Supporting Information

Optical and Electrochemical Properties of Spirobifluorene Iridanaphthalene Complexes

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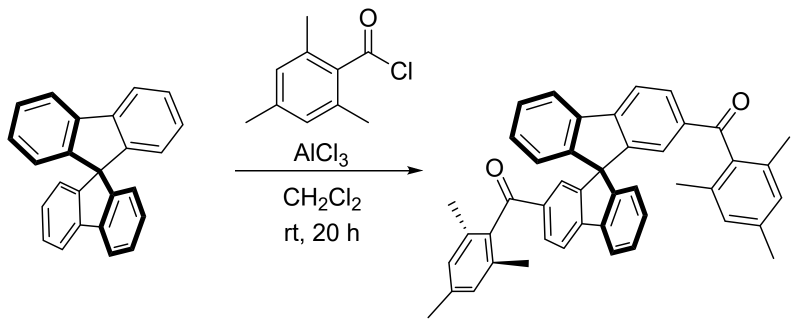
Experimental Section

General Procedures, Methods and Materials

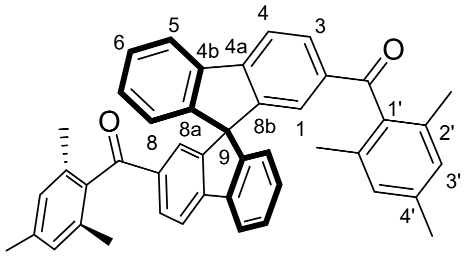
All experiments were carried out under an atmosphere of argon by Schlenk techniques. Solvents were dried by the usual procedures[1] and, prior to use, distilled under argon. All reagents were obtained from commercial sources. The starting material $[IrCp^*Cl(NCMe)(PMe_3)]PF_6$ was prepared as described in the literature.[2] Unless stated, NMR spectra were recorded in CD_2Cl_2 (organometallic complexes) or $CDCl_3$ (organic compounds) at room temperature on Bruker ARX–400 instrument, with resonating frequencies of 400 MHz (^1H), 161 MHz ($^{31}P\{^1H\}$), and 100 MHz ($^{13}C\{^1H\}$) using the solvent as the internal lock. ^1H and $^{13}C\{^1H\}$ signals are referred to internal TMS and those of $^{31}P\{^1H\}$ to 85% H_3PO_4; downfield shifts (expressed in ppm) are considered positive. ^1H and $^{13}C\{^1H\}$ NMR (or JMOD, J-modulated spin echo experiment) signal assignments were confirmed by $\{^1H,^1H\}$ COSY, $\{^1H,^1H\}$ NOESY, $\{^1H,^{13}C\}$ HSQC, $\{^1H,^{13}C\}$ HMBC and DEPT experiments. Coupling constants are given in hertz. Mass spectra are referred to the most abundant isotopes and they were acquired using an Apex–Qe or a SolariX XR spectrometer by high or low resolution electrospray technique. UV-Vis spectra were measured on a Jasco V-670 spectrophotometer while cyclic voltammetry experiments were measured on an Autolab potentiostat/galvanostat (PGSTAT100).

Synthesis of 2,2'-(2,4,6-trimethylbenzoyl)-9,9'-spirobifluorene (I)



I

To a solution of spirobifluorene (5 g, 15.8 mmol) in dicloroethane (100 mL), pulverized $AlCl_3$ (8.4 g, 63 mmol) and 2,4,6-trimethylbenzoyl chloride (10.5 mL, 63 mmol) were added and the mixture was refluxed under inert atmosphere for 24 h. After that, the reaction mixture was extracted three times with CH_2Cl_2 and the combined organic phases were washed once with H_2O and once with saturated NaCl. Then, it was dried over Na_2SO_4 and the solvent removed by evaporation under reduced pressure. The crude was purified by column chromatography (SiO_2, gradient hex/AcOEt from 90/10 to 85/15) affording the expected diketone as a white solid. Yield: 9.0 g (93%).



$C_{45}H_{36}O_2$ (608.76 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{45}H_{37}O_2$ [M+H]$^+$ 609.2788 found 609.2774. **^{1}H NMR**: δ 7.89 (d, $^3J_{HH}$ = 8.1 Hz, 1H, H^5); 7.82 (d, $^3J_{HH}$ = 8.0 Hz, 1H, H^4); 7.60 (d, $^3J_{HH}$ = 8.3 Hz, 1H, H^3); 7.49 (s, 1H, H^1); 7.41 (t, $^3J_{HH}$ = 7.5 Hz, 1H, H^6); 7.19 (t, $^3J_{HH}$ = 7.5 Hz, 1H, H^7); 6.85 (s, 2H, $H^{3'}$); 6.76 (d, $^3J_{HH}$ = 8.3 Hz, 1H, H^8); 2.31 (s, 3H, $C^{4'}CH_3$); 2.02 (s, 6H, $C^{2'}CH_3$) ppm. **^{13}C NMR**: δ 200.4 (s, *C*=O); 149.5 (s, C^{8a}); 148.9 (s, C^{8b}); 147.5 (s, C^{4a}); 140.6 (s, C^{4b}); 138.6 (s, $C^{4'}$); 137.0 (s, $C^{1'}$); 136.9 (s, C^2); 134.4 (s, 2C, $C^{2'}$); 131.7 (s, C^3); 129.6 (s, C^7); 128.5 (s, 2C, $C^{3'}$); 128.4 (s, C^6); 124.4 (s, C^8); 124.2 (s, C^1); 121.4 (s, C^5); 120.3 (s, C^4); 66.0 (s, C^9); 21.3 (s, $C^{4'}CH_3$); 19.6 (s, 2C, $C^{2'}CH_3$) ppm.

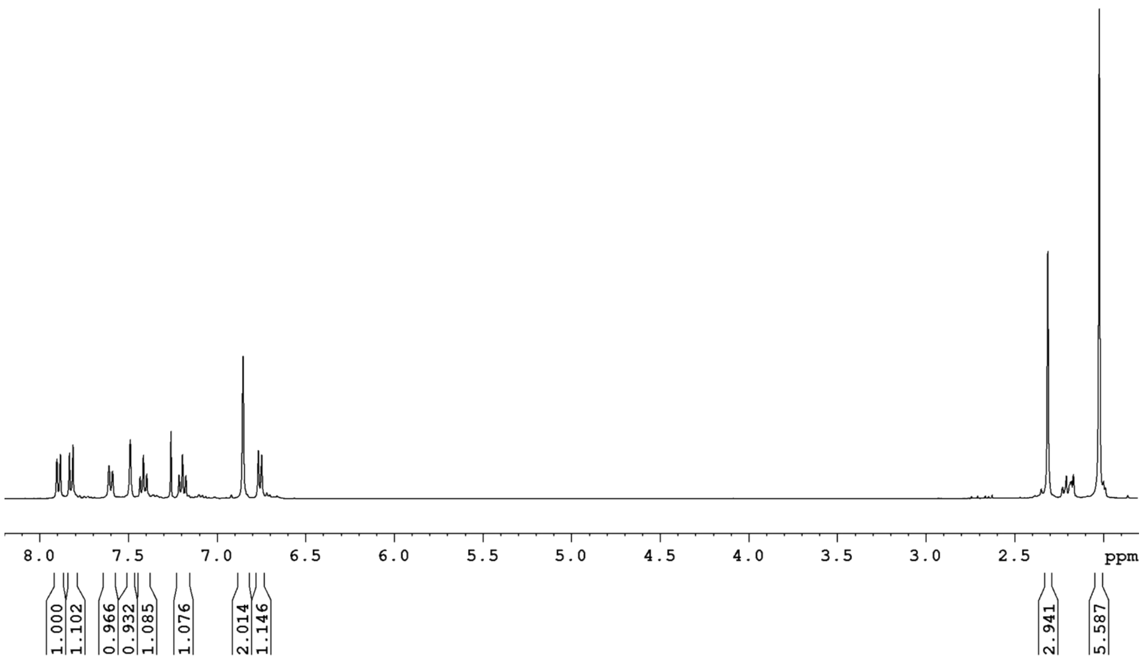


Figure S1. ^{1}H NMR spectrum of **I**.

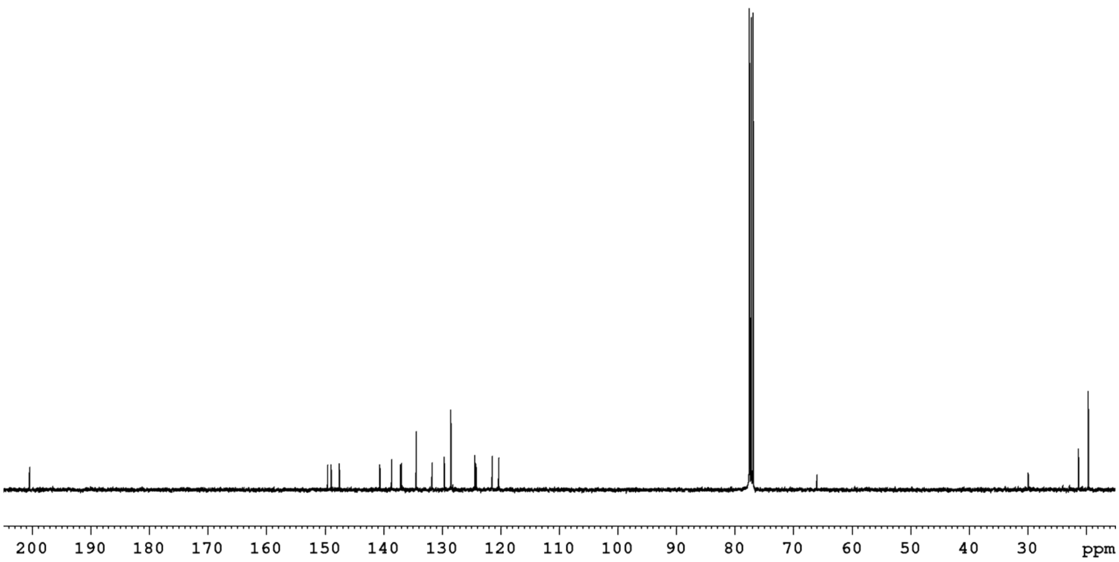


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **I**.

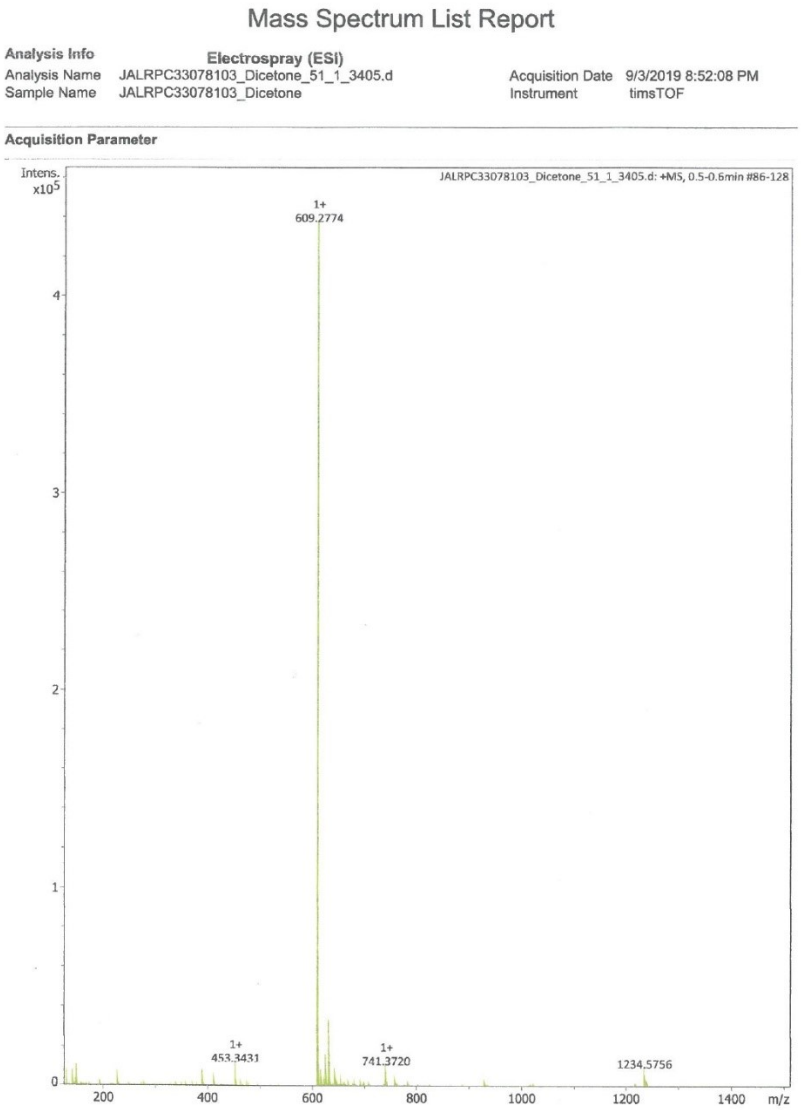
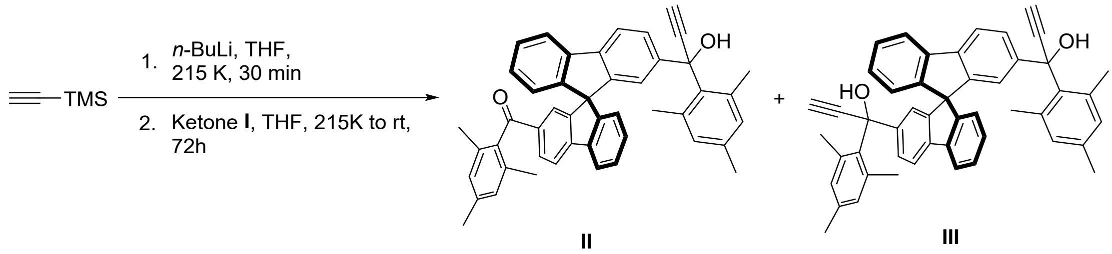
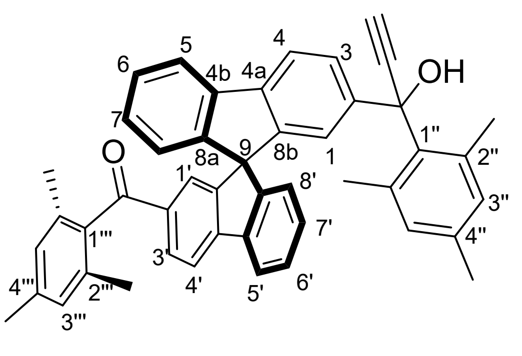


Figure S3. HR-ESI-MS spectrum of **I**.

Synthesis of 2-(1-hydroxy-1-mesitylprop-2-yn-1-yl)-2'-(2,4,6-trimethylbenzoyl)-9,9'-spirobifluorene (II) and 2,2'-(1-hydroxy-1-mesitylprop-2-yn-1-yl)-9,9'-spirobifluorene (III)



To a solution of trimethylsilylacetilene (2.2 mL, 21.3 mmol) in THF (15 mL) at –78 ºC, *n*-buthyllithium 1.6 M in hexanes (12 mL, 19.2 mmol) was added dropwise and the reaction mixture was stirred for 30 minutes. After that, a solution of the diketone **I** (1.3 g, 2.13 mmol) in THF (20 mL) was added via cannula and the mixture was allowed to warm up to room temperature and stirred for 72h. Then, MeOH (20 mL) and K_2CO_3 (2.9 g, 21.3 mmol) were added and the mixture was stirred again for 3 hours. The solution was filtrated through a pad of SiO_2, washed with AcOEt and concentrated under vacuum. The residue was purified and the two obtained products separated by a column chromatography (SiO_2, gradient hex/AcOEt from 85/15 to 0/100). Thus, a mixture of the two diastereoisomers (*R,M*)* and (*R,P*)* of the monopropargylic alcohol **II** and a second mixture with the three possible diastereoisomers (*R,M,R*)*, (*R,M,S*)* and (*R,P,R*)* of the dipropargylic alcohol **III** were obtained as white foams. Yield monoalcohol (**II**): 351 mg (26%). Yield dialcohol (**III**): 492 mg (35%).



$C_{47}H_{38}O_2$ (634.80 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{47}H_{38}O_2Na$ $[M+Na]^+$ 657.2770, found 657.2758; Calcd. for $C_{47}H_{37}O$ $[M-H_2O+H]^+$ 617.2844, found 617.2828. **^{1}H NMR**: δ 8.03 (d, $^3J_{HH}$ = 7.4 Hz, 1H, $H_B{}^{5'}$); 8.02 (d, $^3J_{HH}$ = 7.4 Hz, 1H, $H_A{}^{5'}$); 7.99 (d, $^3J_{HH}$ = 7.5 Hz, 2H, $H_A{}^{4'}$ + $H_{A/B}{}^{5}$); 7.97 (d, $^3J_{HH}$ = 7.8 Hz, 1H, $H_{A/B}{}^{5}$); 7.94 (d, $^3J_{HH}$ = 8.2 Hz, 2H, $H_{A/B}{}^{4}$ + $H_B{}^{4'}$); 7.90 (d, $^3J_{HH}$ = 8.0 Hz, 1H, $H_{A/B}{}^{4}$); 7.80 (d, $^3J_{HH}$ = 7.6 Hz, 1H, $H_A{}^{3'}$); 7.72 (d, $^3J_{HH}$

= 8.0 Hz, 1H, $H_B^{3'}$); 7.66 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.4 Hz, 1H, $H_{A/B}^3$); 7.62 (s, 1H, $H_B^{1'}$); 7.53 (s, 1H, $H_A^{1'}$); 7.54 (m, 2H, $H_{A+B}^{6'}$); 7.51 (m, 2H, H_{A+B}^6); 7.50 (dd, $^3J_{HH}$ = 8.0, $^4J_{HH}$ = 1.5 Hz, 1H, $H_{A/B}^3$); 7.337 (t, $^3J_{HH}$ = 7.2 Hz, 1H, $H_B^{7'}$); 7.332 (t, $^3J_{HH}$ = 7.2 Hz, 1H, $H_A^{7'}$); 7.261 (t, $^3J_{HH}$ =7.4 Hz, 1H, $H_{A/B}^7$); 7.26 (s, 1H, $H_{A/B}^1$); 7.258 (t, $^3J_{HH}$ = 7.4 Hz, 1H, $H_{A/B}^7$); 7.18 (s, 1H, $H_{A/B}^1$); 7.01 (s, 2H, $H_B^{3'''}$); 6.98 (s, 2H, $H_A^{3'''}$); 6.91 (d, $^3J_{HH}$ = 7.0 Hz, 2H, $H_{A+B}^{8'}$); 6.89 (s, 2H, $H_{A/B}^{3''}$); 6.87 (s, 2H, $H_{A/B}^{3''}$); 6.86 (d, $^3J_{HH}$ = 7.0 Hz, 1H, $H_{A/B}^8$); 6.83 (d, $^4J_{HH}$ = 7.6 Hz, 1H, $H_{A/B}^8$); 2.86 (s, 1H, ≡C$H_{A/B}$); 2.80 (s, 1H, ≡C$H_{A/B}$); 2.47 (s, 3H, C$^{4'''}$CH_3^B); 2.46 (s, 3H, C$^{4'''}$CH_3^A); 2.37 (s, 3H, C$^{4''}$C$H_3^{A/B}$); 2.35 (s, 3H, C$^{4''}$C$H_3^{A/B}$); 2.33 (s, 12H, C$^{2''}$CH_3^{A+B}); 2.18 (s, 6H, C$^{2'''}$CH_3^B); 2.14 (s, 6H, C$^{2'''}$CH_3^A) ppm. **^{13}C NMR**: δ 200.3 (s, CO^A); 200.2 (s, CO^B); 150.15 (s, $C_A^{8a'}$); 150.10 (s, $C_B^{8a'}$); 149.54 (s, $C_A^{2'}$); 149.52 (s, $C_B^{2'}$); 148.6 (s, $C_{A/B}^{8a}$); 148.5 (s, $C_{A/B}^{8a}$); 148.15 (s, $C_{A/B}^2$); 148.12 (s, $C_{A/B}^2$); 147.33 (s, $C_A^{4a'}$); 147.29 (s, $C_B^{4a'}$); 145.5 (s, $C_{A/B}^{8b}$); 145.3 (s, $C_{A/B}^{8b}$); 142.2 (s, $C_{A/B}^{4a}$); 142.0 (s, $C_{A/B}^{4a}$); 141.3 (s, $C_{A/B}^{4b}$); 141.2 (s, $C_{A/B}^{4b}$); 140.44 (s, $C_{A/B}^{4b'}$); 140.40 (s, $C_{A/B}^{4b'}$); 138.5 (s, 2C, $C_{A+B}^{4'''}$); 137.1 (s, 3C, $C_A^{8b'}$ + $C_{A+B}^{2''}$); 137.0 (s, 2C, $C_{A/B}^{1'''}$); 136.89 (s, $C_{A/B}^{4''}$); 136.87 (s, 2C, $C_B^{8b'}$+ $C_{A/B}^{2''}$); 136.8 (s, $C_{A/B}^{2''}$); 136.74 (s, $C_{A/B}^{1''}$); 136.70 (s, $C_{A/B}^{1''}$); 136.6 (s, $C_{A/B}^{4''}$); 134.32 (s, $C_{A/B}^{2''}$); 134.29 (s, $C_{A/B}^{2''}$); 131.7 (s, 2C, $C_{A/B}^{3''}$); 131.6 (s, 2C, $C_{A/B}^{3''}$); 131.2 (s, $C_B^{3'}$); 130.9 (s, $C_A^{3'}$); 129.45 (s, $C_B^{7'}$); 129.42 (s, $C_A^{7'}$); 128.5 (s, 4C, $C_A^{3'''}$+ $C_B^{3'''}$); 128.2 (s, 2C, C_{A+B}^7); 128.1 (s, 4C, C_{A+B}^6 + $C_{A+B}^{6'}$); 126.8 (s, $C_{A/B}^3$); 126.7 (s, $C_{A/B}^3$); 124.4 (s, $C_A^{1'}$); 124.3 (s, 2C, $C_{A+B}^{8'}$); 124.0 (s, 2C, $C_B^{1'}$ + $C_{A/B}^8$); 123.96 (s, $C_{A/B}^8$); 122.16 (s, $C_{A/B}^1$); 122.15 (s, $C_{A/B}^1$); 121.2 (s, 2C, $C_{A+B}^{5'}$); 120.5 (s, 3C, $C_{A/B}^4$ + $C_B^{4'}$ + $C_{A/B}^5$); 120.4 (s, $C_{A/B}^4$); 120.2 (s, $C_A^{4'}$ or $C_{A/B}^5$); 120.1 (s, $C_A^{4'}$ or $C_{A/B}^5$); 86.05 (s, ≡$C_{A/B}$); 86.02 (s, ≡$C_{A/B}$); 76.4 (s, $C_{A/B}$-OH); 76.3 (s, $C_{A/B}$-OH); 75.9 (s, ≡CH$_{A/B}$); 75.8 (s, ≡CH$_{A/B}$); 66.14 (s, $C_{A/B}^9$); 66.12 (s, $C_{A/B}^9$); 24.0 (s, C$^{2''}$$C_{A/B}H_3$); 23.9 (s, C$^{2''}$$C_{A/B}H_3$); 21.3 (s, 2C, C$^{4'''}$$C_{A+B}H_3$); 20.6 (s, 2C, C$^{4''}$$C_{A+B}H_3$); 19.6 (s, C$^{2'''}$$C_{A/B}H_3$); 19.5 (s, C$^{2'''}$$C_{A/B}H_3$) ppm.

