875890 -2.2568230
H 6.8520690 -1.4503700 1.4982170
H 7.8283090 -0.5332300 -0.5962190

Complex *Z*-4

C -2.2681580 -1.9083690 1.3910660
C -3.1904210 -2.1222680 0.2730170
C -2.4245980 -2.3830050 -0.8842600
C -1.0083810 -2.4297140 -0.4980080
C -0.9346340 -2.2375980 0.9088310
C -2.6637130 -1.8379570 2.8380450
H -1.9071110 -1.3274710 3.4382330
H -2.7899080 -2.8469190 3.2509680
H -3.6089290 -1.3085030 2.9744480
C -4.6827320 -2.1876910 0.3986420
H -4.9684750 -3.1656190 0.8054580
H -5.1819220 -2.0797350 -0.5657640
H -5.0795350 -1.4327310 1.0813880
C -2.9187920 -2.6490000 -2.2723000
H -2.3982270 -2.0164680 -2.9966070
H -3.9892300 -2.4578660 -2.3669160
H -2.7389890 -3.6959450 -2.5436360
C 0.0996060 -2.7948450 -1.4377540
H 1.0840310 -2.5829450 -1.0158730
H 0.0081800 -2.2378320 -2.3739550
H 0.0593780 -3.8647150 -1.6763470
C 0.2563660 -2.4538710 1.7926710
H 0.1582300 -3.4311970 2.2815230
H 0.3312270 -1.7055780 2.5859130
H 1.1949040 -2.4684780 1.2356330
C 1.0519010 0.6083900 0.4204290
Ir -1.7531450 -0.2649510 -0.0307660
C -0.3549640 0.8773410 0.7505670
P -3.3775100 1.4204490 0.1685980
C -4.1614310 1.6012270 1.8235180
H -4.8913810 2.4163620 1.8099440
H -3.3892970 1.8206600 2.5637050
H -4.6724190 0.6803480 2.1124570
C -4.7782830 1.1464000 -0.9893740
H -5.4942890 1.9705440 -0.9166710
H -5.2918270 0.2111920 -0.7638340
H -4.3790190 1.0977930 -2.0050800
C -2.8642470 3.1329490 -0.2486280
H -3.7393590 3.7888760 -0.2222920
H -2.4330280 3.1400090 -1.2509960
H -2.1243170 3.4938000 0.4655260
H 1.2607280 -0.4463500 0.5804470
O -0.6599030 1.7416280 1.6987370
C 0.3153360 2.3776920 2.5742310
H -0.0805050 2.2624450 3.5837550
H 0.3731700 3.4354640 2.3169680
H 1.2907810 1.9053800 2.4729830
C 2.0804340 1.2973470 -0.1396020
C 2.0941640 2.7198420 -0.7245990
Cl -1.3728980 0.5796310 -2.3123350
C 3.3443150 0.4861120 -0.2785900
C 3.4792830 -0.4402880 -1.3536970
C 4.3606590 0.5841260 0.6534290
C 4.6070160 -1.2201440 -1.4726560
H 2.6846530 -0.5144990 -2.0897540
C 5.5379590 -0.2062540 0.5563720
H 4.2701470 1.2687600 1.4926700
C 5.6668070 -1.1295690 -0.5309500
H 4.7000920 -1.9175290 -2.3011100
C 6.8435500 -1.9195250 -0.6285800
C 6.5892550 -0.1124960 1.5077960
C 7.7174350 -0.8918590 1.3853330
C 7.8461290 -1.8030610 0.3077250
H 6.4916490 0.5886780 2.3325620
H 6.9407050 -2.6162990 -1.4568120
H 8.7427290 -2.4094780 0.2234200
H 8.5169480 -0.8096390 2.1153540
C 2.6210250 2.6431600 -2.1821070
H 3.6305400 2.2304640 -2.2311410

Complex *E*-4a

C 3.1009430 1.1868700 -0.1760130
C 3.5023720 0.0378470 -0.9867420
C 2.6168360 -0.0573790 -2.0801170
C 1.7054280 1.0938780 -2.0333310
C 2.0701310 1.8992030 -0.9262260
C 3.9144750 1.7675430 0.9453050
H 3.3045850 2.3846870 1.6086590
H 4.7204190 2.3994960 0.5512720
H 4.3761360 0.9858840 1.5524500
C 4.7221100 -0.7948050 -0.7323100
H 5.6127500 -0.2350970 -1.0437430
H 4.7113490 -1.7268640 -1.2995160
H 4.8518480 -1.0333670 0.3261420
C 2.6174370 -1.0700720 -3.1820720
H 1.6180230 -1.4926800 -3.3193680
H 3.3083610 -1.8914360 -2.9830330
H 2.9194370 -0.6005720 -4.1258440
C 0.7007940 1.3988630 -3.0997800
H 0.0736390 2.2511590 -2.8331280
H 0.0529700 0.5367480 -3.2804530
H 1.2104410 1.6407140 -4.0404850
C 1.5998270 3.2910610 -0.6402240
H 2.2301260 4.0001290 -1.1914490
H 1.6799230 3.5424130 0.4190680
H 0.5674240 3.4489310 -0.9530460
C -0.7000230 1.8487050 1.1451350
Ir 1.3097870 -0.1376780 -0.0601420
C 0.1613700 0.6666910 1.3039570
P 1.7081170 -2.0063210 1.3101860
C 2.8648730 -1.7685460 2.7218850
H 2.9701650 -2.7007230 3.2853120
H 2.4773210 -0.9894890 3.3798000
H 3.8513080 -1.4669140 2.3616100
C 2.4393830 -3.3963840 0.3570300
H 2.5717590 -4.2664980 1.0071340
H 3.4081500 -3.1130120 -0.0557740
H 1.7606880 -3.6477750 -0.4604640
C 0.2225880 -2.7817430 2.0631020
H 0.5077170 -3.7174130 2.5529620
H -0.5026310 -2.9838680 1.2729650
H -0.2226450 -2.1102720 2.7964970
H -0.3435160 2.6851230 1.7439800
O 0.3418100 0.2943110 2.5751910
C -0.3806710 0.8927050 3.6830630
H -0.2710300 0.1903750 4.5089520
H -1.4328770 1.0353940 3.4341260
H 0.0750300 1.8492290 3.9506840
C -1.8585810 2.0076760 0.4593880
C -2.6027920 3.3686340 0.4729390
Cl -0.2383290 -1.6480120 -1.2003820
C -2.5524780 0.8327920 -0.1468600
C -2.8855000 0.7571320 -1.5318530
C -2.9666560 -0.1939100 0.6873920
C -3.6064220 -0.3025670 -2.0268290
H -2.5342110 1.5217930 -2.2133030
C -3.7253180 -1.2937890 0.2093920
H -2.7541140 -0.1441390 1.7521370
C -4.0580510 -1.3504440 -1.1812430
H -3.8349440 -0.3520210 -3.0880640
C -4.8201500 -2.4461750 -1.6636670
C -4.1750230 -2.3327610 1.0676270
C -4.9138800 -3.3831540 0.5701020
C -5.2380580 -3.4411520 -0.8076310
H -3.9326570 -2.2841960 2.1264220
H -5.0699130 -2.4876730 -2.7203150
H -5.8221430 -4.2745690 -1.1857640
H -5.2556900 -4.1711870 1.2343450
C -4.0177960 3.1547490 1.0661820
H -4.5569930 4.1069700 1.0846540