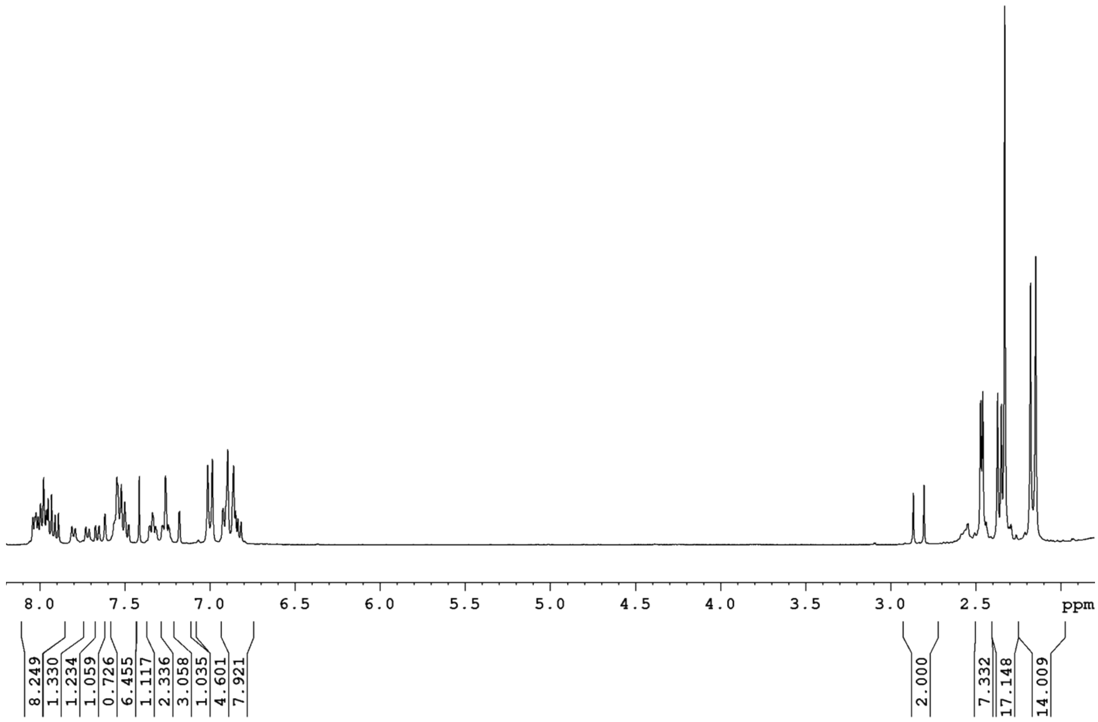


Figure S4. ^{1}H NMR spectrum of **II**.

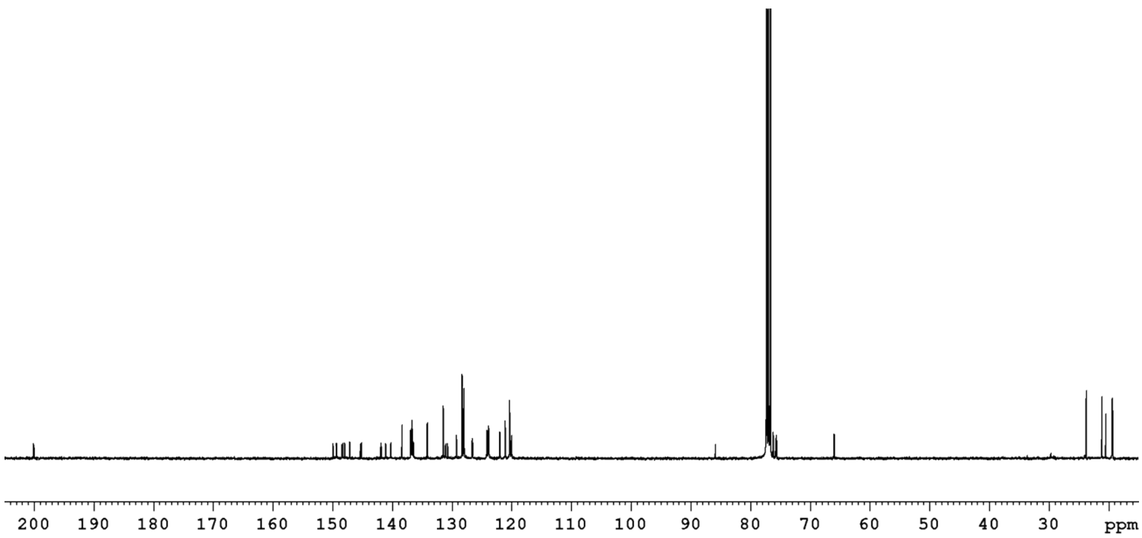


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **II**.

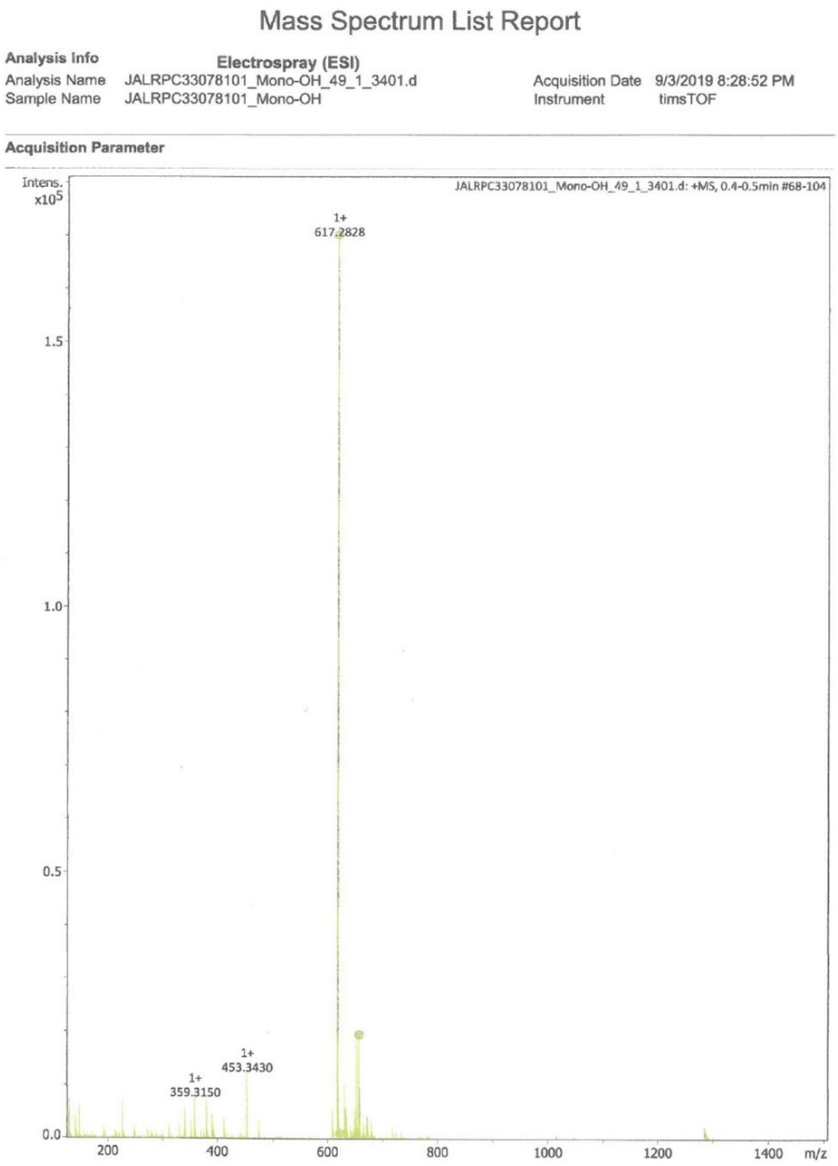


Figure S6. HR-ESI-MS spectrum of **II**.

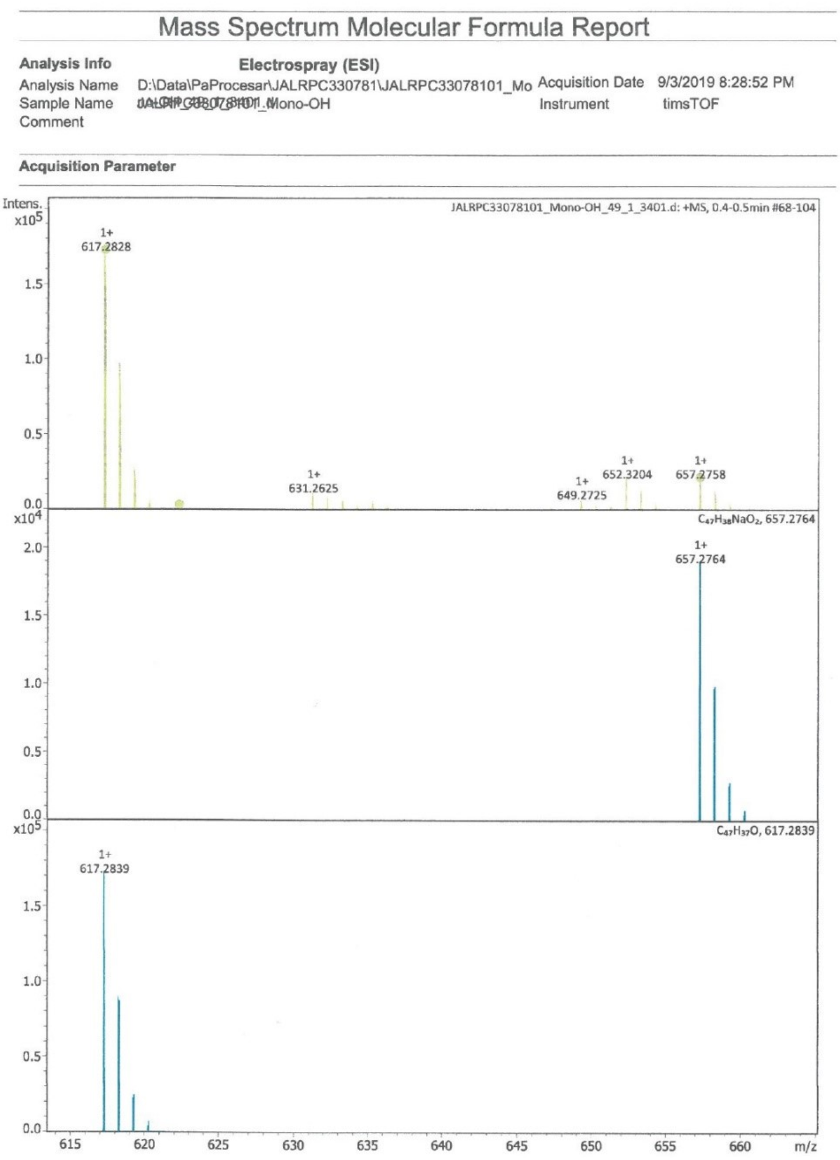
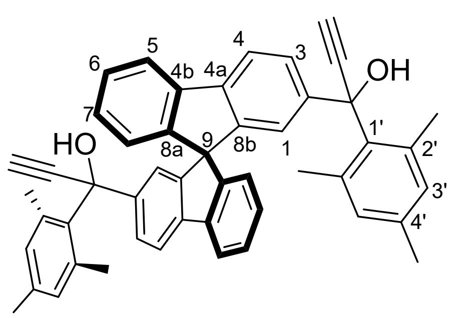


Figure S7. Comparison between experimental (top) and theoretical (middle and bottom) HR-ESI-MS spectra of **II**.



$C_{37}H_{28}O$ (660.62 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{49}H_{39}O$ $[M\text{-}OH]^+$ 643.3001, found 643.29956; Calcd. for $C_{47}H_{37}O$ $[M\text{-}OH,\text{-}C{\equiv}CH,\text{-}H]^+$ 617.2844, found 617.28393. **^{1}H NMR**: δ 7.81 (d, $^3J_{HH}$ = 7.8 Hz, 2H, $H_B{}^5 + H_C{}^5$); 7.79 (d, $^3J_{HH}$ = 7.7 Hz, 1H, $H_A{}^4$); 7.78 (d, $^3J_{HH}$ = 7.3 Hz, 1H, $H_A{}^5$); 7.73 (d, $^3J_{HH}$ = 8.0 Hz, 1H, $H_B{}^4$); 7.70 (d, $^3J_{HH}$ = 8.1 Hz, 1H,

H_{C}^{4}); 7.55 (dd, $^{3}J_{HH} = 8.0$, $^{4}J_{HH} = 1.8$ Hz, 1H, H_{A}^{3}); 7.48-7.30 (m, 3H, $H_{A}^{6} + H_{B}^{6} + H_{C}^{6}$); 7.27 (d, $^{4}J_{HH} =1.5$ Hz, 1H, H_{C}^{1}); 7.24 (dd, $^{3}J_{HH} = 8.1$, $^{4}J_{HH} = 1.8$ Hz, 1H, H_{C}^{3}); 7.20 (dd, $^{3}J_{HH} = 8.0$, $^{4}J_{HH} = 1.8$ Hz, 1H, H_{B}^{3}); 7.17 (d, $^{4}J_{HH} =1.8$ Hz, 1H, H_{B}^{1}); 7.11 (dd, $^{3}J_{HH} = 8.1$, $^{4}J_{HH} = 1.8$ Hz, 1H, H_{A}^{7}); 7.08 (t, $^{3}J_{HH} = 7.8$ Hz, 2H, $H_{B}^{7} + H_{C}^{7}$); 7.01 (d, $^{4}J_{HH} =1.5$ Hz, 1H, H_{A}^{1}); 6.76 (s, 2H, $H^{3'}$); 6.75 (s, 2H, $H^{3'}$); 6.72-6.70 (m, 3H, $H^{3'} + H_{A}^{8}$); 6.66 (t, $^{3}J_{HH} = 7.6$ Hz, 2H, $H_{B}^{8} + H_{C}^{8}$); 4.38 (s br, observed by {^{1}H, ^{1}H} COSY, 1H, OH); 2.75 (s, 1H, C≡CH_{A}); 2.66 (s, 1H, C≡CH_{B}); 2.62 (s, 1H, C≡CH_{C}); 2.23 (s, 6H, $C^{2'}CH_{3}^{A}$); 2.20 (s, 12H, $C^{2'}CH_{3}^{B} + C^{2'}CH_{3}^{C}$); 2.18 (s, 6H, $C^{4'}CH_{3}^{B} + C^{4'}CH_{3}^{C}$); 2.17 (s, 3H, $C^{4'}CH_{3}^{A}$) ppm. **^{13}C NMR**: δ 149.4, 149.3 and 149.2 (all s, C^{8a}); 148.7 (s, C_{A}^{2}); 148.6 (s, $C_{B}^{2} + C_{C}^{2}$); 145.6 (s, C_{A}^{8b}); 145.3 and 145.2 (both s, C_{B}^{8b} and C_{C}^{8b}); 142.1 (s, C_{A}^{4a}); 142.0 (s, C_{B}^{4a}); 141.9 (s, C_{C}^{4a}); 141.1 and 141.0 (both s, C_{B}^{4b} and C_{C}^{4b}); 140.9 (s, C_{A}^{4b}); 137.0-135.5 (all s, mesityl ring); 128.1 (s, C^{7}); 126.6 (s, C_{A}^{3}); 126.5 (s, C_{B}^{3}); 126.4 (s, C_{C}^{3}); 127.9 and 127.8 (both s, C^{6}); 131.7 and 131.6 (both s, $C^{3'}$); 124.1 (s, C_{A}^{8}); 124.9 (s, $C_{B}^{8} + C_{C}^{8}$); 122.1 (s, $C_{B}^{1} + C_{C}^{1}$); 122.0 (s, C_{A}^{1}); 120.5, 120.4, 120.34, 120.32 and 120.2 (all s, C^{4} and C^{5}); 86.0 (s, ≡C_{A}); 85.9 (s, ≡C_{B}); 85.7 (s, ≡C_{A}); 76.6 (s, C_{C}-OH); 76.4 (s, C_{B}-OH); 76.2 (s, ≡C_{A}H); 75.8 (s, C_{A}-OH); 75.6 (s, ≡C_{B}H + ≡C_{C}H); 66.3 (s, C_{C}^{9}); 66.2 (s, C_{B}^{9}); 66.1 (s, C_{A}^{9}); 24.01 (s, $C_{A}^{2'}CH_{3}$); 23.96 (s, $C_{A}^{4'}CH_{3} + C_{B}^{2'}CH_{3} + C_{C}^{2'}CH_{3}$); 20.6 (s, $C_{B}^{4'}CH_{3} + C_{C}^{4'}CH_{3}$)ppm.

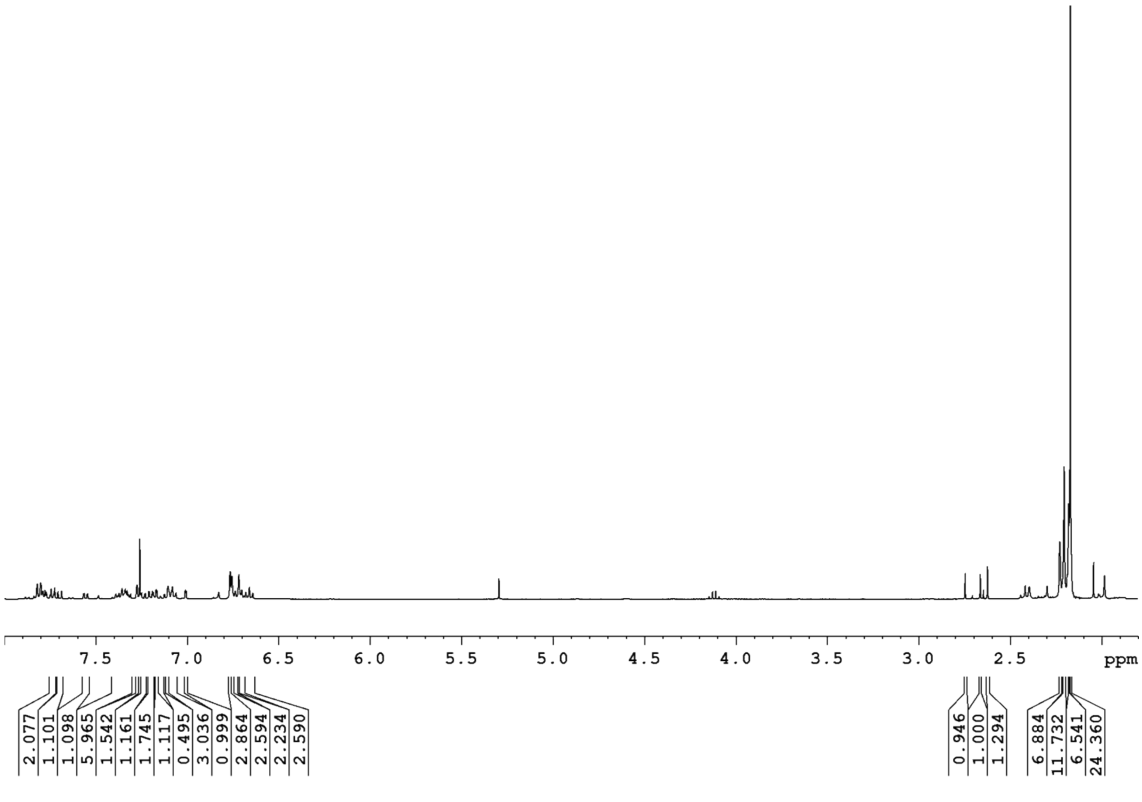


Figure S8. ^{1}H NMR spectrum of **III**.

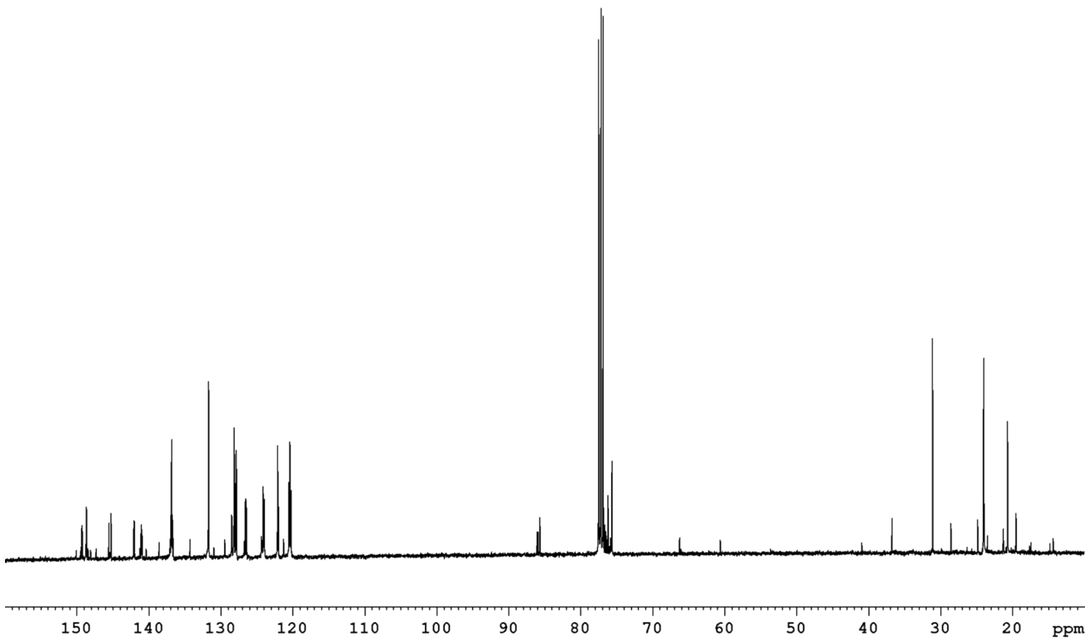


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **III**.

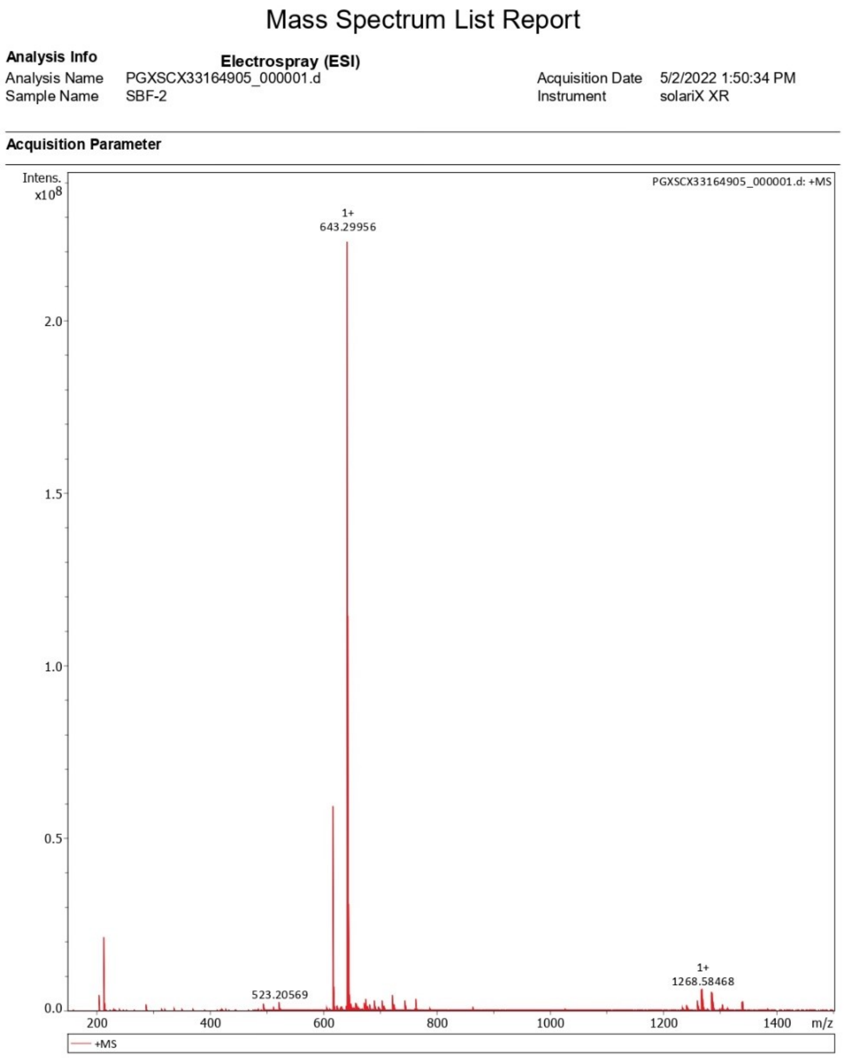
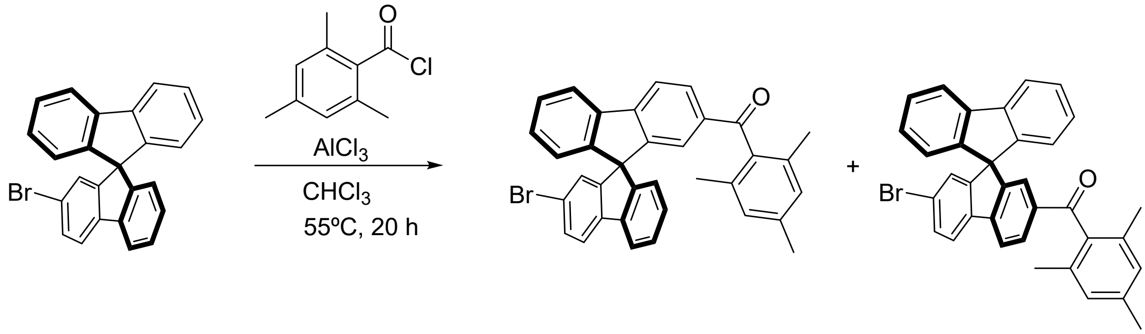


Figure S10. HR-ESI-MS spectrum of **III**.

Synthesis of 2-bromo-2'-(2,4,6-trimethylbenzoyl)-9,9'-spirobifluorene (IV) and 2-bromo-7-(2,4,6-trimethylbenzoyl)-9,9'-spirobifluorene (IV-b)

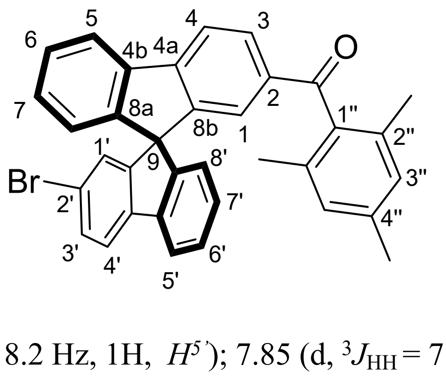


IV : **IV-b**

2.8 : 1

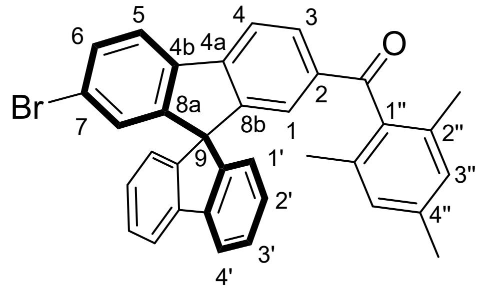
To a solution of 2-bromo-spirobifluorene (1.2 g, 3.03 mmol) in chloroform (30 mL), pulverized $AlCl_3$ (1.2 g, 9.0 mmol) and 2,4,6-trimethylbenzoyl chloride (1.5 mL, 8.7 mmol) were added and the mixture was heated under inert atmosphere for 20 h. After that, the reaction mixture was extracted three times with CH_2Cl_2 and the combined organic phases were washed once with H_2O and once with saturated NaCl. Then, it was dried over Na_2SO_4 and the solvent was removed by evaporation under reduced pressure. The crude was purified by column chromatography (SiO_2, gradient hex/AcOEt from 95/5 to 85/15) affording a mixture of ketones **IV** and **IV-b** in a 2.8:1 ratio, respectively, as a white solid. Yield: 1.26 g (76%).

$C_{35}H_{25}OBr$ (541.48 g/mol).



^{1}H NMR: δ 7.90 (d, $^3J_{HH}$ = 8.2 Hz, 1H, $H^{5'}$); 7.85 (d, $^3J_{HH}$ = 7.9 Hz, 1H, $H^{4'}$); 7.84 (d br, $^3J_{HH}$ = 7.6 Hz, 1H, H^5); 7.73 (d, $^3J_{HH}$ = 8.0 Hz, 1H, H^4); 7.65 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.8 Hz, 1H, $H^{3'}$); 7.55 (s, 1H, $H^{1'}$); 7.521 (dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 1.8 Hz, 1H, H^3); 7.44-7.37 (m, 2H, $H^6 + H^{6'}$); 7.20 (td, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.1 Hz, 1H, H^7); 7.14 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.0 Hz, 1H, $H^{7'}$); 6.90 (d, $^4J_{HH}$ = 1.8 Hz, 1H, H^1); 6.88 (s, 2H, $H^{3''}$); 6.78 (d br, $^3J_{HH}$ = 7.8 Hz, 1H, $H^{8'}$); 6.74 (d, 1H, $^3J_{HH}$ = 7.8 Hz, H^8); 2.32 (s, 3H, $C^{4''}CH_3$); 2.06 (s, 6H,

$C^{2''}CH_3$) ppm. **^{13}C NMR**: δ 200.1 (s, *C*O); 149.9 (s, $C^{2'}$); 149.5 (s, $C^{8a'}$); 148.9 (s, $C^{8b'}$); 147.6 (s, C^{8a}); 147.1 (s, $C^{4a'}$); 141.0 (s, C^{8b}); 140.9 (s, C^{4a}); 140.3 (s, C^{4b}); 138.5 (s, $C^{4''}$); 136.9 (s, $C^{1''}$); 134.3 (s, $C^{2''}$); 131.5 (s, C^{3}); 131.3 (s, $C^{3'}$); 129.5 (s, $C^{7'}$); 128.44 and 128.4 (both s, $C^{3''}$ + $C^{6'}$ + C^{6}); 128.3 (s, C^{7}); 127.2 (s, C^{1}); 124.4 (s, $C^{8'}$); 124.2 (s, $C^{1'}$); 124.0 (s, C^{8}); 121.7 (s, C^{4}); 121.5 (s, C^{2}); 121.3 (s, $C^{5'}$); 120.4 and 120.14 (both s, C^{5} + $C^{4'}$); 65.8 (s, C^{9}); 21.2 (s, $C^{4''}CH_3$); 19.6 (s, $C^{2''}CH_3$) ppm.



^{1}H NMR: δ 7.88 (d, $^{3}J_{HH}$ = 7.6 Hz, 2H, $H^{4'}$); 7.81 (d, $^{3}J_{HH}$ = 8.0 Hz, 1H, H^{5}); 7.75 (d, $^{3}J_{HH}$ = 8.0 Hz, 1H, H^{4}); 7.64 (dd, $^{3}J_{HH}$ = 7.9, $^{4}J_{HH}$ = 1.7 Hz, 1H, $H^{6'}$); 7.54-7.52 (m, overlapped, 1H, H^{8}); 7.517 (dd, $^{3}J_{HH}$ = 8.1, $^{4}J_{HH}$ = 1.4 Hz, 1H, H^{3}); 7.44-7.37 (m, 2H, $H^{3'}$); 7.14 (td, $^{3}J_{HH}$ = 7.5, $^{4}J_{HH}$ = 1.0 Hz, 1H, $H^{2'}$); 6.92 (d, $^{4}J_{HH}$ = 1.8 Hz, 1H, H^{1});6.75 (d br, $^{3}J_{HH}$ = 7.8 Hz, 2H, $H^{1'}$); 6.86 (s, 2H, $H^{3''}$); 6.75 (d br, $^{3}J_{HH}$ = 7.8 Hz, 1H, $H^{1'}$); 2.31 (s, 3H, $C^{4''}CH_3$); 2.03 (s, 6H, $C^{2''}CH_3$) ppm. **^{13}C NMR**: δ 200.0 (s, *C*O); 152.4 (s, C^{7}); 146.0 (s, C^{4b}); 142.0 (s, $C^{4a'}$); 139.3 (s, C^{4a}); 137.2 (s, C^{8a}); 138.5 (s, $C^{4''}$); 136.8 (s, $C^{1''}$); 134.3 (s, $C^{2''}$); 131.3 (s, C^{6}); 131.0 (s, C^{8b}); 131.3 (s, C^{3}); 128.1 (s, $C^{3'}$); 128.44 (s, $C^{3''}$); 128.4 (s, $C^{2'}$);127.6 (s, C^{1}); 124.34 (s, C^{8}); 123.98 (s, $C^{1'}$); 123.3 (s, C^{2}); 122.4 (s, C^{4}); 120.5 (s, $C^{4'}$); 120.1 (s, C^{5}); 65.9 (s, C^{9}); 21.2 (s, $C^{4''}CH_3$); 19.5 (s, $C^{2''}CH_3$) ppm.

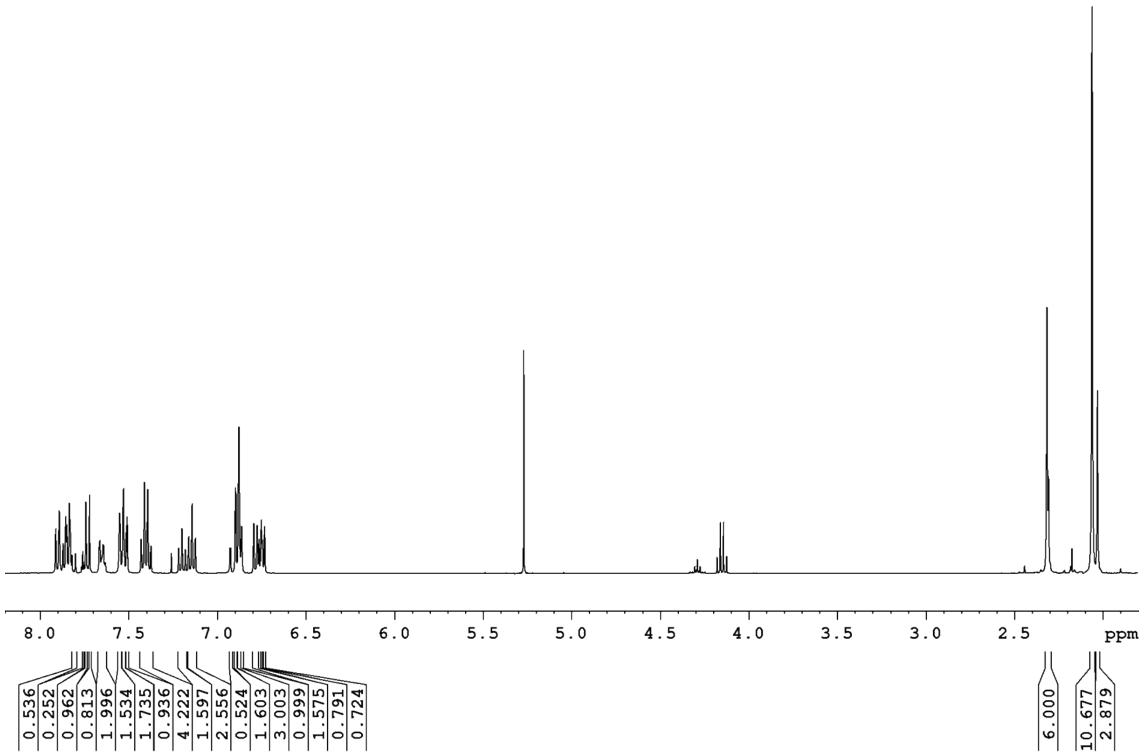


Figure S11. [1]H NMR spectrum of the mixture of **IV** and **IV-b**.

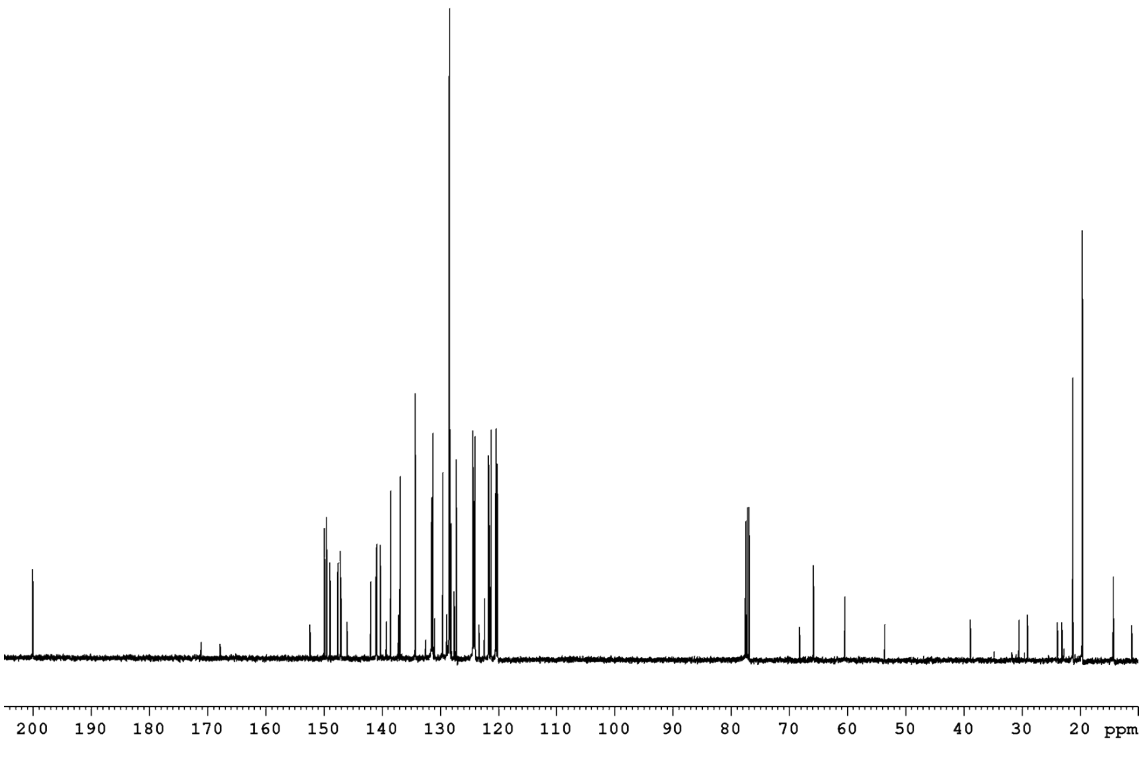
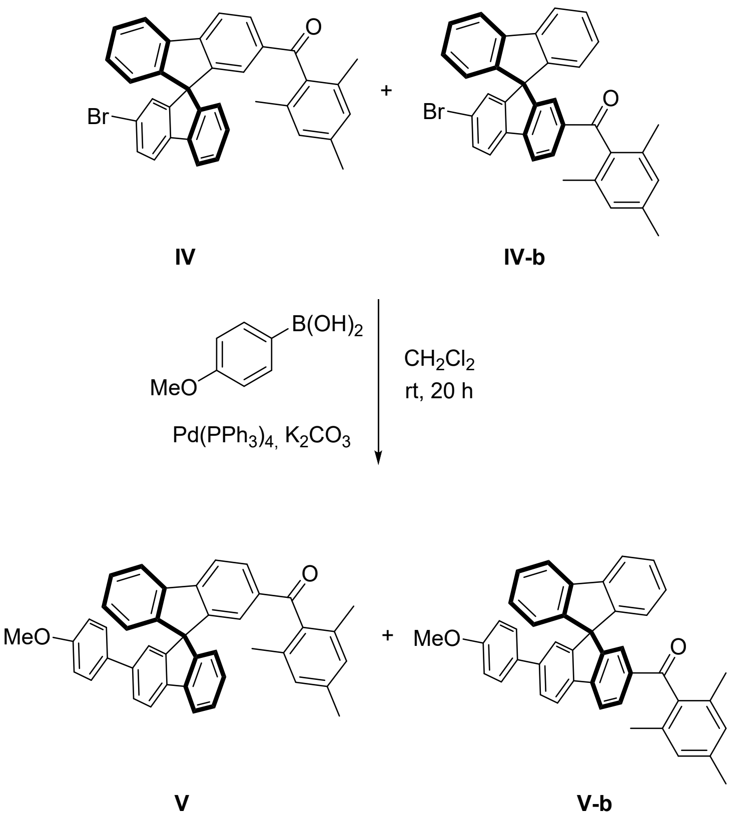


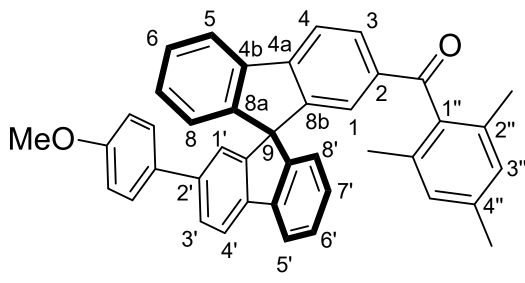
Figure S12. $^{13}C\{^1H\}$ NMR spectrum of the mixture of **IV** and **IV-b**.