Complex *E*-4b

C 2.8271220 0.9508190 -1.3253330
C 3.1647720 -0.4510470 -1.5654830
C 2.0536850 -1.0717390 -2.1728930
C 1.0333760 -0.0447070 -2.4201880
C 1.5491870 1.2017720 -1.9860350
C 3.8102290 2.0081510 -0.9114590
H 3.3116080 2.8807320 -0.4837120
H 4.3933320 2.3502990 -1.7758710
H 4.5161250 1.6324000 -0.1680590
C 4.5124510 -1.0572980 -1.3141690
H 5.2000850 -0.7505440 -2.1121000
H 4.4799220 -2.1478970 -1.3164030
H 4.9533600 -0.7242590 -0.3714590
C 1.9179770 -2.4975760 -2.6068130
H 0.9734640 -2.9209750 -2.2538540
H 2.7308860 -3.1195390 -2.2277530
H 1.9305740 -2.5618580 -3.7015230
C -0.2408440 -0.3038840 -3.1600870
H -0.8913410 0.5724070 -3.1619590
H -0.7856640 -1.1386690 -2.7104720
H -0.0249220 -0.5633710 -4.2036570
C 0.9720160 2.5539300 -2.2688160
H 1.3121790 2.8885660 -3.2567720
H 1.3013370 3.2992860 -1.5423770
H -0.1184690 2.5431610 -2.2749400
C -0.5883580 2.1930280 0.5409160
Ir 1.3207420 -0.1360540 -0.0822660
C 0.4271470 1.2276240 0.9956160
P 2.3112000 -1.0721850 1.8361450
C 3.7289740 -0.1471000 2.5558160
H 4.1189160 -0.6725600 3.4328320
H 3.3998180 0.8513410 2.8471440
H 4.5304030 -0.0525690 1.8194840
C 2.9866200 -2.7484540 1.4994490
H 3.3358610 -3.2008110 2.4325450
H 3.8216290 -2.7030990 0.7992460
H 2.1890160 -3.3600510 1.0727960
C 1.1956240 -1.3899390 3.2610430
H 1.7325020 -1.9657690 4.0206190
H 0.3349300 -1.9592720 2.9060280
H 0.8527030 -0.4511340 3.6937140
H -0.2021790 3.2108870 0.5709230
O 0.9184750 1.4976380 2.2075480
C 0.3805300 2.5358580 3.0686780
H 0.7592480 2.3048780 4.0639450
H -0.7097790 2.5267920 3.0586340
H 0.7522510 3.5130290 2.7509360
C -1.8889390 2.0238100 0.2029500
C -2.7692430 3.2476540 -0.1621720
Cl -0.2351280 -2.0107060 0.1333380
C -2.5749450 0.7043320 0.3698670
C -2.7373850 0.1861130 1.6887540
C -3.1178840 -0.0037380 -0.6883000
C -3.4281550 -0.9811150 1.9151300
H -2.3358820 0.7438920 2.5297220
C -3.8239240 -1.2179960 -0.4895570
H -2.9929100 0.3482840 -1.7062820
C -3.9932080 -1.7171920 0.8416740
H -3.5540230 -1.3510140 2.9292730
C -4.7161790 -2.9235860 1.0394560
C -4.3801750 -1.9493690 -1.5741640
C -5.0744710 -3.1163390 -1.3504830
C -5.2445030 -3.6077740 -0.0317930
H -4.2544110 -1.5692490 -2.5848050
H -4.8452480 -3.2987020 2.0511030
H -5.7960940 -4.5290350 0.1289530
H -5.4988950 -3.6657700 -2.1853360
C -3.9073890 3.3619880 0.8832840
H -4.5488330 4.2135470 0.6358450