Synthesis of 2-(*p*-methoxyphenyl)-2'-(2,4,6-trimethylbenzoyl)-9,9'-spirobifluorene (V)



To a solution of the mixture of ketones **IV** and **IV-b** (1.26 g, 2.32 mmol, 2.8:1 ratio) in toluene (18 mL), the palladium (0) complex $Pd(PPh_3)_4$ (213 mg, 0.18 mmol) and *p*-methoxyphenylboronic acid (422 mg, 2.78 mmol) were added. Then, a 1M solution of K_2CO_3 (9.25 ml, 9.25 mmol) in water was added. The biphasic mixture was then refluxed under inert atmosphere for 16 h. After that, the reaction mixture was extracted three times with ethylacetate and the combined organic phases were washed once with H_2O and once with saturated NaCl. Then, it was dried over Na_2SO_4 and the solvent removed by evaporation under reduced pressure. The crude was purified by column chromatography (SiO_2, gradient hex/AcOEt from 95/5 to 90/10) affording the mixture of ketones **V** and **V-b** in a 2.8:1 ratio as a yellow solid. The desired ketone **V** was enriched to a 90% by column chromatography (SiO_2, hex/CH_2Cl_2 1:1). Yield: 583 mg (60% based on ketone **IV**).

$C_{42}H_{32}O_2$ (568.70 g/mol). **HRMS** (ESI^+): *m/z* Calcd. for $C_{42}H_{33}O_2$ $[M+H]^+$ 569.2475 found 569.2475.



^{1}**H NMR**: δ 7.93-7.90 (m, 2H, $H^{5'}$ + H^{5}); 7.84-7.80 (m, 2H, $H^{4'}$+ H^{4}); 7.63 (dd, $^{3}J_{HH}$ = 8.3, $^{4}J_{HH}$ = 1.3 Hz, 1H, H^{3}); 7.62 (dd, $^{3}J_{HH}$ = 8.1, $^{4}J_{HH}$ = 1.6 Hz, 1H, $H^{3'}$); 7.55 (d, $^{4}J_{HH}$ = 1.3 Hz, 1H, H^{1}); 7.44-7.40 (m, 2H, $H^{6'}$ + H^{6}); 7.40-7.35 (m, 2H, $H^{2'''}$); 7.21 (td, $^{3}J_{HH}$ = 7.6, $^{4}J_{HH}$ = 1.0 Hz, 1H, $H^{7'}$); 7.13 (td, $^{3}J_{HH}$ = 7.6, $^{4}J_{HH}$ = 1.0 Hz, 1H, H^{7}); 6.90-6.85 (m, 5H, $H^{3'''}$ + $H^{1'}$ + $H^{3''}$); 6.83 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, $H^{8'}$); 6.74 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, H^{8}); 3.81 (s, 3H, OMe); 2.32 (s, 3H, $C^{4'}CH_3$); 2.03 (s, 6H, $C^{2'}CH_3$) ppm. ^{13}**C NMR**: δ 200.2 (s, *C*=O); 159.1 (s, $C^{4'''}$); 150.5 (s, C^{8a}); 149.7 (s, C^{8b}); 148.5 (s, $C^{8b'}$); 148.0 (s, $C^{4a'}$); 147.2 (s, C^{4a}); 141.7 (s, $C^{8a'}$); 140.7 (s, $C^{4b'}$); 140.6 (s, C^{4b}); 140.2 (s, 2C, $C^{2'}$); 136.9 (s, $C^{1''}$); 136.8 (s, C^{2}); 134.2 (s, $C^{4''}$); 133.6 (s, $C^{1'''}$+ $C^{2''}$); 131.2 (s, C^{3}); 129.4 (s, C^{7} + C^{7}); 128.3 (s, 2C, $C^{3''}$); 128.1 (s, 2C, $C^{2'''}$); 127.7 (s, $C^{6'}$ + C^{6}); 126.8 (s, 2C, $C^{3'}$); 124.4 (s, $C^{8'}$); 124.3 (s, C^{1}); 123.9 (s, C^{8}); 122.2 (s, 2C, $C^{1'}$); 121.0 (s, $C^{5'}$ + C^{5}); 120.5 (s, $C^{4'}$); 119.7 (s, C^{4}); 114.1 (s, 2C, $C^{3'''}$); 66.0 (s, C^{9}); 55.3 (s, OMe); 21.1 (s, $C^{4''}CH_3$); 19.5 (s, 2C, $C^{2''}CH_3$) ppm.

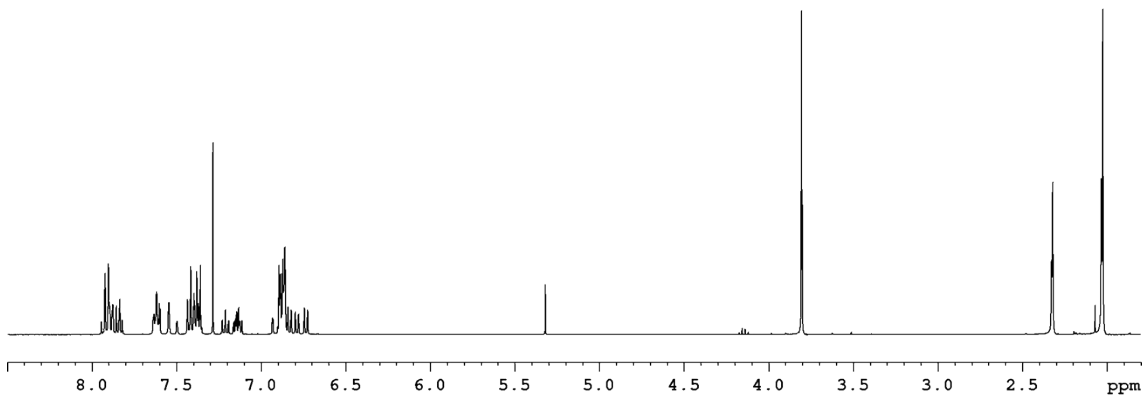


Figure S13. ^{1}H NMR spectrum of **V**.

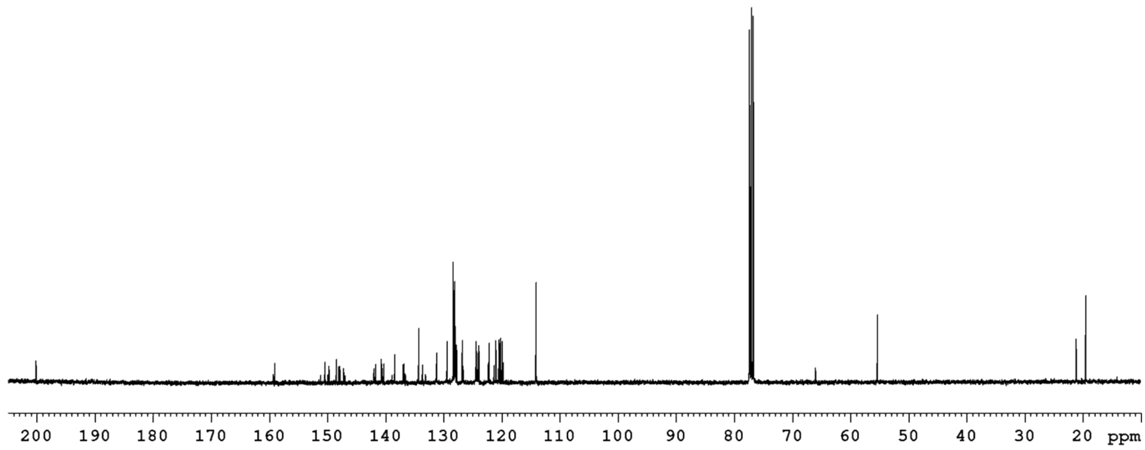
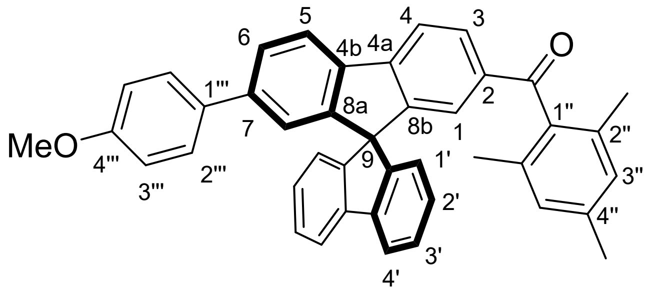


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **V**.



^{1}H NMR: δ 7.92 (dd, $^{3}J_{HH}$ = 8.04, 0.40 Hz, 1H, H^{5}); 7.88 (dt, $^{3}J_{HH}$ = 7.74, 0.73 Hz, 2H, $H^{4'}$); 7.82 (dd, $^{3}J_{HH}$ = 8.04, 0.52 Hz, 1H, H^{4}); 7.63-7.58 (m, 2H, H^{3}+H^{6}); 7.50 (s br, 1H, H^{1}); 7.40 (td, $^{3}J_{HH}$ = 7.59, 1.07 Hz, 2H, $H^{3'}$); 7.38-7.34 (dm, $^{3}J_{HH}$ = 8.95 Hz, 2H, $H^{2'''}$); 7.13 (td, $^{3}J_{HH}$ = 7.61, 1.09 Hz, 2H, $H^{2'}$); 6.93 (d br, $^{3}J_{HH}$ = 1.49 Hz, 1H, H^{8}); 6.88-6.83 (m, 4H, $H^{3''}$+$H^{3'''}$); 6.78 (dt, $^{3}J_{HH}$ = 7.85, 0.77 Hz, 2H, $H^{1'}$); 3.78 (s, 3H, OMe); 2.31 (s, 3H, $C^{4''}CH_3$); 2.03 (s, 6H, $C^{2''}CH_3$) ppm. **^{13}C NMR**: δ 200.1 (s, *C*=O); 159.3 (s, $C^{4'''}$); 151.2 (s, C^{8a}); 150.0 (s, C^{8b}); 147.9 (s, 2C, $C^{4b'}$); 147.0 (s, C^{4a}); 142.1 (s, C^{7}); 142.0 (s, 2C, $C^{4a'}$); 138.9 (s, C^{4b}); 138.4 (s, $C^{4''}$); 137.0 (s, $C^{1''}$); 136.6 (s, C^{2}); 134.3 (s, 2C, $C^{2''}$); 133.1 (s, $C^{1'''}$); 131.3 (s, C^{3}); 128.4 (s, 2C, $C^{3''}$); 128.2 (s, 2C, $C^{2'''}$); 128.0 (s, 2C, $C^{3'}$); 127.9 (s, 2C, $C^{2'}$); 126.7 (s, C^{6}); 124.2 (s, C^{1}); 124.1 (s, 2C, $C^{1'}$); 122.4 (s, C^{8}); 121.3 (s, C^{5}); 120.3 (s, 2C, $C^{4'}$); 119.8 (s, C^{4}); 114.1 (s, 2C, $C^{3'''}$); 66.0 (s, C^{9}); 55.3 (s, OMe); 21.2 (s, $C^{4''}CH_3$); 19.5 (s, 2C, $C^{2''}CH_3$) ppm.

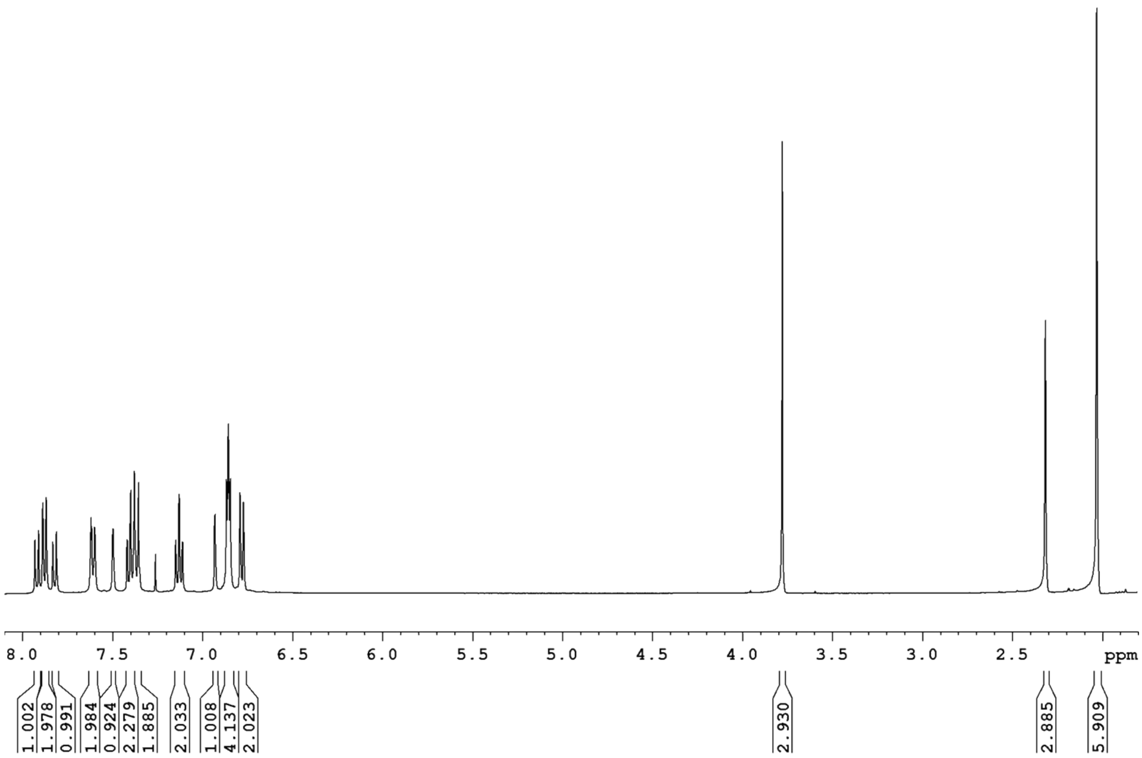


Figure S15. ^{1}H NMR spectrum of **V-b**.

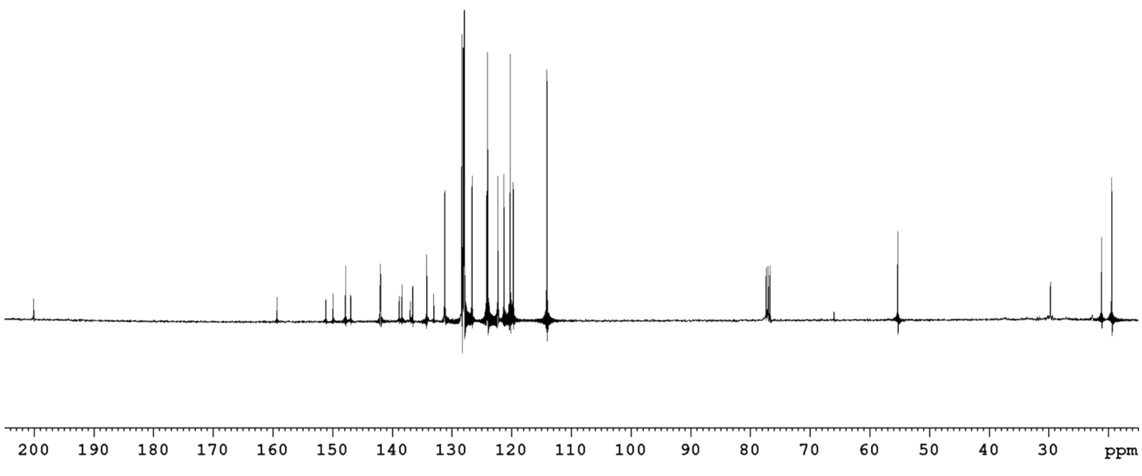


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **V-b**.

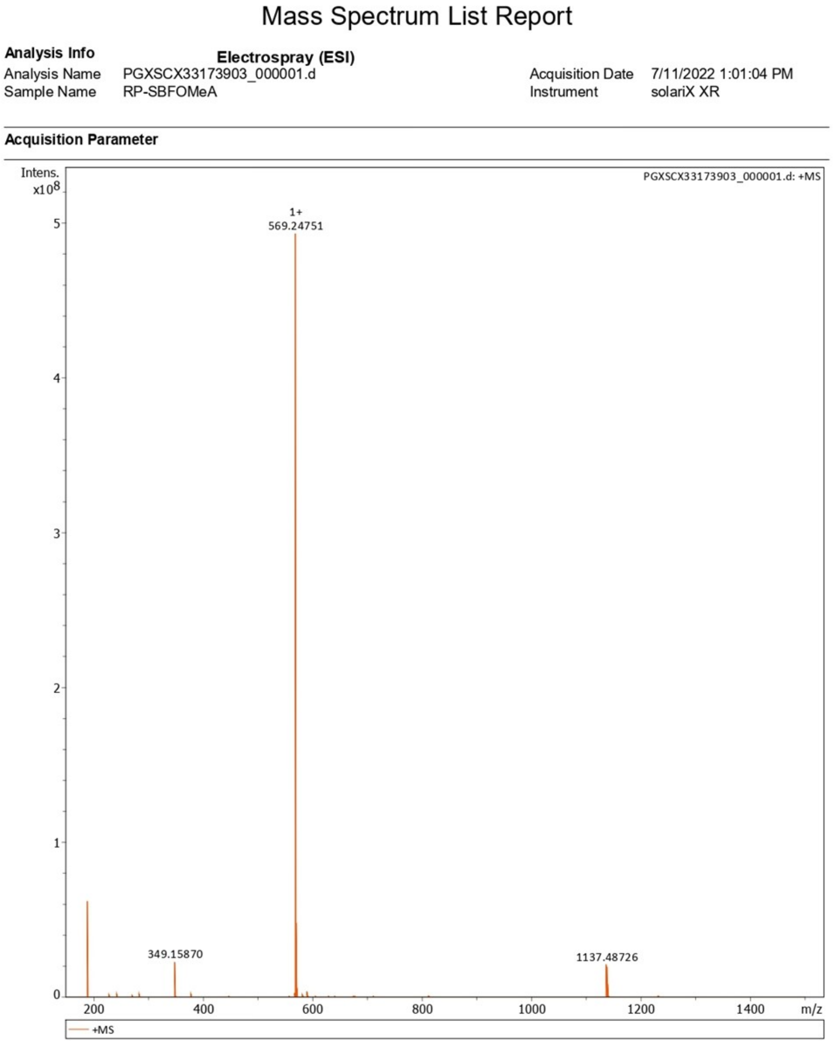
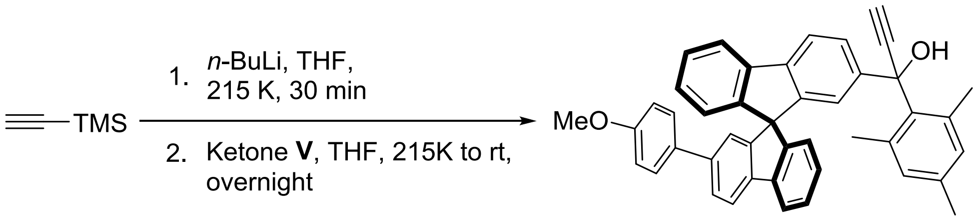


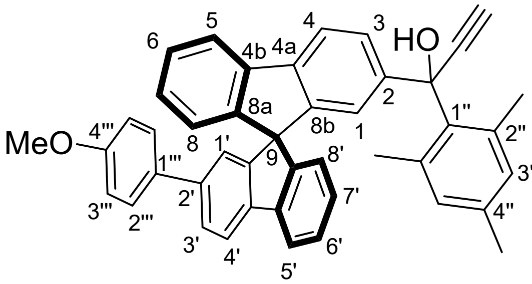
Figure S17. HR-ESI-MS spectrum of the mixture of **V** and **V-b**.

Synthesis of 2-(*p*-methoxyphenyl)-2'-(1-hydroxy-1-mesitylprop-2-yn-1-yl)-9,9'-spirobifluorene (VI)



VI

To a solution of trimethylsilylacetilene (0.3 mL, 2.9 mmol) in THF (5 mL) at –78 ºC, *n*-buthyllithium 1.6 M in hexanes (1.6 mL, 2.64 mmol) was added dropwise and the reaction mixture was stirred for 30 minutes. After that, a solution of the ketone **V** obtained above (110 mg, 0.19 mmol) in THF (5 mL) was added via cannula and the mixture was allowed to warm up to room temperature and stirred overnight. Then, MeOH (5 mL) and K_2CO_3 (400 mg, 2.9 mmol) were added and the mixture was stirred again for 3 hours. The solution was filtrated through a pad of SiO_2, washed with AcOEt and concentrated under vacuum to provide a mixture of the two diastereoisomers (*R,M*)* and (*R,P*)* in a 1:1.2 ratio of the monopropargylic alcohol **VI** as white foams with an 8% impurity of the possible isomer derived from **IV-b**. Yield: 110 mg (96%).



$C_{44}H_{33}O_2$ (593.74 g/mol). **HRMS** (ESI^+): *m/z* Calcd. for $C_{44}H_{33}O$ $[M-OH+H]^+$ 577.2526 found 577.2526; Calcd. for $C_{44}H_{34}O_2$ $[M+H]^+$ 594.2553 found 594.2553. **^{1}H NMR**: 7.90 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 0.4 Hz, 1H, $H_A{}^{4'}$); 7.89 (dd, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 0.5 Hz, 1H, $H_B{}^{4'}$); 7.89-7.84 (m, ^{4}H, $H_{A+B}{}^{5'}$ + $H_{A+B}{}^{5}$); 7.81 (m, ^{2}H, $H_{A/B}{}^{4}$); 7.60 (dt apparent, $^3J_{HH}$ = 8.0, J_{HH} = 1.7 Hz, 2H, $H_{A+B}{}^{3'}$); 7.45 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.9 Hz, 1H, $H_A{}^{3}$); 7.42 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.8 Hz, 1H, $H_B{}^{3}$); 7.41-7.35 (m, 8H, $H_{A+B}{}^{6}$ + $H_{A+B}{}^{6'}$ + $H_{A+B}{}^{2'''}$); 7.26 (dd, $^4J_{HH}$ = 1.7, $^5J_{HH}$ = 0.4 Hz, 1H, $H_A{}^{1}$); 7.21 (dd, $^4J_{HH}$ = 1.8, $^5J_{HH}$ = 0.4 Hz, 1H, $H_B{}^{1}$); 7.18-7.10 (m, ^{4}H, $H_{A+B}{}^{7}$ + $H_{A+B}{}^{7'}$); 6.95-6.93 (m, 2H, $H_{A+B}{}^{1'}$); 6.89 (2d, $^3J_{HH}$ = 8.8 Hz, 4H, $H_{A+B}{}^{3'''}$); 6.80-6.77 (m, 3H, $H_B{}^{8'}$ + $H_{A+B}{}^{8}$); 6.78 (s, 2H, $H_B{}^{3''}$); 6.75 (m, 1H, $H_A{}^{8'}$); 6.74 (s, 2H, $H_A{}^{3''}$); 3.82 (s, 3H, OMe^B); 3.821 (s, 3H, OMe^A); 2.70 (s, 1H, ≡CH_B); 2.68 (s, 1H, ≡CH_A); 2.25 (s, 9H, Mes$CH_3{}^A$); 2.23 (s, 9H, Mes$CH_3{}^B$) ppm. **^{13}C NMR**: δ 159.1 (s, 2C, $C_{A+B}{}^{4'''}$); 149.6, 149.3, 149.2, 148.9, 148.85, 148.8 and 148.7 (all s, $C_{A+B}{}^{8a'}$ + $C_{A+B}{}^{8a}$ + $C_{A+B}{}^{8b}$ + $C_{A+B}{}^{8b'}$); 145.5 (s, $C_{A+B}{}^{2}$); 141.8 and 141.6 (both s, $C_{A+B}{}^{4b}$ + $C_{A+B}{}^{4b'}$); 140.6 (s, $C_{A+B}{}^{4a'}$); 140.5 (s, $C_{A+B}{}^{2'}$); 141.0 (s, $C_{A+B}{}^{4a}$); 136.8 (s, $C_{A+B}{}^{2''}$); 136.6 (s, $C_{A+B}{}^{4''}$ + $C_{A+B}{}^{1''}$); 133.6 (s, $C_{A+B}{}^{1'''}$); 131.6 (s, $C_{A+B}{}^{3''}$); 128.1, 128.0, 127.82, 127.76 and 127.7 (all s, $C_{A+B}{}^{7'}$ + $C_{A+B}{}^{7}$ + $C_{A+B}{}^{6}$ + $C_{A+B}{}^{6'}$ + $C_{A+B}{}^{2'''}$); 126.6 (s, $C_{A+B}{}^{3'}$); 126.5 (s, $C_{A+B}{}^{3}$); 124.1, 124.0 and 123.9 (s, $C_{A+B}{}^{8'}$ + $C_{A+B}{}^{8}$); 122.3 (s, $C_{A+B}{}^{1'}$); 122.1 (s, $C_B{}^{1}$); 122.0 (s, $C_A{}^{1}$); 120.4, 120.3, 120.2 and 120.1 (all s, $C_{A+B}{}^{5'}$ + $C_{A+B}{}^{4}$ + $C_{A+B}{}^{4'}$ + $C_{A/+B}{}^{5}$); 114.1 (s, $C_A{}^{3'''}$); 85.8 (s, ≡C_{A+B}); 76.3 (s, C_{A+B}-OH); 76.0 (s, ≡CH_A); 75.9 (s, ≡CH_B); 66.2 (s, $C_{A+B}{}^{9}$); 55.3 (s, $OC_{A+B}H_3$); 23.9 (s, Mes$C_{A+B}H_3$) ppm.

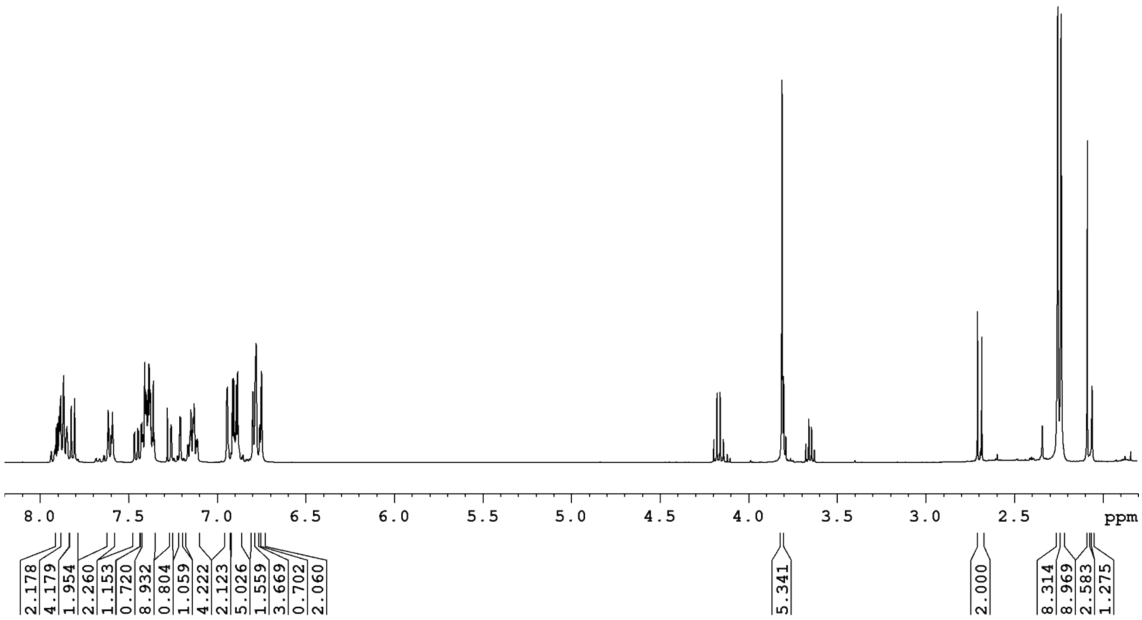


Figure S18. ^{1}H NMR spectrum of **VI**.

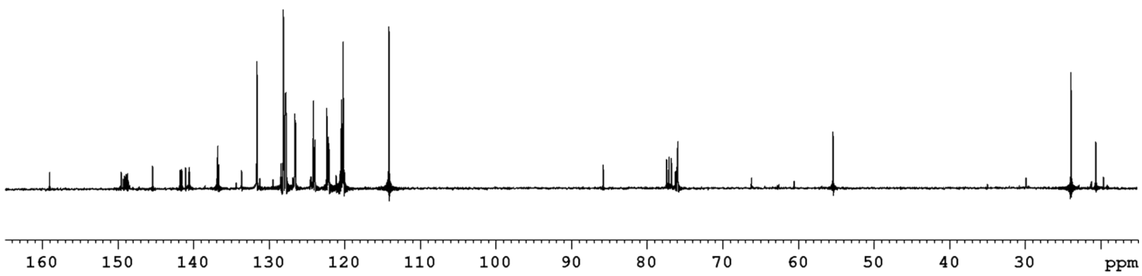


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of **VI**.

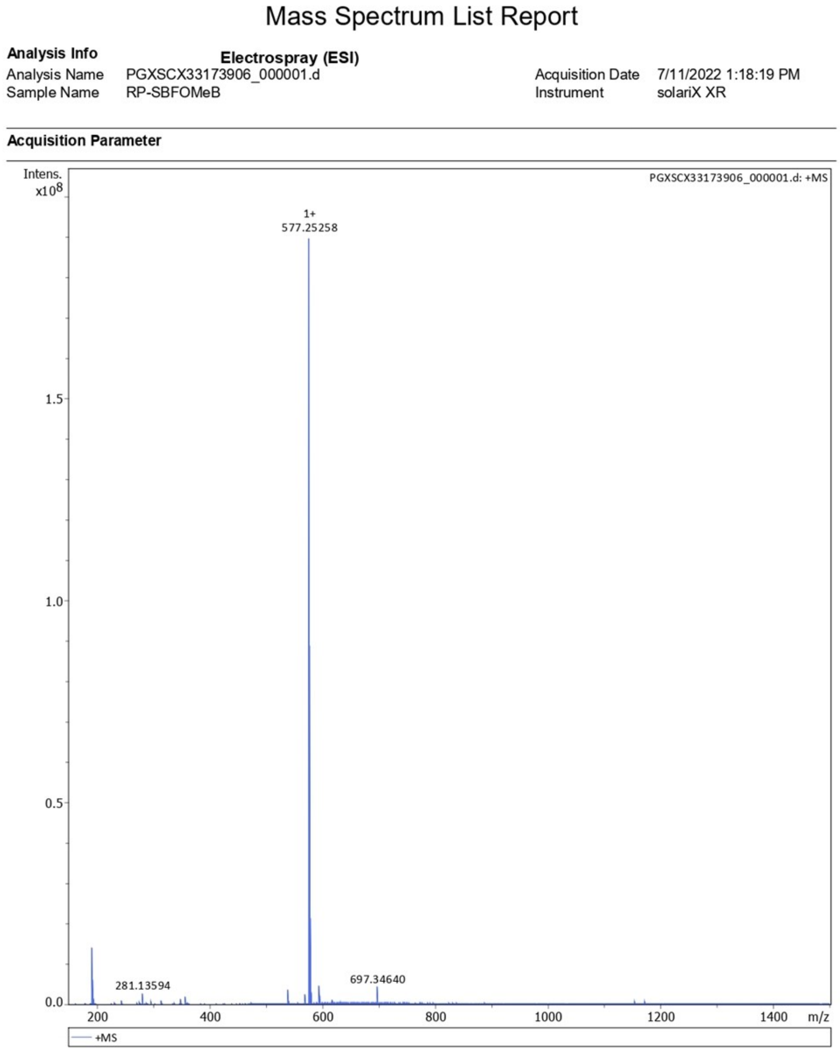
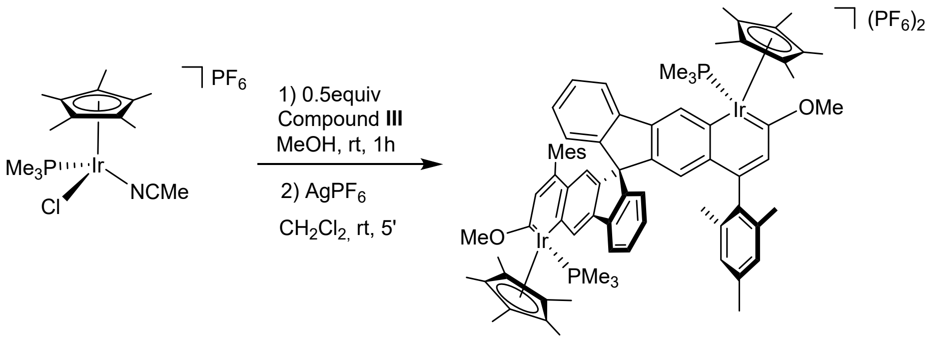


Figure S20. HR-ESI-MS spectrum of **VI**.

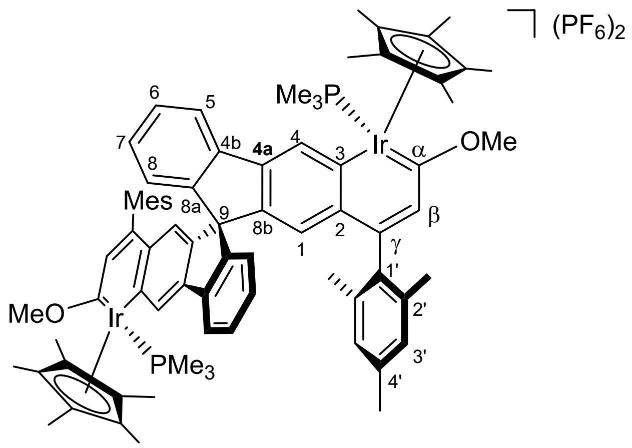
Preparation of $[IrCp^*(PMe_3)\{=C(OMe)–CH=C(2,4,6\text{-}Me_3C_6H_2)(\kappa^4\text{-}2,3,2',3'\text{-}SBF)C=CH–C(OMe)=\}(PMe_3)Cp^*Ir](PF_6)_2$ (2)



2

To a yellow solution of $[IrCp^*Cl(NCMe)(PMe_3)]PF_6$ (515 mg, 0.82 mmol) in 22 ml of methanol, the propargylic alcohol **III** (271 mg, 0.41 mmol) was added and the mixture was stirred for 1 h at room temperature. The dark suspension obtained was vacuum concentrated obtaining a red solid which was washed with a mixture of Et_2O/pentane 1/5 (3 × 10 mL) and dried in vacuum. Then, the dark brown solid (708 mg, 0.38 mmol) was dissolved in 20 mL of dichloromethane and treated with $AgPF_6$ (116 mg, 0.46 mmol). The solution was stirred for 10 min at room temperature, filtered and vacuum concentrated, obtaining a brown solid that was washed with Et_2O/pentane (1/5) (3 × 4 mL) and dried in vacuum. The residue was purified by column chromatography (SiO_2, gradient CH_2Cl_2/MeCN from 100/0 to 90/10) affording complex **2**. Yield: 613.3 mg (84 % from acetonitrile complex).

There are 3 possible diasteroisomers which can provide 4 groups of signals. (*R,M,R*)*-**2** and (*S,M,S*)*-**2** will show both branches as equivalents, thus, one signal for each isomer will be observed. However, (*R,M,S*)*-**2** presents two different iridium atoms and therefore, the resonances of each fluorene branch will be slightly different. Therefore a 2:1:1 ratio of isomers can be determined, where (*R,M,S*)*-**2** is the diastereoisomer in the largest amount. Due to the very similar nature of all the resonances and the spatial arrangement of the SBF moiety, it was not possible to differentiate the isomers.



$C_{77}H_{90}O_2F_{12}Ir_2P_4$ (1783.85 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{77}H_{90}O_2Ir_2P_2$ $[M]^{+2}$ 747.2814 found 747.28352. **^{1}H NMR (300 MHz)**: δ 8.30, 8.29, 8.28 and 8.26 (all s, 1H, H^4); 7.86 and 7.85 (both dm, 2H, $^3J_{HH}$ = 7.6 Hz, H^5); 7.425 and 7.422 (both t, 1H, $^3J_{HH}$ = 7.6 Hz, H^6); 7.419 (t, 2H, $^3J_{HH}$ = 7.5 Hz, H^6); 7.200, 7.198, 7.184 and 7.17 (all td, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 1.2 Hz, 1H, H^7); 6.75, 6.73, 6.71 (all s br, 1H, $H^{3'}$); 6.703 and 6.698 (both s, 1H, H^1); 6.68 (s br, 2H, H^8); 6.67 and 6.66 (both s br, 2H, H^1 + H^8); 6.66-6.62 (m, 5H, $H^{3'}$); 6.50 and 6.47 (both d, $^4J_{HP}$ = 1.0 Hz, 1H, H^β); 6.49 (d, $^4J_{HP}$ = 0.7 Hz, 2H, H^β); 4.285, 4.276, 4.27 and 4.26 (all s br, 3H, OCH_3); 2.21 (s, 6H, $C^{4'}CH_3$); 2.18 and 2.17

(both s, 3H, $C^{4'}CH_3$); 1.86 (d, 30H, $^4J_{HP}$ = 1.7 Hz, $C_5(CH_3)_5$); 1.82 and 1.81 (both d, 15H, $^4J_{HP}$ = 1.7 Hz, $C_5(CH_3)_5$); 1.70, 1.67 and 1.64 (all s br, 6H, $C^{2'}CH_3$); 1.69 and 1.58 (both s br, 3H, $C^{2'}CH_3$); 1.355, 1.350, 1.31 and 1.29 (all d, 9H, $^2J_{HP}$ = 10.9 Hz, $P(CH_3)_3$) ppm. **$^{31}P\{^1H\}$ NMR (162 MHz)**: δ –33.36 (s, $P(CH_3)_3$); –33.63 (s, $P(CH_3)_3$); –144.24 (sept, $^1J_{PF}$ = 707.5 Hz, PF_6) ppm. **$^{13}C\{^1H\}$ NMR (125.7 MHz)**: δ 245.44, 245.37, 245.2 and 245.1 (all d, $^2J_{CP}$ = 10.9 Hz, C^α); 179.33, 179.32, 179.12 and 179.09 (all s, C^γ); 157.4, 157.3, 157.15 and 157.13 (all d, $^2J_{CP}$ = 10.6 Hz, C^3); 151.3, 151.2, 151.13 and 151.06 (all s, C^{8a}); 145.5, 145.45, 145.43 and 145.39 (all s, C^{4a}); 144.65, 144.59, 144.32 and 144.30 (all s, C^{8b}), 139.7, 139.65 and 139.57 (2C) (all s, C^{4b}); 138.32, 138.28, 138.16 and 138.15 (all s, $C^{1'}$); 138.06, 138.04 (2C) and 138.02 (all s, $C^{4'}$); 134.5 (2C), 134.23, 134.19, 133.8, 133.7, 133.4 and 133.3 (all s, $C^{2'}$); 133.9 and 133.79 both d, $^4J_{CP}$ = 1.8 Hz, C^4); 133.83 (s br, 2C, C^4); 133.1, 132.99 and 132.96 (2C) (all s, C^2); 130.6 and 130.3 (all s, 2C, C^1); 130.49 and 130.47 (both s, 2C, C^7); 128.70, 128.67 (2C), 128.62, 128.60, 128.52, 128.49, 128.3 (2C) and 128.1 (2C) (all s, C^6 and $C^{3'}$); 124.4, 124.3, 124.2 and 124.1 (all s, C^8); 121.7, 121.60, 121.56 and 121.5 (all s, C^5); 117.6 and 117.4 (both d, $^3J_{CP}$ = 2.2 Hz, C^β); 117.2 and 117.1 (m, 2C C^β); 100.2 (d br, $^2J_{CP}$ = 1.5 Hz, 2C $C_5(CH_3)_5$); 100.05 and 100.02 (both d, $^2J_{CP}$ = 1.8 Hz, $C_5(CH_3)_5$); 65.2 and 65.1 (both s, C^9); 63.6 (2C), 63.54 and 63.51 (all s, OCH_3); 21.12 (2C), 21.09 and 21.08 (all s, $C^{4'}CH_3$); 20.2, 20.1 (2C), 20.2, 20.0, 19.90, 19.87, 19.73 and 19.67 (all s, $C^{2'}CH_3$); 14.30, 14.29, 14.2 and 14.1 (all d, $^1J_{CP}$ = 41.1 Hz, $P(CH_3)_3$); 9.9 (2 signals), 9.82 and 9.76 (all s, $C_5(CH_3)_5$) ppm.

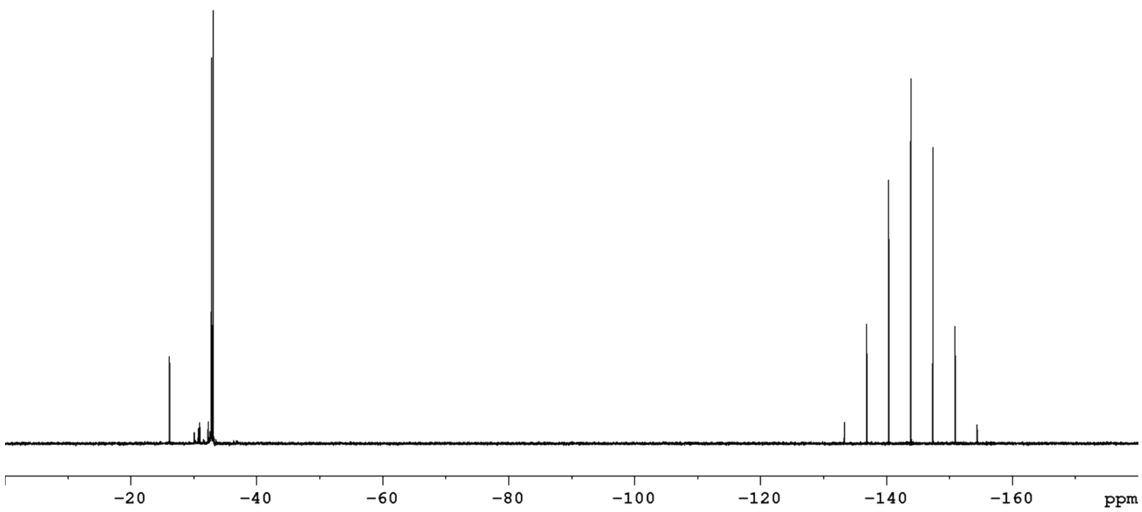


Figure S21. $^{31}P\{^1H\}$ NMR spectrum of **2**.