Complex 5

C 1.9088780 -0.5796940 -2.0369370
C 2.7248910 -0.8536690 -0.8655360
C 2.1573320 -2.0396480 -0.2098090
C 0.9623850 -2.3852460 -0.8780800
C 0.8088490 -1.4858420 -2.0236360
C 2.2713380 0.3704430 -3.1357720
H 1.3993510 0.6995340 -3.7040210
H 2.9493180 -0.1330160 -3.8361860
H 2.7942840 1.2484260 -2.7536220
C 4.1181530 -0.3321460 -0.6770320
H 4.7814190 -0.7974710 -1.4167180
H 4.5213690 -0.5665930 0.3082540
H 4.1669080 0.7482470 -0.8229040
C 2.8390470 -2.8543380 0.8455150
H 2.1354000 -3.4567610 1.4226890
H 3.4382040 -2.2527000 1.5313360
H 3.5308670 -3.5503660 0.3536710
C 0.1209210 -3.5956200 -0.6161300
H -0.9141770 -3.4508660 -0.9261550
H 0.1209610 -3.8766470 0.4383160
H 0.5178960 -4.4463440 -1.1844810
C -0.1560620 -1.6926190 -3.1436630
H 0.2790160 -2.4148400 -3.8470270
H -0.3546800 -0.7737600 -3.6975700
H -1.1039590 -2.1058300 -2.8010590
C -0.2561690 2.7585890 -0.2495930
Ir 0.7932640 -0.0912560 -0.0885240
C 0.8802680 1.8800640 -0.3404770
P 1.3142740 0.3286180 2.2114160
C 3.0744000 0.7867670 2.4756900
H 3.2113180 1.1321120 3.5045120
H 3.3609720 1.5825700 1.7854620
H 3.7266960 -0.0712830 2.3112550
C 1.0319870 -1.0541670 3.3893430
H 1.3069350 -0.7315810 4.3981410
H 1.6377750 -1.9205980 3.1221720
H -0.0180290 -1.3489340 3.3852140
C 0.4486300 1.7421270 3.0197130
H 0.7891530 1.8095300 4.0569930
H -0.6361470 1.6228070 3.0252220
H 0.6924290 2.6771590 2.5117640
H -0.1016570 3.8275520 -0.1692000
O 2.0729160 2.4028140 -0.5377160
C 2.2905860 3.8204540 -0.8313360
H 3.3464060 3.8918570 -1.0847050
H 2.0779440 4.4243250 0.0530710
H 1.6740930 4.1309930 -1.6761220
C -1.5161190 2.2499110 -0.2191700
C -2.7580580 3.1381650 -0.0364600
C -1.7120510 0.7712240 -0.3913520
C -2.3407910 0.3207940 -1.6021730
C -1.6607500 -0.1063350 0.7154770
C -2.9850060 -0.8855760 -1.6471540
H -2.3434250 0.9723190 -2.4676600
C -2.3419900 -1.3815820 0.6744680
H -1.4674850 0.3055060 1.6969900
C -3.0259410 -1.7644110 -0.5195710
H -3.5078250 -1.1800960 -2.5535490
C -3.7588290 -2.9753200 -0.5471000
C -2.4499820 -2.2103600 1.8127360
C -3.1769070 -3.3876280 1.7645960
C -3.8287980 -3.7776990 0.5764440
H -1.9862090 -1.9047060 2.7457720
H -4.2797180 -3.2579610 -1.4574390
H -4.4005470 -4.6996430 0.5530190
H -3.2610280 -4.0078740 2.6513370
C -3.7610740 2.4570840 0.9270200
H -4.6401510 3.0978030 1.0344990
H -4.1035300 1.4876280 0.5566670

H 1.9633520 2.0318120 -2.8075620
H 2.6469050 3.6517020 -2.6065120
C 3.0555720 3.6169390 0.0953210
H 3.0660130 4.6223820 -0.3370510
H 2.7405050 3.7090130 1.1404630
H 4.0790980 3.2365320 0.0784870
C 0.7043080 3.3723940 -0.7766040
H -0.0044120 2.7416340 -1.3198300
H 0.3032130 3.5932540 0.2147110
H 0.7736840 4.3279950 -1.3052140

H -4.6016220 2.4453570 0.4757630
H -3.9663690 2.7793340 2.0938610
C -1.8819880 4.4343080 1.3229830
H -1.7923620 4.1360150 2.3729940
H -0.8834140 4.6699770 0.9397750
H -2.4610970 5.3616690 1.3026630
C -2.7530780 3.9372940 -0.9614260
H -3.4108400 3.3272500 -1.5813050
H -3.1957550 4.9365850 -0.9044630
H -1.7855660 4.0338520 -1.4665100

H -4.5289120 2.4642090 0.9053900
H -3.5086860 3.5255140 1.8904010
C -1.9850640 4.5745230 -0.1672960
H -1.5716120 4.8167720 0.8175460
H -1.1699600 4.5743670 -0.8987360
H -2.6607600 5.3907180 -0.4374830
C -3.4085840 3.0720240 -1.5624070
H -4.1009470 2.2299720 -1.5962760
H -3.9775570 3.9733060 -1.8104610
H -2.6515520 2.9349440 -2.3427100

H -3.3341900 2.3189490 1.9260070
C -2.3793220 4.5202860 0.5378810
H -1.8278180 4.4378830 1.4799050
H -1.7912750 5.1184300 -0.1650710
H -3.2936660 5.0833620 0.7408840
C -3.4542020 3.3623520 -1.4102210
H -3.9009060 2.4486800 -1.8056030
H -4.2619480 4.0865440 -1.2705740
H -2.7628070 3.7724190 -2.1527550

Complex *E*-4b- η²

C 3.1896000 0.1641260 -0.1112390
C 2.9624850 -1.2006280 -0.6042820
C 2.2310560 -1.1177440 -1.8102230
C 2.0428260 0.3036670 -2.1306290
C 2.6923050 1.0786250 -1.1310360
C 4.1440040 0.5532400 0.9766210
H 3.8087020 1.4483360 1.5030960
H 5.1269900 0.7702470 0.5402540
H 4.2833640 -0.2426790 1.7085180
C 3.5726900 -2.4441040 -0.0337530
H 4.5875460 -2.5557020 -0.4364310
H 3.0169640 -3.3416690 -0.3115640
H 3.6679520 -2.4118610 1.0527700
C 1.9174210 -2.2580730 -2.7329610
H 1.0951740 -2.0284250 -3.4138580
H 1.6761960 -3.1757410 -2.1921330
H 2.7924580 -2.4702580 -3.3601510
C 1.4690290 0.8212610 -3.4147330
H 1.1295600 1.8555250 -3.3271050
H 0.6365530 0.2125230 -3.7768240
H 2.2401290 0.7979430 -4.1947720
C 2.9311410 2.5569370 -1.1589640
H 3.8843220 2.7570700 -1.6635690
H 3.0051770 2.9756130 -0.1537490
H 2.1536340 3.0920560 -1.7078320
C -2.1673370 0.6655900 -0.3164290
C -1.9530260 2.1079090 -0.0427670
C -1.2049550 0.0137370 -1.1796950
C -0.7511190 2.4942760 0.4893640
C -3.0344830 3.1391380 -0.4025590
Ir 0.9701700 -0.0398120 -0.0655450
C 0.3637400 1.6414140 0.8299710
P 0.5017070 -1.2584200 1.9179560
C 1.8173480 -1.0552090 3.1850550
H 1.5095230 -1.5382630 4.1170640
H 1.9858930 0.0078760 3.3666670
H 2.7523010 -1.5080870 2.8534290
C 0.3455920 -3.0755900 1.7027780
H 0.1676180 -3.5488930 2.6732920
H 1.2612800 -3.4874500 1.2751290
H -0.4894500 -3.3006820 1.0365210
C -1.0081280 -0.8070150 2.8636720
H -1.0205070 -1.3660990 3.8039960
H -1.9037710 -1.0531700 2.2946530
H -1.0122480 0.2612490 3.0914350
C -1.3240390 -1.3619730 -1.4279710
H -0.6301980 3.5446140 0.7244080
O 1.2099030 2.0993130 1.7391730
C 1.0245910 3.3495750 2.4739020
H 1.7980650 3.3365230 3.2395010
H 0.0348610 3.3809910 2.9320930
H 1.1731590 4.2037590 1.8098630
C -2.3409870 -2.1454730 -0.8308730
C -3.3050840 -1.4843420 0.0014590
C -3.1791850 -0.0812950 0.2422390
H -3.8949110 0.3776340 0.9133220
H -0.6835230 -1.8266210 -2.1688350
C -2.4768790 -3.5356700 -1.0901100
C -4.3580860 -2.2446680 0.5629580
C -4.4622660 -3.5973520 0.2970000
H -5.2808870 -4.1689920 0.7227050
C -3.5198970 -4.2473170 -0.5352760
H -3.6284850 -5.3069820 -0.7418530
H -5.0931730 -1.7529190 1.1933300
H -1.7609060 -4.0273670 -1.7428180
H -0.7153740 0.6310960 -1.9254980
C -2.5560870 4.5889750 -0.1887140
H -2.3720930 4.8153280 0.8669350
H -1.6541180 4.8198180 -0.7645700
H -3.3371380 5.2738230 -0.5276420
C -3.3707630 2.9478260 -1.9080840
H -3.7536300 1.9458370 -2.1178290
H -4.1418760 3.6679920 -2.1956260
H -2.4962240 3.1293390 -2.5416740
C -4.3296060 2.9352380 0.4289720
H -4.8665810 2.0259200 0.1547910
H -4.1281840 2.9251710 1.5049550
H -5.0034600 3.7724510 0.2276920

Complex B

C 3.1966500 -0.6602340 -0.9378750
C 2.3273940 -1.8006030 -1.2344840
C 1.2848340 -1.3544200 -2.0855600
C 1.4375060 0.0784510 -2.2728900
C 2.6736590 0.4716490 -1.6168360
C 4.5311190 -0.7386860 -0.2535960
H 4.7953470 0.2033000 0.2321970
H 5.3212610 -0.9662800 -0.9805720
H 4.5592580 -1.5279830 0.5014780
C 2.6329450 -3.2279070 -0.8801470
H 3.2928890 -3.6728670 -1.6355280
H 1.7307100 -3.8423170 -0.8348850
H 3.1491190 -3.3113520 0.0796080
C 0.2625580 -2.2048350 -2.7770290
H -0.7142930 -1.7186730 -2.8158670
H 0.1350610 -3.1733210 -2.2891040
H 0.5809580 -2.3969260 -3.8093000
C 0.6488700 0.9119250 -3.2421150
H 0.6679470 1.9702510 -2.9714100
H -0.3967630 0.5972250 -3.2775170
H 1.0571900 0.8222000 -4.2566710
C 3.3225760 1.8202280 -1.7125090
H 4.0294250 1.8358410 -2.5511600
H 3.8767690 2.0668160 -0.8048090
H 2.5902830 2.6110720 -1.8910280
C -2.0103130 0.6769650 0.0260910
C -1.6395840 2.0983090 0.0670270
C -1.0157160 -0.3836790 0.0225000
C -0.3604750 2.4988200 0.4090180
C -2.6595260 3.2402820 -0.2340350
Ir 1.0358050 -0.1478210 -0.0497430
C 0.7823320 1.6809930 0.5989420
P 1.1502250 -0.9051430 2.1730340
C 2.7338590 -0.5276050 3.0337520
H 2.6794770 -0.8200440 4.0868490
H 2.9333290 0.5431610 2.9597950
H 3.5576890 -1.0652810 2.5595240
C 0.9388510 -2.7118290 2.4663350
H 1.0350780 -2.9268670 3.5348320
H 1.6943500 -3.2820950 1.9218780
H -0.0511120 -3.0249930 2.1292080
C -0.1142490 -0.1765940 3.2945510
H -0.0115360 -0.5848320 4.3040620
H -1.1111490 -0.4021160 2.9110700
H 0.0066280 0.9083230 3.3357600
C -1.4773590 -1.6928840 -0.0027140
H -0.2020040 3.5602820 0.5241660
O 1.8746110 2.2438260 1.1396070
C 1.9091870 3.6137960 1.6032170
H 2.8812570 3.7264170 2.0819040
H 1.1125220 3.8038290 2.3269110
H 1.8321740 4.3108680 0.7642960
C -2.8455690 -2.0633430 -0.0102440
C -3.8195810 -1.0200050 0.0215800
C -3.3657410 0.3105830 0.0324960
H -4.1311800 1.0692230 0.0661480
H -0.7542980 -2.5035520 -0.0273550
C -3.2861300 -3.4130840 -0.0382540
C -5.2049440 -1.3546230 0.0350940
C -5.6014700 -2.6700840 0.0088750
H -6.6565800 -2.9243160 0.0159520
C -4.6315200 -3.7068940 -0.0291670
H -4.9600980 -4.7417120 -0.0510390
H -5.9410470 -0.5554690 0.0611310
H -2.5485570 -4.2109310 -0.0674650
C -3.6556460 3.4296470 0.9453420
H -4.3220390 4.2680470 0.7197920
H -4.2789170 2.5616660 1.1581170
H -3.1124650 3.6754240 1.8635020
C -3.3884420 2.9841840 -1.5832710
H -3.9734340 2.0674830 -1.6163330
H -4.0651460 3.8192360 -1.7880290
H -2.6625650 2.9398860 -2.4019250
C -1.9695730 4.6176470 -0.4130970
H -1.5330160 5.0016900 0.5141080
H -1.1954490 4.5957520 -1.1861620
H -2.7233370 5.3456390 -0.7242860