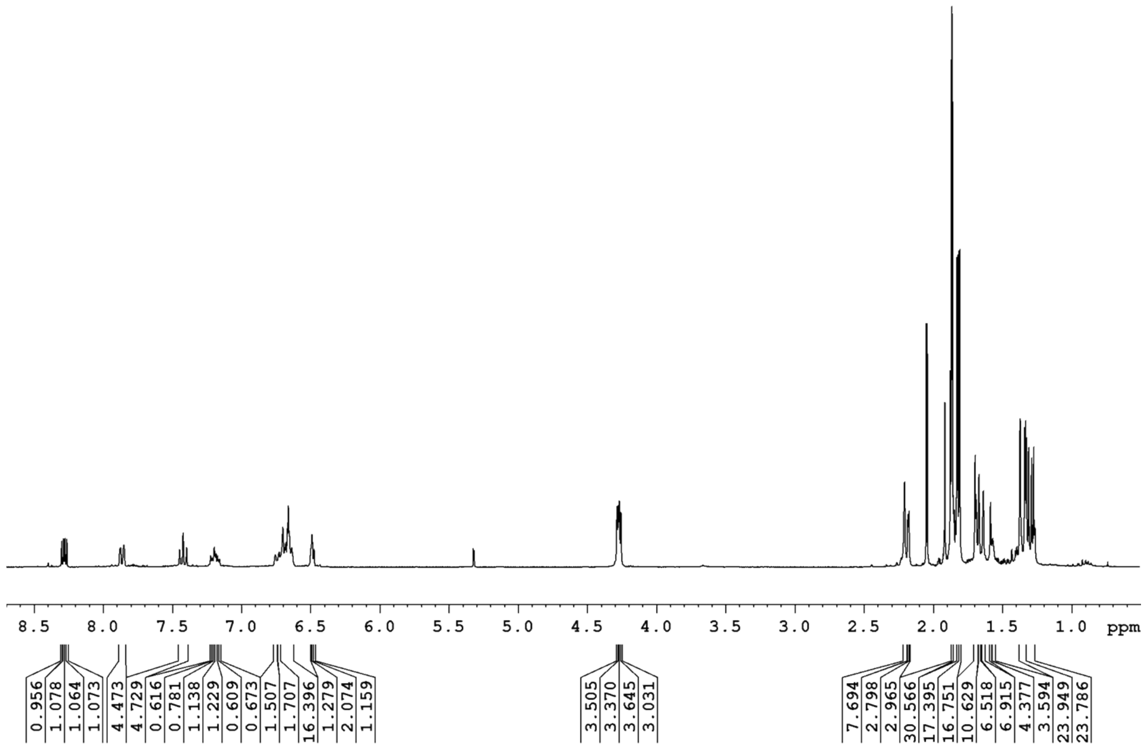


Figure S22. ^{1}H NMR spectrum of **2**.

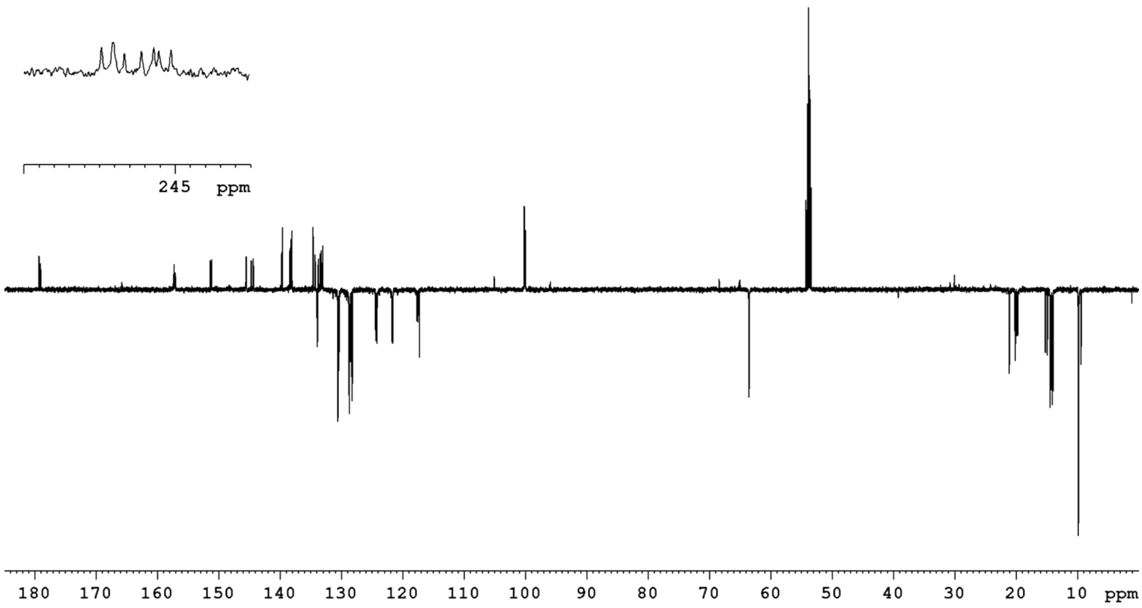


Figure S23. JMOD NMR spectrum of **2**.

Mass Spectrum List Report

Analysis Info	**Electrospray (ESI)**		
Analysis Name	PGXSCX33088801_000001.d	Acquisition Date	29/01/2020 10:49:57
Sample Name	SBF4_B	Instrument	solariX XR

Acquisition Parameter

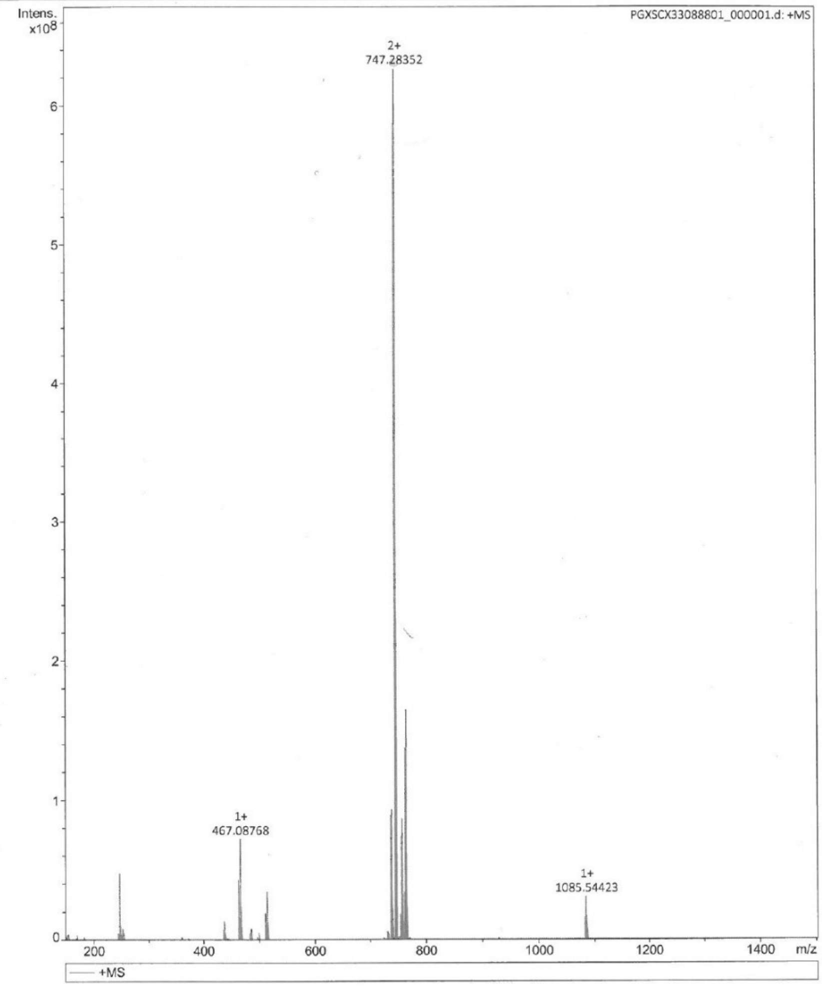


Figure S24. HR-ESI-MS spectrum of **2**.

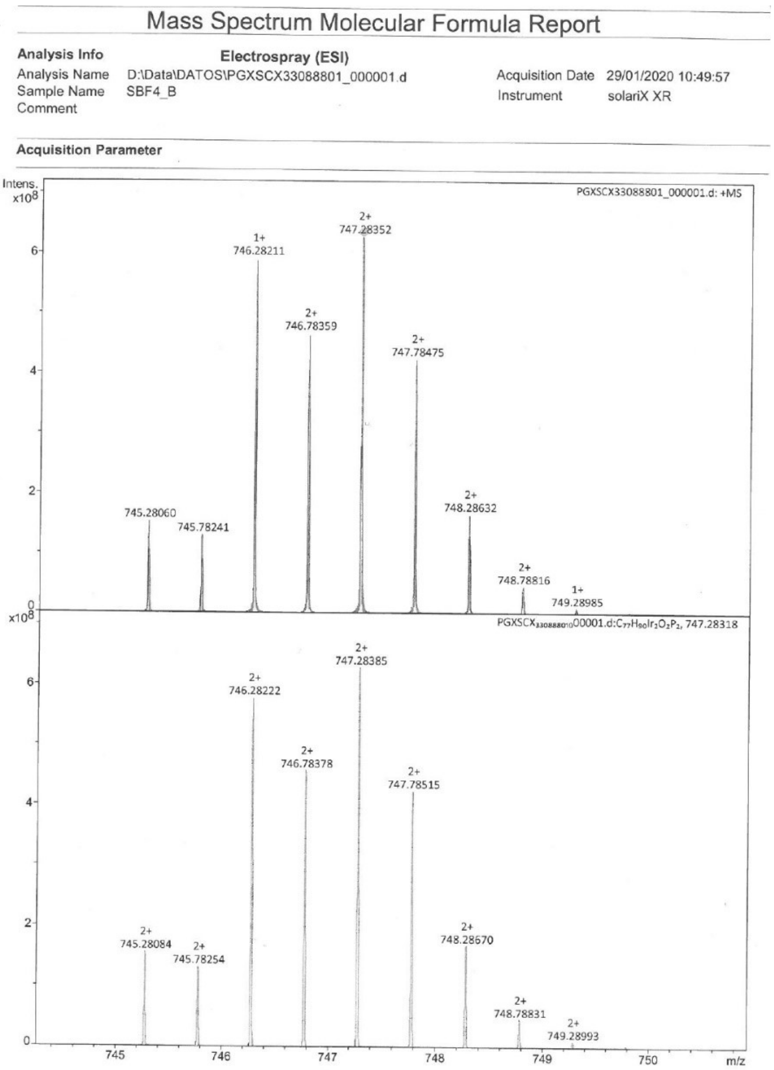
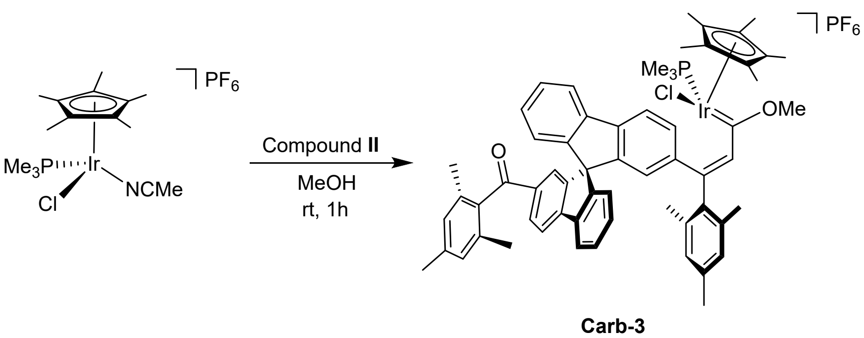


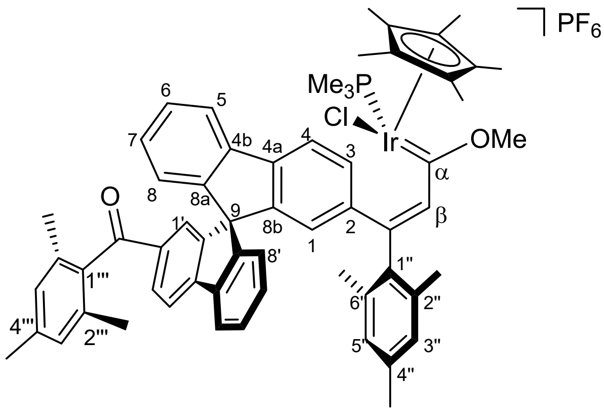
Figure S25. Comparison between experimental (top) and theoretical (bottom) HR-ESI-MS spectra of **2**.

Preparation of [IrCp*Cl(PMe$_3$){=C(OMe)–CH=C(2,4,6-Me$_3$C$_6$H$_2$)(2-(2'-CO-mesityl)-SBF)}]PF$_6$ (Carb-3)



Carb-3

To a yellow solution of [IrCp*Cl(NCMe)(PMe$_3$)]PF$_6$ (500 mg, 0.8 mmol) in 35 ml of methanol, the propargylic alcohol **II** (539 mg, 0.85 mmol) was added and the mixture was stirred for 1 h at room temperature. The dark red suspension obtained was vacuum concentrated obtaining a red solid which was washed with a mixture of Et_2O/pentane 1/3 (3 × 10 mL) and dried in vacuum. Yield: 887 mg (90%). Complex **Carb-3** was isolated as a mixture of isomers together with small impurities. Therefore, its nature was confirmed via mass spectrometry and its reactivity to provide complex **3**.



$C_{61}H_{64}O2ClF_6IrP_2$ (1232.77 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{61}H_{64}O_2ClIrP$ $[M]^+$ 1087.3953 found 1087.3963.

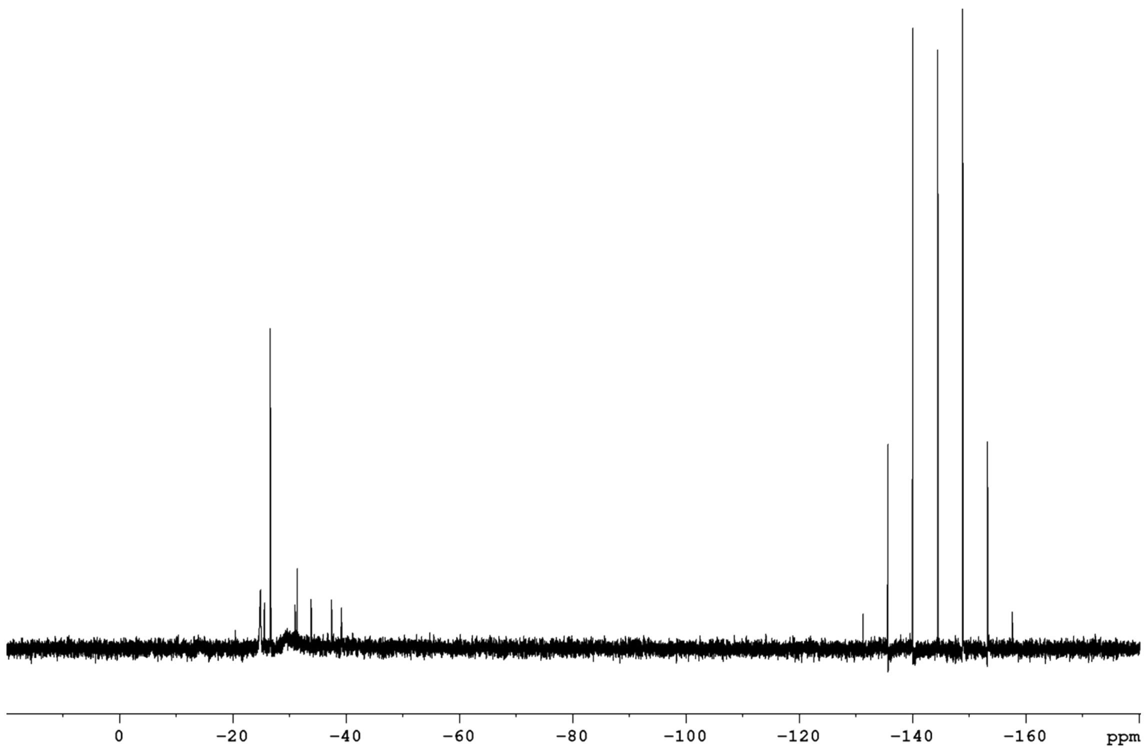


Figure S26. $^{31}P\{^1H\}$ NMR spectrum of **Carb-3**.

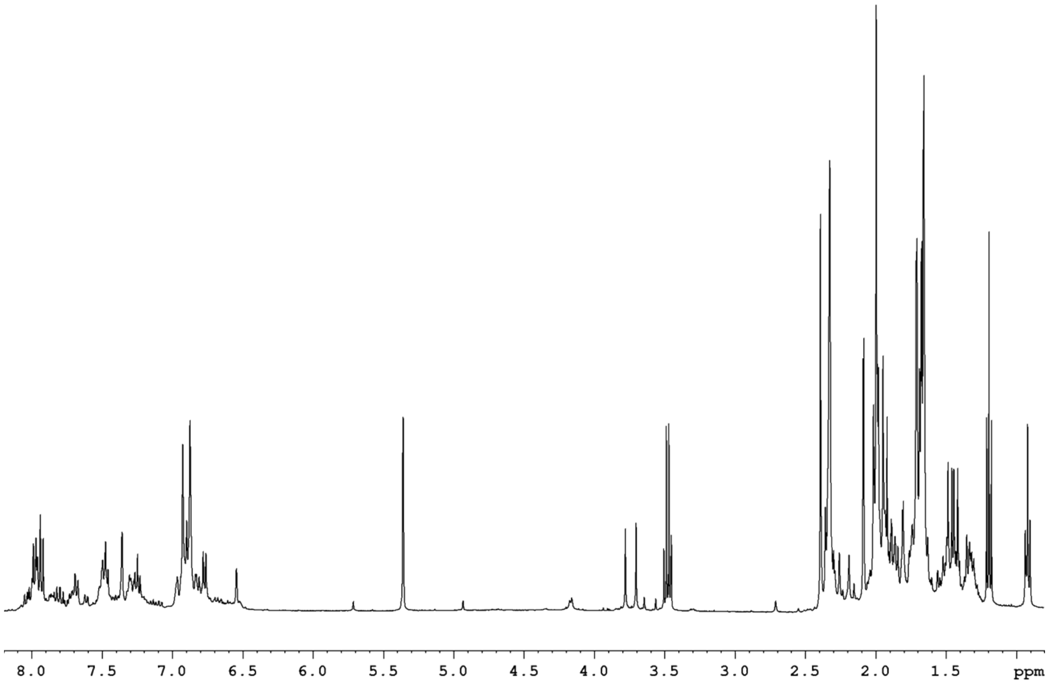


Figure S27. [1]H NMR spectrum of **Carb-3**.

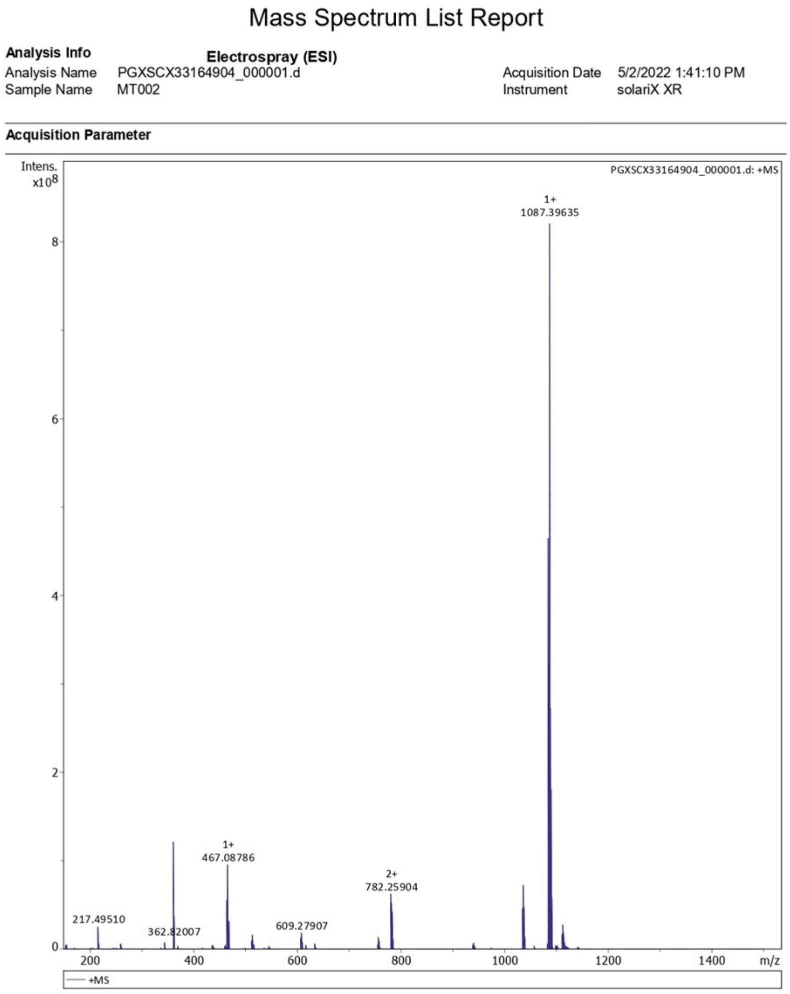


Figure S28. HR-ESI-MS spectrum of **Carb-3**.