Complex C

C -2.5554070 -1.4836130 -1.0758240
C -2.5522590 -0.1108240 -1.5820410
C -1.3438800 0.0929360 -2.2937860
C -0.5517150 -1.1227190 -2.1988650
C -1.3628630 -2.1150620 -1.5149570
C -3.7297330 -2.1637350 -0.4333500
H -3.4189330 -3.0117650 0.1811290
H -4.4162790 -2.5462250 -1.1993270
H -4.3052540 -1.4802130 0.1961450
C -3.7421160 0.8054060 -1.5556620
H -4.4362800 0.5384390 -2.3625760
H -3.4637230 1.8506170 -1.7051150
H -4.3016230 0.7327730 -0.6194390
C -0.9646010 1.2838610 -3.1221700
H 0.0970080 1.5228320 -3.0247260
H -1.5318670 2.1752110 -2.8523300
H -1.1600610 1.0697000 -4.1803950
C 0.6946020 -1.3997210 -2.9898690
H 1.2947550 -2.1910620 -2.5349080
H 1.3231850 -0.5096810 -3.0692900
H 0.4435580 -1.7199530 -4.0090450
C -1.0327640 -3.5721170 -1.3843400
H -1.4446850 -4.1229400 -2.2388530
H -1.4520520 -4.0062370 -0.4746910
H 0.0459130 -3.7442500 -1.3781170
C 2.1683340 0.8387010 0.1390400
C 2.7444110 -0.5097810 0.1738900
C 0.7691310 1.0891950 0.0608630
C 2.0007830 -1.6043090 0.5781580
Ir -0.6690130 -0.4087730 -0.0450420
C 0.6096560 -1.6290910 0.7967750
P -1.5324280 0.1444190 2.0913340
C -2.3030050 -1.2692130 2.9910850
H -2.6154570 -0.9493370 3.9897480
H -1.5908720 -2.0895820 3.0740490
H -3.1797500 -1.6249340 2.4445480
C -2.8620340 1.4151290 2.2293450
H -3.1995310 1.4705430 3.2686960
H -3.7128850 1.1438270 1.5999510
H -2.4919460 2.3930890 1.9208930
C -0.2653400 0.7544790 3.2784270
H -0.7187110 0.9585680 4.2527100
H 0.1883320 1.6687200 2.8904380
H 0.5195190 0.0037480 3.3985800
C 0.3493770 2.4801160 -0.0038420
H 2.5318310 -2.5338830 0.7231460
O 0.0818770 -2.6818550 1.4409600
C 0.8996960 -3.7179990 2.0303890
H 0.2097870 -4.3352040 2.6050990
H 1.6596560 -3.2912130 2.6898600
H 1.3724500 -4.3264800 1.2543120
C 1.2951820 3.5561260 0.1059710
C 2.6691220 3.2459080 0.2622830
C 3.0782140 1.9487140 0.2544430
H 4.1299670 1.7581470 0.3833400
C 0.8644050 4.9060790 0.0642870
C -1.0114530 2.8679870 -0.1749910
C -0.4652830 5.2259620 -0.0928480
C -1.4126850 4.1874780 -0.2170290
H -2.4628020 4.4292200 -0.3551970
H -0.7828230 6.2634720 -0.1281430
H -1.7534160 2.0925630 -0.2918160
H 1.6123910 5.6889130 0.1547800
H 3.3880890 4.0509610 0.3819050
C 4.2354660 -0.7965330 -0.1878820
C 5.1810430 -0.4705960 1.0035350
H 6.2026040 -0.7608080 0.7382970
H 5.2037810 0.5807070 1.2903140
H 4.8901300 -1.0460910 1.8882600
C 4.4732600 -2.2975840 -0.5046840
H 4.4102660 -2.9398440 0.3789530
H 3.7805360 -2.6741880 -1.2635090
H 5.4870550 -2.4131030 -0.8970990
C 4.6533830 -0.0475930 -1.4830330
H 4.5680930 1.0356090 -1.4285540
H 5.6958000 -0.2876030 -1.7130030
H 4.0440840 -0.3845130 -2.3284130

Complex D-a

C -2.7920890 -2.3057020 0.3822540
C -3.7306980 -1.5962320 -0.4827750
C -3.1034880 -1.3800550 -1.7304560
C -1.8086030 -2.0669680 -1.7134010
C -1.6521500 -2.6890800 -0.4489490
C -3.1383080 -2.9133360 1.7113250
H -2.2503430 -3.0716120 2.3274480
H -3.6251640 -3.8873100 1.5760570
H -3.8232440 -2.2782820 2.2772540
C -5.1532450 -1.2829720 -0.1315020
H -5.7621890 -2.1834130 -0.2804830
H -5.5743360 -0.5019710 -0.7666330
H -5.2749360 -0.9889900 0.9127620
C -3.6611730 -0.6855800 -2.9347550
H -2.9358710 0.0260670 -3.3390940
H -4.5771390 -0.1387680 -2.7021720
H -3.8978060 -1.4132340 -3.7202330
C -0.9306320 -2.1811270 -2.9195230
H -0.0341380 -2.7656880 -2.7160670
H -0.6304240 -1.1918340 -3.2792500
H -1.4783490 -2.6773660 -3.7294820
C -0.5837170 -3.6620640 -0.0515890
H -0.8706700 -4.6698490 -0.3766310
H -0.4521240 -3.7006090 1.0319440
H 0.3796520 -3.4267550 -0.5045120
C 1.1112420 -0.8971450 1.0203260
Ir -1.7385810 -0.3852400 -0.0509700
C -0.2510630 -0.3855430 1.2382580
P -2.7652990 1.4150230 1.0468080
C -3.6786370 1.0108840 2.5920820
H -4.1116220 1.9182840 3.0238710
H -2.9869850 0.5604970 3.3059960
H -4.4831210 0.3018270 2.3889480
C -3.9979650 2.2554300 -0.0233570
H -4.4364800 3.1074170 0.5048410
H -4.7935120 1.5648030 -0.3067370
H -3.4888130 2.6019500 -0.9251770
C -1.6596410 2.7879520 1.5505140
H -2.2564270 3.6178670 1.9407640
H -1.0877510 3.1198100 0.6828760
H -0.9744180 2.4457280 2.3273530
H 1.2864650 -1.8287350 1.5634830
O -0.5751940 -0.1873590 2.5187980
C 0.3910770 -0.3048770 3.5981050
H -0.0766240 0.1809950 4.4537660
H 1.3289630 0.1857490 3.3360900
H 0.5697480 -1.3587980 3.8245080
C 2.1775440 -0.4077320 0.3298080
C 3.4326820 -1.2453650 0.2611870
C 3.6375080 -2.1757970 -0.7748940
C 4.4362980 -1.0655770 1.2471960
C 4.8210280 -2.9281350 -0.7965040
C 5.5957800 -1.8375360 1.1844030
C 5.8115330 -2.7807510 0.1710170
H 4.9681100 -3.6428550 -1.6034600
Cl -0.9347050 1.2835900 -1.6501810
H 6.3574280 -1.6967420 1.9480320
C 2.2649410 0.9589820 -0.2274740
C 2.9561490 1.1896100 -1.4555030
C 1.7822800 2.0520840 0.4781750
C 3.0817040 2.4570910 -1.9640110
H 3.3726090 0.3483730 -1.9965520
C 1.9396010 3.3787740 0.0024780
H 1.3216450 1.9049740 1.4503920
C 2.5846180 3.5879010 -1.2591540
H 3.5865700 2.6136950 -2.9132440
C 2.7351170 4.9120150 -1.7448960
C 1.4981870 4.5094910 0.7428560
C 1.6606660 5.7835270 0.2456510
C 2.2792830 5.9862370 -1.0119540
H 1.0363230 4.3561700 1.7146980
H 3.2216730 5.0666600 -2.7039300
H 2.4012020 6.9956040 -1.3927360
H 1.3207630 6.6400620 0.8199340
C 2.6489690 -2.3789230 -1.9020630
H 2.3239980 -3.4251140 -1.9547770
H 1.7657320 -1.7477200 -1.8011020
H 3.1096660 -2.1496620 -2.8698290
C 4.2765530 -0.0786760 2.3824570
H 3.9410890 0.9017750 2.0318730
H 3.5482230 -0.4318430 3.1232250
H 5.2244130 0.0607750 2.9075550
C 7.0841880 -3.5913500 0.1292260
H 7.9581540 -2.9466240 -0.0176660
H 7.2405820 -4.1343070 1.0677060
H 7.0679780 -4.3217770 -0.6836820

Complex D-b

C -1.9069720 -0.3691280 -2.2633110
C -3.2315030 0.1671130 -1.9914870
C -3.0799810 1.4652070 -1.4340120
C -1.6595760 1.7990540 -1.4690560
C -0.9508030 0.7068460 -2.0374780
C -1.6331410 -1.6333560 -3.0249410
H -0.6352100 -2.0209990 -2.8097200
H -1.6931190 -1.4522710 -4.1057260
H -2.3555360 -2.4153410 -2.7790600
C -4.5081410 -0.5013720 -2.4038430
H -4.5948390 -0.4449550 -3.4961150
H -5.3888150 -0.0111670 -1.9875390
H -4.5371260 -1.5612910 -2.1400650
C -4.1541520 2.4265700 -1.0212410
H -3.9392420 2.8533390 -0.0372400

Complex E

C -3.4854440 -1.2368700 -0.9657930
C -3.7201900 0.1970700 -0.9103490
C -2.7631180 0.8520620 -1.7351250
C -1.8943780 -0.1667640 -2.2979680
C -2.3928390 -1.4524020 -1.8628190
C -4.3817310 -2.3008250 -0.3984690
H -3.8206390 -3.1996640 -0.1327850
H -5.1507810 -2.5921180 -1.1252390
H -4.9021500 -1.9582710 0.4992030
C -4.8992630 0.8427700 -0.2431530
H -5.7809440 0.7626960 -0.8913420
H -4.7340160 1.9054040 -0.0533770
H -5.1565250 0.3581820 0.7023340
C -2.7573860 2.3002160 -2.1266980
H -1.7450780 2.6694660 -2.3020760

Complex F

C -3.2183330 -1.5489580 -0.8487980
C -3.3455760 -0.1418050 -1.2263390
C -2.2803120 0.1720490 -2.1082000
C -1.4438120 -1.0068490 -2.2475400
C -2.0958790 -2.0890040 -1.5268190
C -4.2478080 -2.3242820 -0.0784330
H -3.8238530 -3.2238070 0.3731990
H -5.0608550 -2.6432250 -0.7429910
H -4.7024880 -1.7252470 0.7152490
C -4.5514610 0.7070140 -0.9425970
H -5.3710770 0.4268640 -1.6164430
H -4.3525780 1.7685200 -1.1003780
H -4.9224180 0.5782840 0.0777160
C -2.0918650 1.4374230 -2.8891260
H -1.0352430 1.6875380 -3.0050450