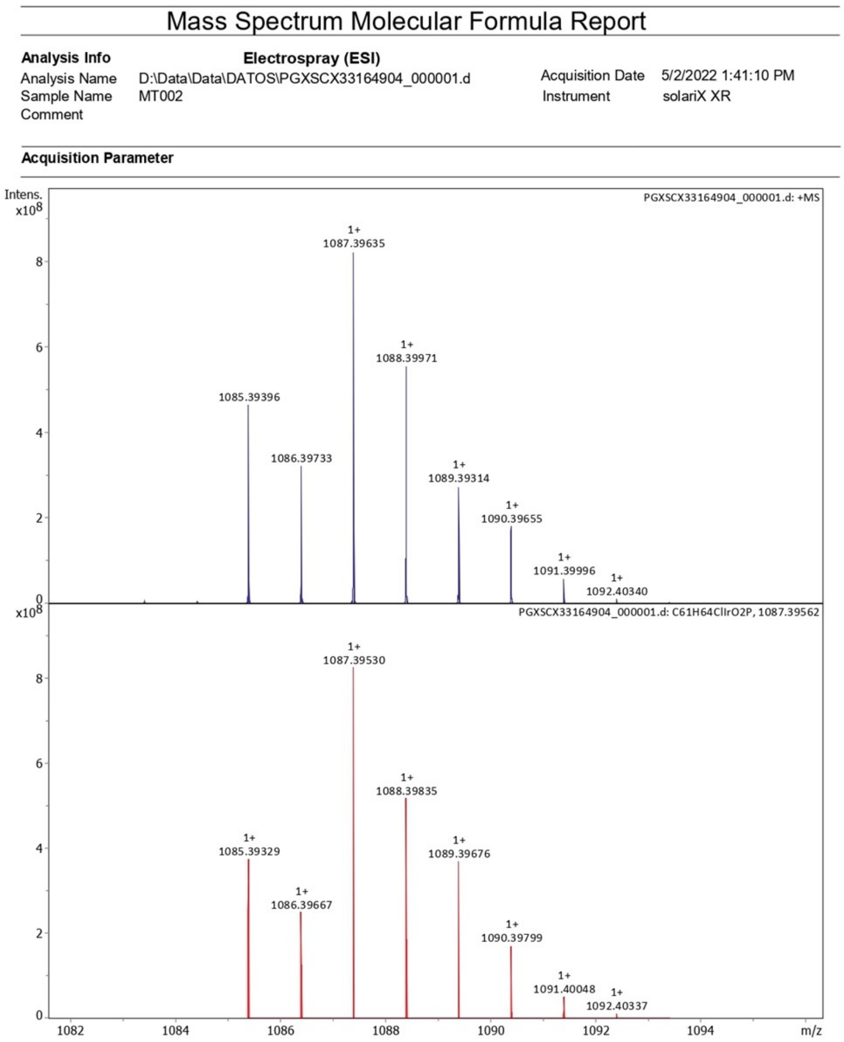
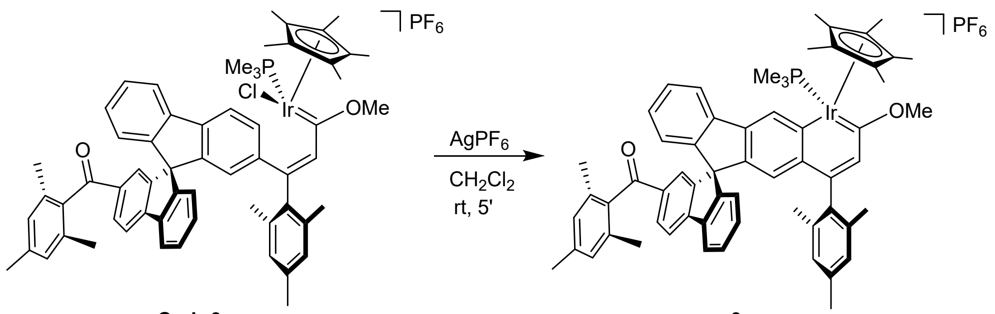


Figure S29. Comparison between experimental (top) and theoretical (bottom) HR-ESI-MS spectra of **Carb-3**.

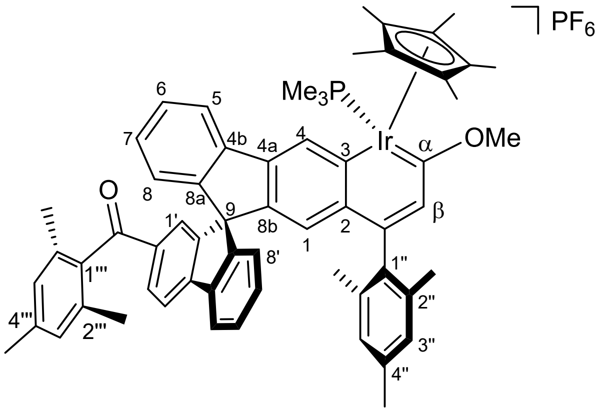
Preparation of [IrCp*Cl(PMe$_3$){=C(OMe)–CH=C(2,4,6-Me$_3$C$_6$H$_2$)(κ^2-2,3-(2'-CO-mesityl)-SBF)}]PF$_6$ (3)



Carb-3 **3**

A dark brown solution of Carb-**3** (887 mg, 0.72 mmol) in 30 mL of dichloromethane was treated with AgPF$_6$ (539 mg, 0.85 mmol). The solution was stirred for 10 min at room temperature, filtered and vacuum concentrated, obtaining a brown solid that was washed with Et_2O/pentane (1/1) (3 × 4 mL) and dried in vacuum. The residue was purified by column chromatography (SiO_2, gradient CH_2Cl_2/MeCN from 100/0 to 90/10) affording complex **3**. Yield: 749 mg (87 % from acetonitrile complex).

There are 2 possible diastereoisomers in a 1:1 ratio. Although it is possible to identify each fluorene branch, due to the lack of correlation between branches at the same complex, the very similar nature of all the resonances and the spatial arrangement of the SBF moiety, it was not possible to separate the signals of each isomer and assign them.



$C_{61}H_{63}O_2F_6IrP_2$ (1196.31 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{61}H_{63}O_2IrP$ [M]$^+$ 1051.4195 found 1051.4208. **^{1}H NMR (300 MHz)**: δ 8.47 and 8.44 (both s, 1H, H^4); 7.99 (apparent t, 2H, $^3J_{HH}$ = 7.1 Hz, H^5); 7.83-7.79 (m 2H, $H^{5'}$); 7.77 and 7.76 (both d, $^3J_{HH}$ = 7.9 Hz, 1H, $H^{4'}$); 7.63 and 7.54 (both d, $^3J_{HH}$ = 8.0 Hz, 1H, $H^{3'}$); 7.47 and 7.46 (both t, 1H, $^3J_{HH}$ = 7.6 Hz, H^6); 7.41-7.33 (m, 2H, $H^{6'}$); 7.40 (s, 1H, $H^{1'}$); 7.25-7.13 (m, 4H, H^7 + $H^{7'}$); 7.19 (s, 1H, $H^{1'}$); 6.87 (s, 2H, $H^{3'''}$); 6.86 (s, 1H, H^1); 6.83 (s br, 3H, $H^1 + H^{3'''}$); 6.75 (s, 1H, $H^{3''}$); 6.73-6.70 (m, 3H, $H^{8'}$+ $H^{3''}$); 6.69-6.66 (m, 3H, H^8 + $H^{3''}$); 6.65 (s, 1H, $H^{3''}$); 6.52 (s, 2H, H^β); 4.29 (s, 6H, OCH_3); 2.31 and 2.29 (both s, 3H, $C^{4'''}CH_3$); 2.19 (s, 6H, $C^{4''}CH_3$); 1.97 and 1.93 (both s, 6H, $C^{2'''}CH_3$); 1.89 (d, 30H, $^4J_{HP}$ = 1.6 Hz, $C_5(CH_3)_5$); 1.80, 1.75, 1.72 and 1.69 (all s, 3H, $C^{2''}CH_3$); 1.42 and 1.39 (both d, 9H, $^2J_{HP}$ = 11.0 Hz, $P(CH_3)_3$) ppm. **^{31}P{^{1}H} NMR (162 MHz)**: δ –33.27 (s, $P(CH_3)_3$); –144.47 (sept, $^1J_{PF}$ = 710.5 Hz, PF_6) ppm. **^{13}C{^{1}H} NMR (125.7 MHz)**: δ 245.2 and 245.1 (both d, $^2J_{CP}$ = 10.1 Hz, C^α); 199.8 and 199.7 (both s, *C*O); 179.4 and 179.3 (both s, C^γ); 158.0 and 157.7 (both d, $^2J_{CP}$ = 10.6 Hz, C^3); 151.2 and 151.1 (both s, C^{8a}); 150.0 and 149.9 (both s, $C^{8a'}$); 149.3 and 149.2 (both s, $C^{8b'}$); 147.2 and 147.1 (both s, $C^{4a'}$); 146.0 and 145.9 (both s, C^{4a}); 143.83 and 143.78 (both s, C^{8b}), 140.3 and 140.2 (both s, $C^{4b'}$); 139.83 and 139.80 (both s, C^{4b}); 138.9 and 138.8 (both s, $C^{4'''}$); 138.3 (s, 2C $C^{4''}$); 138.0 (s, 2C $C^{1''}$); 137.27, 137.24, 137.21 and 137.17 (all s, $C^{2'} + C^{1'''}$); 134.3 (2C), 134.23 and 134.18 (all s, $C^{2'''}$); 134.07, 134.04 (2C) and 133.99 (all s, $C^{2''}$); 133.8 and 133.7 (both s, $C^{2''} + C^{4}$); 133.2 (s, 2C C^{2}); 131.2 and 130.6 (both s, $C^{3'}$); 131.0 and 130.9 (both s, C^{1}); 130.4 (s, 2C, C^{7}); 129.7 (s, 2C, $C^{7'}$); 128.73 and 128.7 (both s, C^{6}); 128.57 (various C), 128.55 (various C), 128.5, 128.43 and 128.40 (all s, $C^{6'} + C^{3''} + C^{3'''}$); 124.4, 124.3, 124.0 and 123.9 (all s, $C^{8'} + C^{8}$); 123.8 and 123.6 (both s, $C^{1'}$); 121.8 (s, 2C C^{5}); 121.60 and 121.57 (both s, $C^{5'}$); 120.7 and 120.6 (both s, $C^{4'}$); 117.4 and 117.5 (both d, $^{3}J_{CP} = 1.8$ Hz, C^{β}); 100.1 and 100.0 (both d, $^{2}J_{CP} = 1.8$ Hz, $C_5(CH_3)_5$); 65.70 and 65.67 (both s, C^{9}); 63.4 (s, OCH_3); 21.31 and 21.29 (all s, $C^{4'''}CH_3$); 21.0 (all s, $C^{4''}CH_3$); 20.1, 20.0 and 19.9 (2C) (all s, $C^{2''}CH_3$); 19.44 and 19.41 (both s, $C^{2'''}CH_3$); 14.4 and 14.2 (both d, $^{1}J_{CP} = 41.0$ Hz, $P(CH_3)_3$); 9.80 and 9.78 (both s, $C_5(CH_3)_5$) ppm.

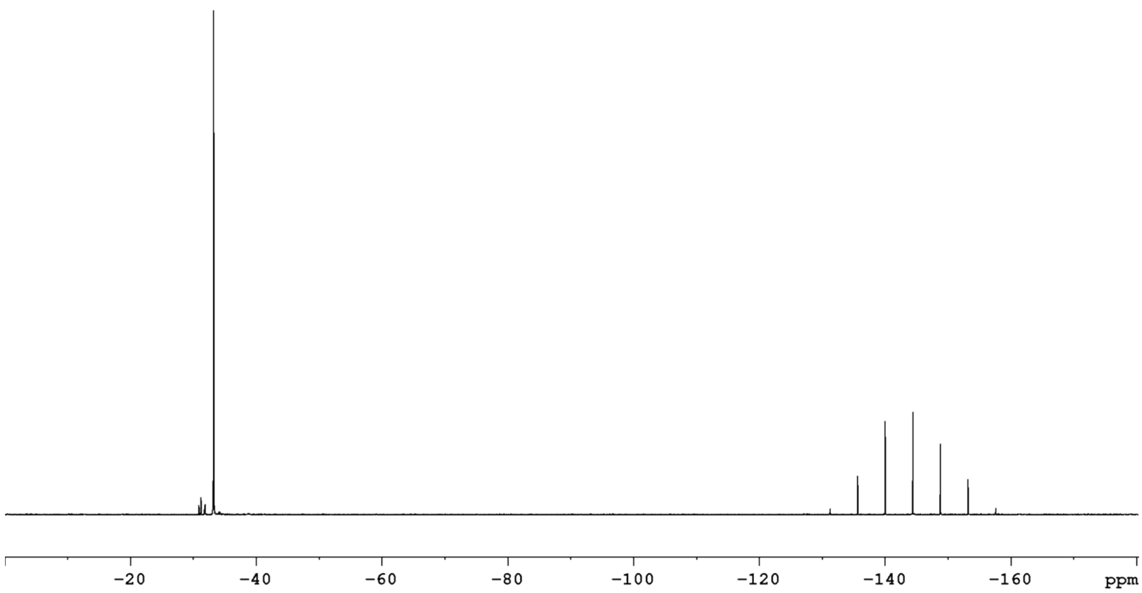


Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum of **3**.

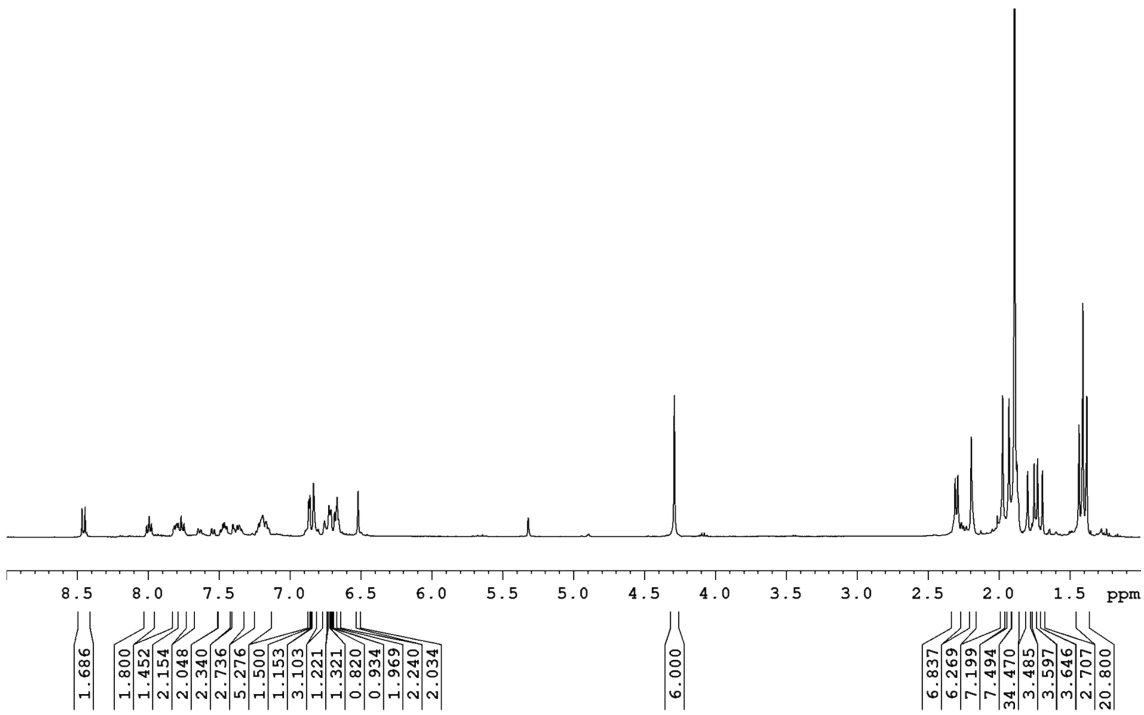


Figure S31. ^{1}H NMR spectrum of **3**.

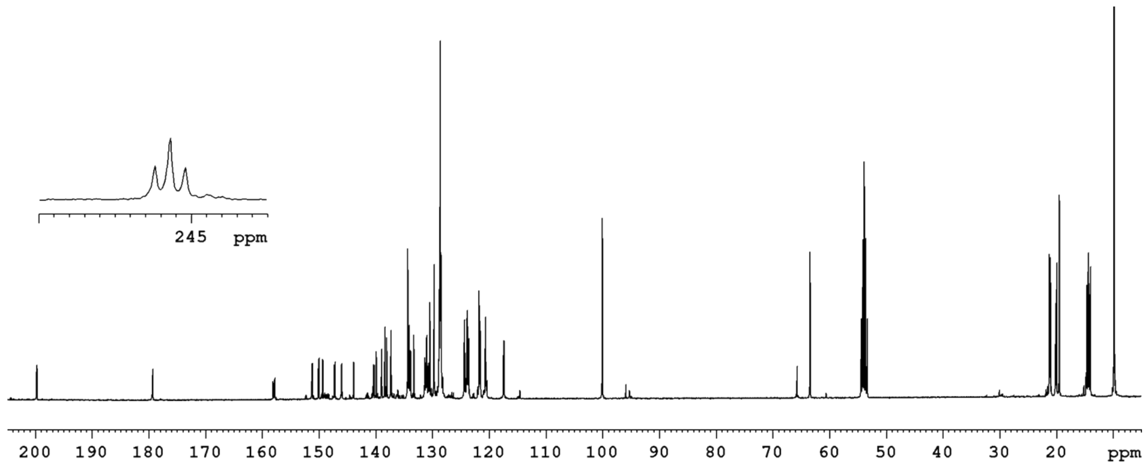


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of **3**.

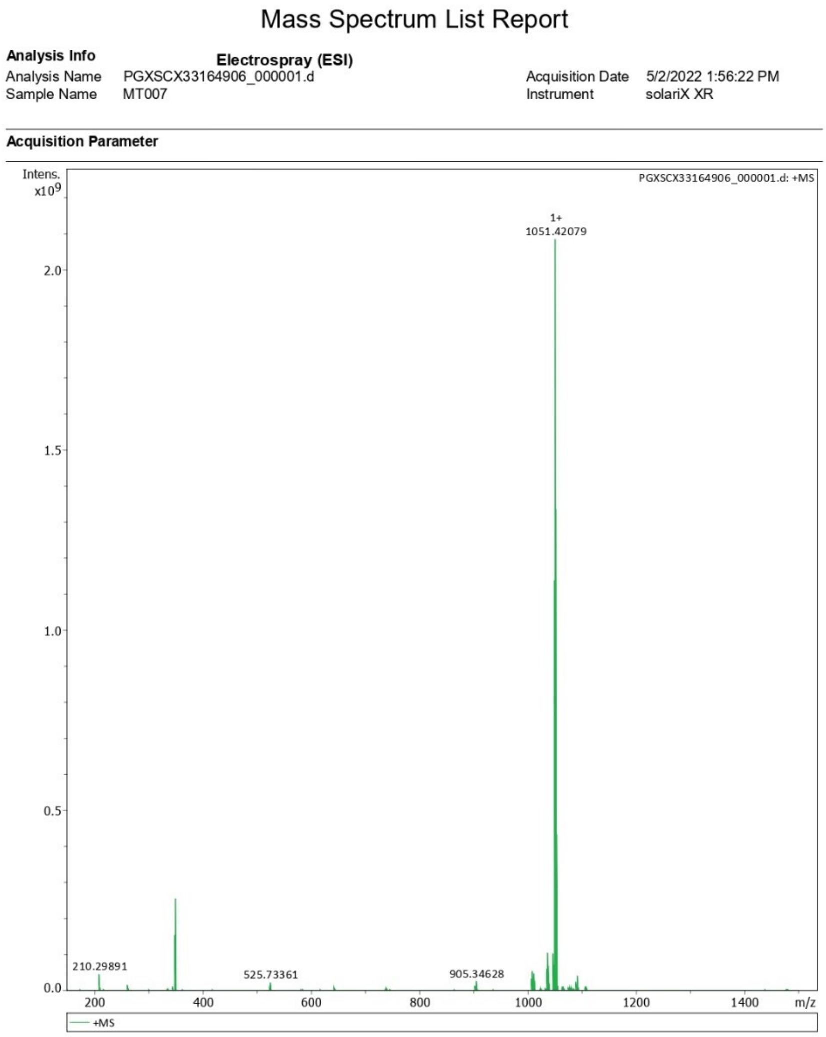


Figure S33. HR-ESI-MS spectrum of **3**.

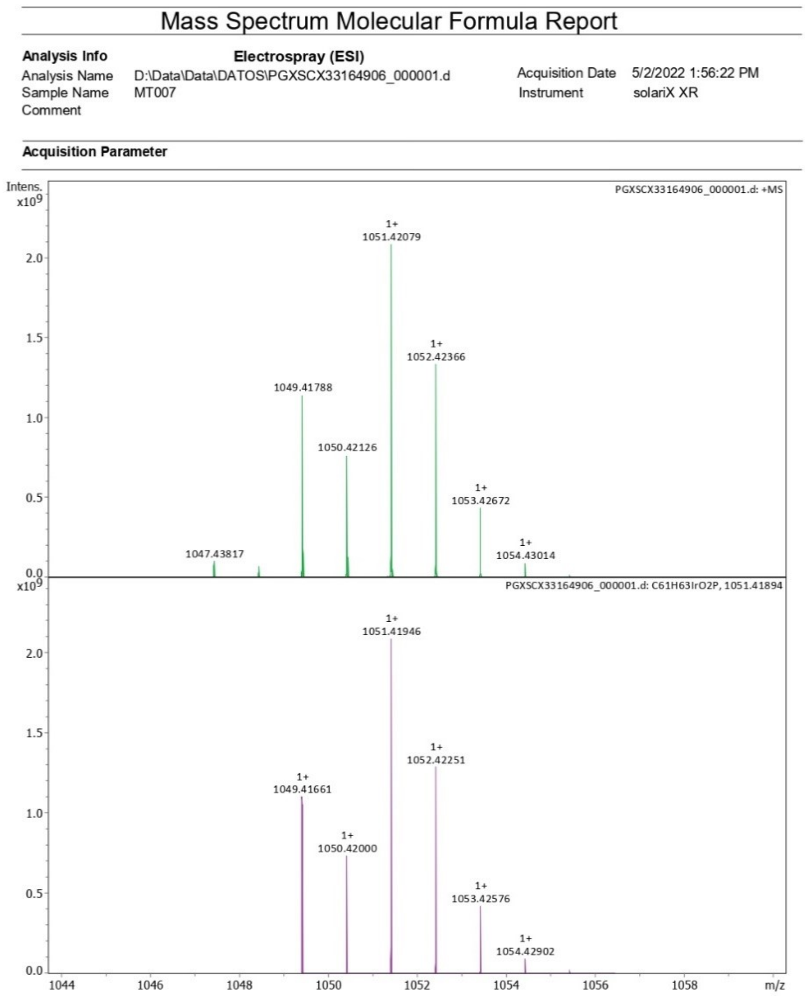
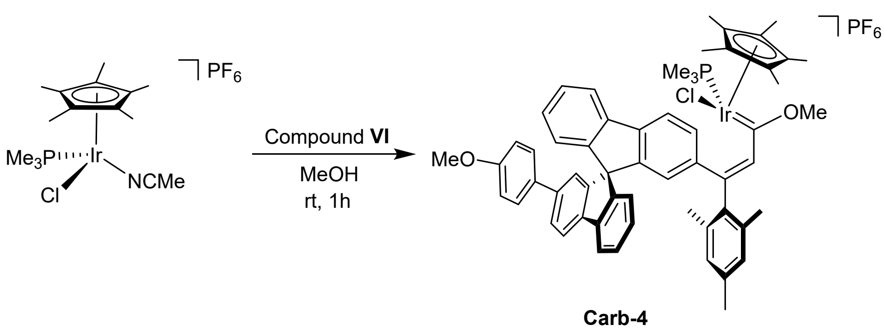


Figure S34. Comparison between experimental (top) and theoretical (bottom) HR-ESI-MS spectra of **3**.