H	-5.1355840	1.9510260	-0.9783570
H	-4.2196000	3.2552180	-1.7362650
C	-1.0986160	3.1291320	-1.0829440
H	-0.0236970	3.0786700	-0.9077510
H	-1.5700590	3.5009560	-0.1706940
H	-1.2848710	3.8553650	-1.8844660
C	0.4544180	0.7448050	-2.5434740
H	0.4455330	1.0987630	-3.5828490
H	0.9156240	-0.2397950	-2.5371630
H	1.0827300	1.4218110	-1.9656590
C	0.8938990	-1.5388800	0.2431530
Ir	-1.9114320	-0.0617900	-0.0428470
C	-0.4949210	-1.2782450	0.6305160
P	-3.5550290	-1.2347750	1.2001900
C	-3.8901880	-2.9573060	0.6475860
H	-4.7089620	-3.3929050	1.2281450
H	-2.9910760	-3.5603560	0.7835100
H	-4.1618400	-2.9688800	-0.4097580
C	-5.1899010	-0.3969290	1.0958060
H	-5.9071120	-0.9042680	1.7478170
H	-5.5775910	-0.4045240	0.0782900
H	-5.0709970	0.6359180	1.4302270
C	-3.3788880	-1.3756810	3.0265490
H	-4.2812390	-1.8467900	3.4280000
H	-3.2660360	-0.3761750	3.4474600
H	-2.5087510	-1.9708390	3.2925690
H	1.0573210	-2.6114250	0.1393980
O	-0.9125800	-2.1824480	1.5338150
C	-0.0352800	-3.0909350	2.2465490
H	-0.6169970	-3.4274680	3.1049840
H	0.8707160	-2.5812040	2.5761230
H	0.2220510	-3.9501400	1.6215720
C	2.0557770	-0.8160420	0.1556280
C	3.3216240	-1.6048380	-0.0799260
C	3.5864890	-2.2943330	-1.2870050
C	4.2537940	-1.6960180	0.9881420
C	4.7735900	-3.0261760	-1.4091080
C	5.4163600	-2.4515240	0.8175800
C	5.7072920	-3.1169310	-0.3761020
H	4.9703590	-3.5424940	-2.3456070
Cl	-2.0039840	1.4777330	1.8745600
H	6.1129010	-2.5266010	1.6492440
C	2.2244660	0.6237480	0.4273240
C	1.3889860	1.3326510	1.3392670
C	3.2625980	1.3108780	-0.1977110
C	1.5897490	2.6690080	1.5859300
H	0.6010130	0.8136770	1.8693780
C	3.4784470	2.6927570	0.0186050
H	3.9245730	0.7823020	-0.8771250
C	2.6264100	3.3934380	0.9358830
H	0.9497190	3.1838850	2.2964580
C	2.8570170	4.7742280	1.1699110
C	4.5248640	3.4036580	-0.6335060
C	4.7196070	4.7431460	-0.3869830
C	3.8788740	5.4334610	0.5224210
H	5.1704310	2.8701120	-1.3259770
H	2.2154570	5.3030580	1.8693650
H	4.0466420	6.4900020	0.7081610
H	5.5214080	5.2781440	-0.8864260
C	4.0315140	-1.0308750	2.3305550
H	4.2428340	0.0424890	2.2915630
H	3.0015610	-1.1359660	2.6856290
H	4.6893750	-1.4703480	3.0841090
C	2.6732530	-2.2451630	-2.4931610
H	1.6234830	-2.4028240	-2.2344890
H	2.7465380	-1.2810030	-3.0095200
H	2.9544860	-3.0158980	-3.2146430
C	6.9899170	-3.8934590	-0.5438090
H	6.9009300	-4.6518160	-1.3264180
H	7.8156850	-3.2281750	-0.8241980
H	7.2797070	-4.3931640	0.3852770

H	-3.2195900	2.9351000	-1.3665550
H	-3.3246300	2.4396680	-3.0556880
C	-0.8583530	0.0707800	-3.3584800
H	-0.1223510	-0.7356030	-3.3914830
H	-0.3199500	1.0055200	-3.1863520
H	-1.3270390	0.1335100	-4.3486360
C	-1.9124740	-2.7858170	-2.3525090
H	-2.4761410	-3.0755970	-3.2476550
H	-2.0573180	-3.5660440	-1.6031140
H	-0.8549570	-2.7624950	-2.6254350
C	1.4749910	0.6767380	0.0249000
C	1.9311980	-0.6980260	0.1100720
C	0.0741880	1.0452890	0.0603820
C	1.1109290	-1.7904950	0.3299380
C	3.3980570	-1.0112120	-0.0013500
Ir	-1.5129760	-0.2811820	-0.0483390
C	-0.3020800	-1.7650690	0.4078470
C	4.1882600	-1.1455590	1.1595150
C	3.9692790	-1.2069260	-1.2779010
C	5.5423180	-1.4684870	1.0192790
C	5.3259260	-1.5320270	-1.3656700
C	6.1321620	-1.6708290	-0.2314130
P	-1.9021680	0.1008970	2.2291360
C	-2.9840180	-1.1505570	3.0379390
H	-3.0645120	-0.9559770	4.1118170
H	-2.5652580	-2.1464130	2.8774830
H	-3.9834790	-1.1226660	2.5979090
C	-2.7081040	1.7015430	2.6511000
H	-2.8782990	1.7647480	3.7302080
H	-3.6657040	1.7912970	2.1344450
H	-2.0608540	2.5257620	2.3441050
C	-0.4067740	0.1115830	3.2997250
H	-0.6857810	0.2939810	4.3415180
H	0.2728730	0.8969770	2.9641790
H	0.1096410	-0.8481300	3.2299570
C	-0.2080010	2.4030250	0.0803670
H	1.6217770	-2.7420370	0.4320160
O	-0.9395430	-2.9066870	0.7180690
C	-0.2436910	-4.1488610	0.9765410
H	-1.0260950	-4.8649240	1.2252830
H	0.4447020	-4.0450590	1.8192190
H	0.2968900	-4.4864400	0.0884190
H	6.1521450	-1.5601900	1.9148650
C	0.7787010	3.4254450	0.0253180
C	2.1569840	3.0454110	-0.0459090
C	2.4616860	1.6743940	-0.0395610
H	5.7640650	-1.6786310	-2.3501560
H	3.5051510	1.3784040	-0.0697280
H	-1.2427980	2.7313880	0.1224900
C	0.4538400	4.8073720	0.0320090
C	3.1624310	4.0533580	-0.1063920
C	2.8144180	5.3828170	-0.0992140
H	3.5802720	6.1503600	-0.1463940
C	1.4475550	5.7599560	-0.0290140
H	1.1866280	6.8141380	-0.0233220
H	4.2052510	3.7527130	-0.1593480
H	-0.5899230	5.1060370	0.0841910
C	3.1462610	-1.0779840	-2.5402850
H	2.3332860	-1.8133040	-2.5667060
H	2.6863440	-0.0876110	-2.6259040
H	3.7654320	-1.2369680	-3.4260660
C	3.6096550	-0.9330190	2.5411600
H	3.1130710	0.0397410	2.6273120
H	2.8652880	-1.6977080	2.7923750
H	4.3935110	-0.9757170	3.3008200
C	7.5883390	-2.0489900	-0.3563520
H	8.1636160	-1.7231910	0.5145290
H	7.7056360	-3.1365130	-0.4379380
H	8.0412600	-1.6074300	-1.2489110

H	-2.5873770	2.2904080	-2.4249280
H	-2.5123980	1.3090500	-3.8945620
C	-0.3376660	-1.1619430	-3.2521020
H	0.3281040	-1.9882200	-2.9939120
H	0.2694640	-0.2570280	-3.3211400
H	-0.7469390	-1.3663890	-4.2496700
C	-1.7218870	-3.5385760	-1.6070190
H	-2.2504510	-4.0051760	-2.4476910
H	-1.9904990	-4.0818350	-0.6996310
H	-0.6524880	-3.6758200	-1.7793050
C	1.4702450	1.0683020	-0.1019450
C	2.1990600	-0.1705940	0.0546950
C	0.0523010	1.1683230	-0.0147310
C	1.6380900	-1.4042050	0.3486620
Ir	-1.2259380	-0.4674960	-0.0502050
C	0.2630590	-1.6602860	0.4636470
P	-1.7415970	-0.2123760	2.2446580
C	-2.1752670	-1.7876670	3.0991870
H	-2.3136840	-1.6058950	4.1692550
H	-1.3856850	-2.5243560	2.9517280
H	-3.1032780	-2.1910150	2.6873770
C	-3.1491180	0.8680120	2.7516700
H	-3.2823110	0.7959670	3.8353280
H	-4.0740130	0.5491970	2.2655480
H	-2.9499800	1.9073090	2.4876940
C	-0.3530670	0.4479830	3.2535070
H	-0.6168980	0.4556150	4.3149780
H	-0.1214140	1.4650060	2.9303840
H	0.5348310	-0.1703060	3.1044360
C	-0.4943440	2.5140740	-0.0032160
H	2.3424890	-2.2135860	0.5065620
O	-0.1286900	-2.8805130	0.8692850
C	0.8097400	-3.9307280	1.1928510
H	0.1959760	-4.7713240	1.5148960
H	1.4774180	-3.6257050	2.0030970
H	1.3939050	-4.2170610	0.3141300
C	0.3501220	3.6688660	-0.1598220
C	1.7494030	3.4931660	-0.3310020
C	2.2826370	2.2436320	-0.2910980
H	3.3533430	2.1155850	-0.3898870
C	-0.2063100	4.9725000	-0.1383850
C	-1.8829880	2.7780880	0.1774190
C	-1.5559530	5.1721080	0.0489380
C	-2.4027780	4.0551760	0.2142550
H	-3.4685680	4.2027460	0.3640390
H	-1.9662900	6.1770100	0.0687430
H	-2.5494700	1.9362670	0.2827400
H	0.4616820	5.8196210	-0.2670720
H	2.3816730	4.3648330	-0.4713430
C	3.7034030	-0.1778930	-0.0182140
C	4.3452630	-0.3682070	-1.2607180
C	4.4651200	-0.0495320	1.1625020
C	5.7416850	-0.4279700	-1.2955770
C	5.8597650	-0.1127600	1.0756840
C	6.5204860	-0.3010760	-0.1412830
H	6.2331600	-0.5779970	-2.2540280
H	6.4443580	-0.0103600	1.9869270
C	3.8098330	0.1578910	2.5102940
H	3.0978890	0.9901160	2.4911920
H	3.2586820	-0.7328750	2.8356350
H	4.5580490	0.3766560	3.2756490
C	3.5562590	-0.5069560	-2.5430630
H	2.8886120	-1.3754970	-2.5165020
H	2.9303190	0.3734190	-2.7283950
H	4.2237850	-0.6266570	-3.3994330
C	8.0280650	-0.3375310	-0.2126250
H	8.4346800	0.6561550	-0.4371540
H	8.4662700	-0.6621690	0.7351780
H	8.3755980	-1.0144450	-0.9984950

References

[1] D. D. Perrin, W. L. F. Armarego, *Purification of Laboratory Chemicals*, 3rd ed., Butterworth/ Heinemann, London/Oxford, **1988**.

[2] M. Talavera, S. Bolaño, J. Bravo, J. Castro, S. García-Fontán, J. M. Hermida-Ramón, *Organometallics* **2013**, *32*, 4402-4408.

[3] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox *Gaussian 09, Revision D.01*, Gaussian, Inc: Wallingford CT, 2013.

[4] D. Geuenich, K. Hess, F. Köhler, R. Herges, *Chem. Rev.* **2005**, *105*, 3758-3772.