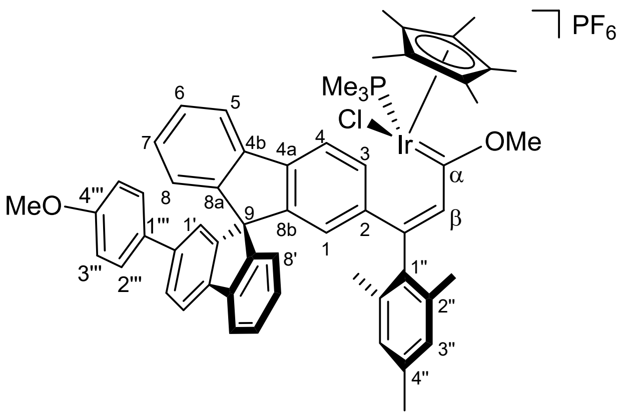
Preparation of [IrCp*Cl(PMe$_3$){=C(OMe)–CH=C(2,4,6-Me$_3$C$_6$H$_2$)(κ^1-2-(2’-*p*-methoxyphenyl)-SBF)}]PF$_6$ (Carb-4)



Carb-4

To a yellow solution of [IrCp*Cl(NCMe)(PMe$_3$)]PF$_6$ ((156 mg, 0.25 mmol) in 20 ml of methanol, the propargylic alcohol **VI** (177 mg, 0.30 mmol) was added and the mixture was stirred for 1 h at room temperature. The dark suspension obtained was vacuum concentrated obtaining a brown solid which was washed with a mixture of Et$_2$O/pentane 1/3 (3 × 5 mL) and dried in vacuum. Yield: 277 mg (≈ 93%). Complex

Carb-**4** was isolated as a mixture of isomers together with small impurities. Therefore, its nature was confirmed via mass spectrometry and its reactivity to provide complex **4**.



$C_{58}H_{60}O_2ClF_6IrP_2$ (1192.70 g/mol). **HRMS** (ESI$^+$): *m/z* Calcd. for $C_{58}H_{60}O_2ClIrP$ $[M]^+$ 1047.3640 found 1047.3644.

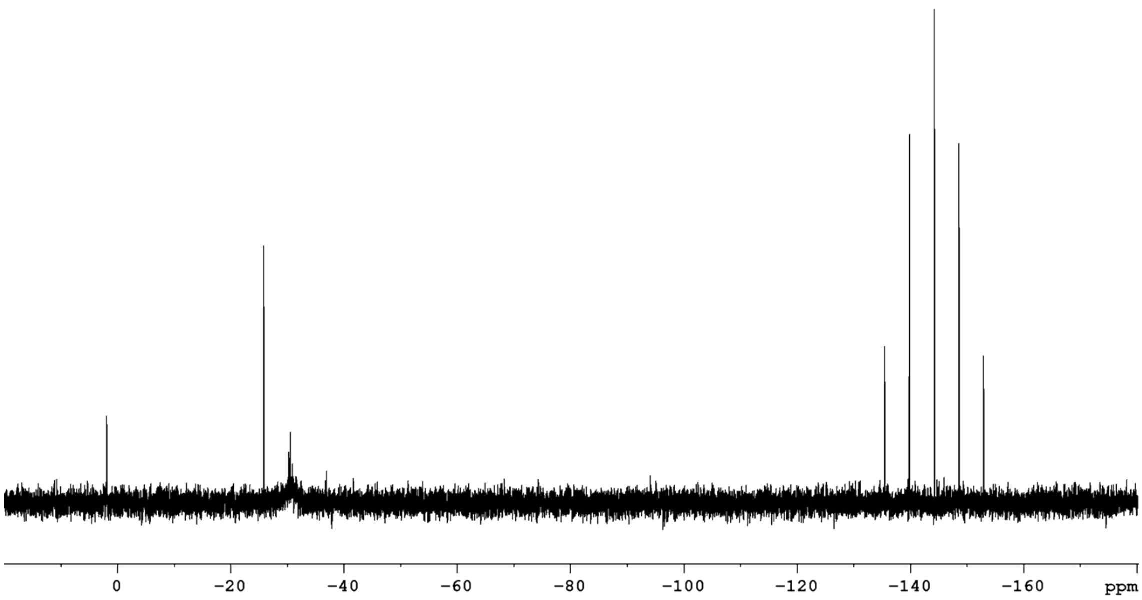


Figure S35. $^{31}P\{^1H\}$ NMR spectrum of **Carb-4**.

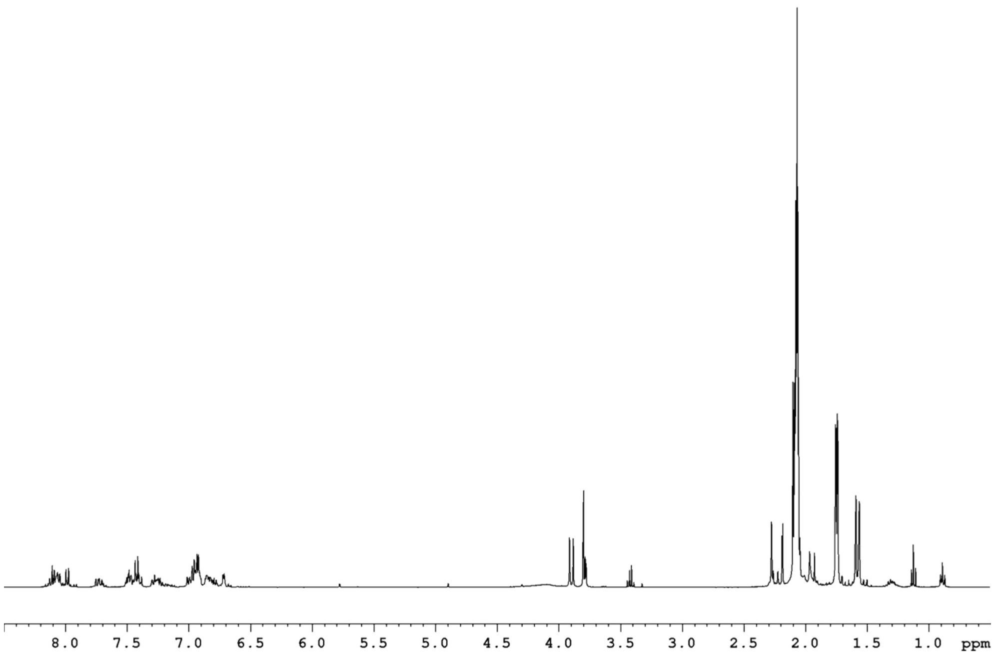


Figure S36. ^{1}H NMR spectrum of **Carb-4**.

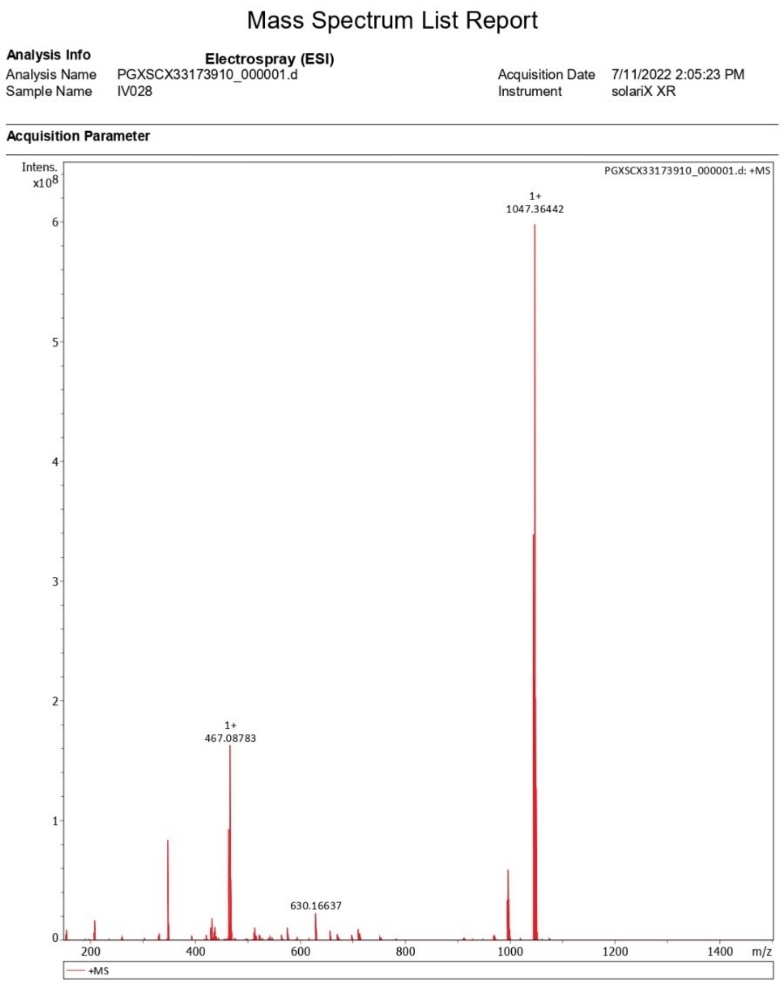


Figure S37. HR-ESI-MS spectrum of **Carb-4**.

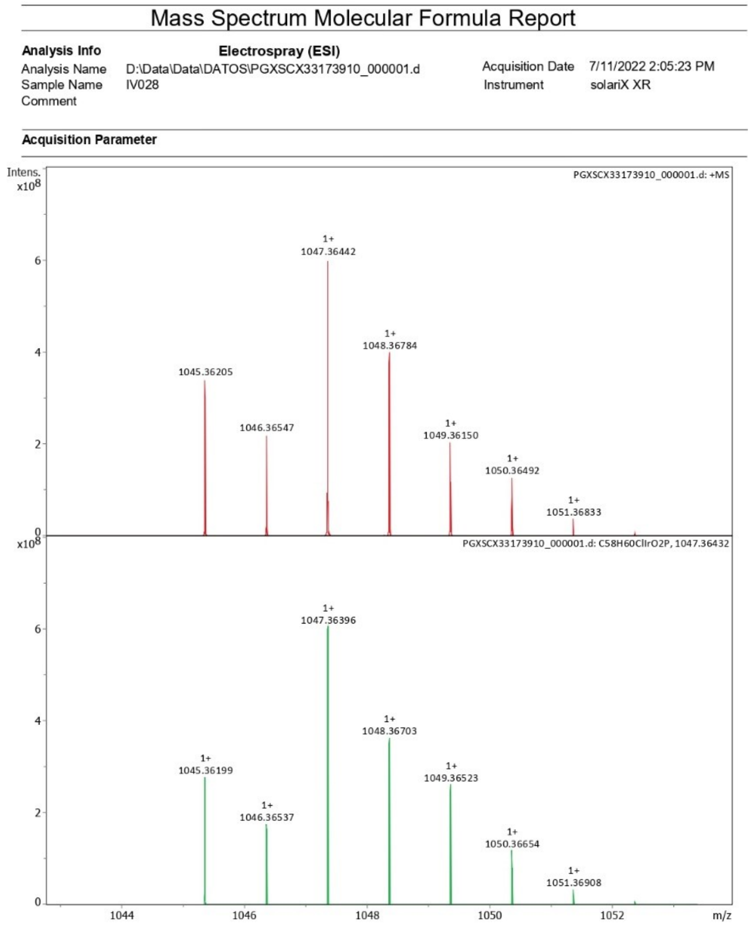
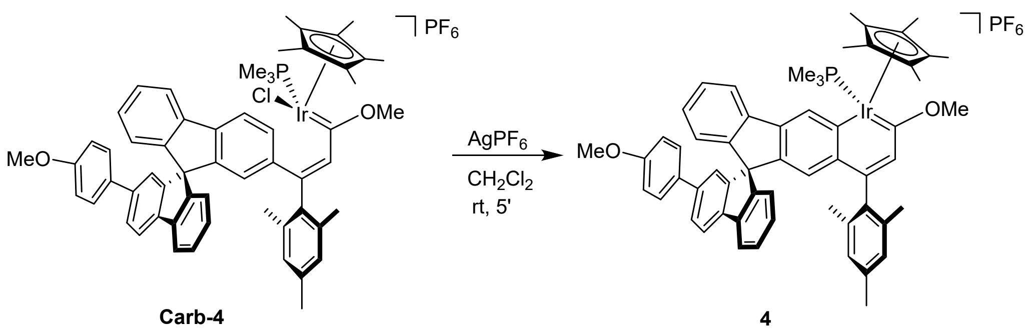


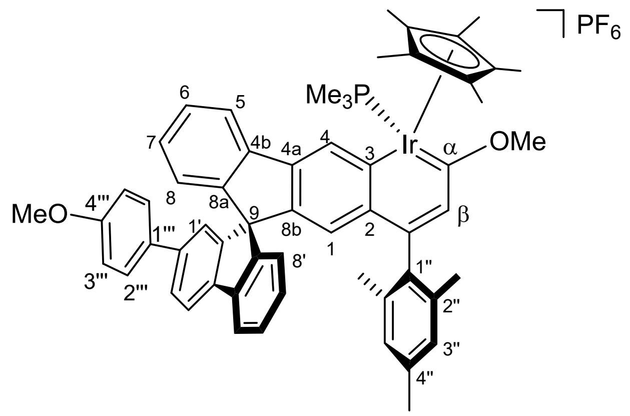
Figure S38. Comparison between experimental (top) and theoretical (bottom) HR-ESI-MS spectra of **Carb-4**.

Preparation of [IrCp*Cl(PMe$_3$){=C(OMe)–CH=C(2,4,6-Me$_3$C$_6$H$_2$)(κ^2-2,3-(2’-*p*-methoxyphenyl)-SBF)}]PF$_6$ (4)



A dark brown solution of **Carb-4** (277 mg, 0.232 mmol) in 10 mL of dichloromethane was treated with AgPF$_6$ (64 mg, 0.25 mmol). The solution was stirred for 10 min at room temperature, filtered and vacuum concentrated, obtaining a brown solid that was washed with Et$_2$O/pentane (1/1) (3 × 4 mL) and dried in vacuum. The residue was purified by column chromatography (SiO_2, gradient CH_2Cl_2/MeCN from 100/0 to 90/10) affording complex **4**. Yield: 233 mg (87 %).

There are 2 possible diastereoisomers in a 1:1.1 ratio. Although it is possible to identify each fluorene branch, due to the lack of correlation between branches at the same complex, the very similar nature of all the resonances and the spatial arrangement of the SBF moiety, it was not possible to separate the signals of each isomer and assign them.



$C_{58}H_{59}O_2F_6IrP_2$ (1156.24 g/mol). **HRMS** (ESI^+): *m/z* Calcd. for $C_{58}H_{59}O_2IrP$ $[M]^+$ 1011.3881 found 1011.3881. **^{1}H NMR (300 MHz)**: 8.69 and 8.68 (both s, 1H, H^{4}); 8.18 (d, 2H, $^3J_{HH}$ = 7.3 Hz, H^{5}); 7.91-7.83 (m, 4H, $H^{5'} + H^{4'}$); 7.61-7.54 (m, 2H, $H^{3'}$); 7.46-7.40 (m, 2H, H^{6}); 7.39-7.33 (m, 2H, $H^{6'}$); 7.33-7.28 (m, 4H, $H^{2'''}$); 7.24-7.18 (m, 2H, H^{7}); 7.15-7.07 (m, 2H, $H^{7'}$); 7.00 and 6.99 (both s, 1H, H^{1}); 6.93-6.84 (m, 7H, $H^{8'} + H^{3''} + H^{1''}$); 6.77-6.67 (m, 2H, H^{β}); 6.67-6.61 (m, 6H, $H^{8} + H^{3'''}$); 4.53 and 4.52 (both s, 3H, C_{α}-OCH_3); 3.76 and 3.75 (both s, 3H, Ph-OCH_3); 2.14 (s, 6H, $C^{4''}CH_3$); 2.00 (d, 30H, $^4J_{HP}$ = 1.5 Hz, $C_5(CH_3)_5$); 1.86, 1.804, 1.797 and 1.71 (all s, 3H, $C^{2''}CH_3$); 1.540 and 1.537 (both d, 9H, $^2J_{HP}$ = 11.0 Hz, $P(CH_3)_3$) ppm. **^{31}P{^{1}H} NMR (162 MHz)**: δ –33.81 (s, $P(CH_3)_3$); –33.82 (s, $P(CH_3)_3$); –144.21 (sept, $^1J_{PF}$ = 703.7 Hz, PF_6) ppm. **^{13}C{^{1}H} NMR (125.7 MHz)**: δ 246.7 and 246.6 (both d, $^2J_{CP}$ = 10.9 Hz, C^{α}); 178.6 (s, 2C C^{γ}); 160.32 and 160.27 (both s, $C^{4'''}$); 158.1 and 158.0 (both d, $^2J_{CP}$ = 8.2 Hz, C^{3}); 152.6 and 152.59 (both s, C^{8a}); 150.4 and 150.3 (both s, $C^{8b'}$); 149.5 and 149.4 (both s, $C^{8a'}$); 146.4 and 146.2 (both s, C^{4a}); 145.0 and 144.9 (both s, C^{8b}), 142.2 and 142.1 (both s, $C^{4b'}$); 141.4 and 141.3 (both s, $C^{4a'}$); 141.0 and 140.9 (both s, $C^{1'''}$); 140.64 and 140.58 (both s, C^{4b}); 139.0 (s, 2C $C^{1''}$); 138.4 and 138.3 (both s, $C^{4''}$); 135.0 (s, C^{4}); 134.94, 134.89, 134.43 and 134.40 (all s, $C^{2''}$); 133.90 and 133.87 (both s, $C^{2'}$); 133.8 (s, 2C, C^{2}); 131.1 (s, 2C C^{1}); 130.6 (s, 2C C^{7}); 129.03, 129.01, 128.94, 128.92, 128.87, 128.61, 128.57, 128.53 and 128.48 (all s,

$C^{2'''}$ + $C^{7'}$ + $C^{6'}$ +C^{6}); 127.33 and 127.27 (both s, $C^{3'}$); 124.3 and 124.2 (s, 2C $C^{3''}$); 124.7 (s, 2C C^{8}); 122.5 (s, 2C C^{5}); 122.4 and 122.2 (both s, $C^{1'}$); 122.1 and 121.9 (both s, $C^{8'}$); 121.6, 121.5, 121.2 and 121.1 (all s, $C^{5'}$ + $C^{4'}$); 118.8 and 118.7 (both d, $^{3}J_{CP}$ = 1.9 Hz, C^{β}); 115.1 and 115.0 (all s, 2C $C^{3'''}$); 100.5 (d, $^{2}J_{CP}$ = 1.8 Hz, $C_5(CH_3)_5$); 66.5 (s, C^{9}); 64.2 and 64.1 (both s, C^{α}-OCH$_3$); 55.6 (s br, Ph-OCH$_3$); 20.9 (s, $C^{4''}$$CH_3$); 20.3, 20.2, 20.1 and 20.0 (all s, $C^{2''}$$CH_3$); 14.2 and 14.1 (both d, $^{1}J_{CP}$ = 40.9 Hz, P(CH$_3$)$_3$); 9.8 (s, C_5(CH$_3$)$_5$) ppm.

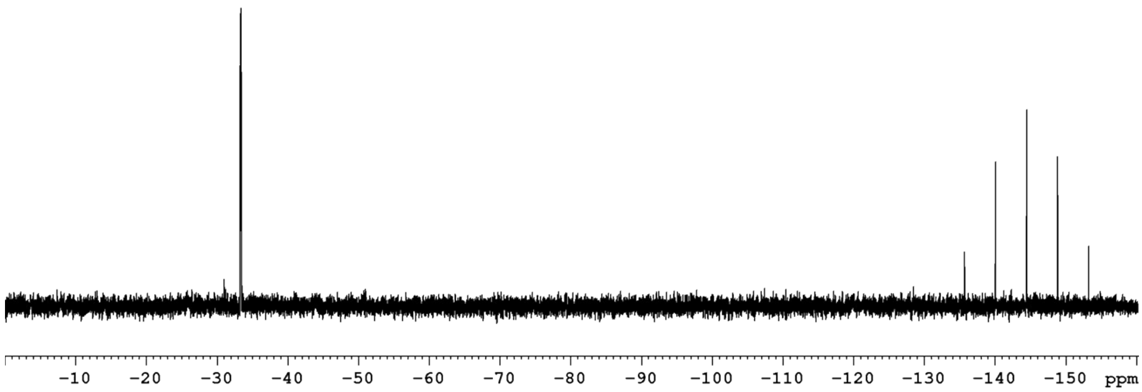


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum of **4**.

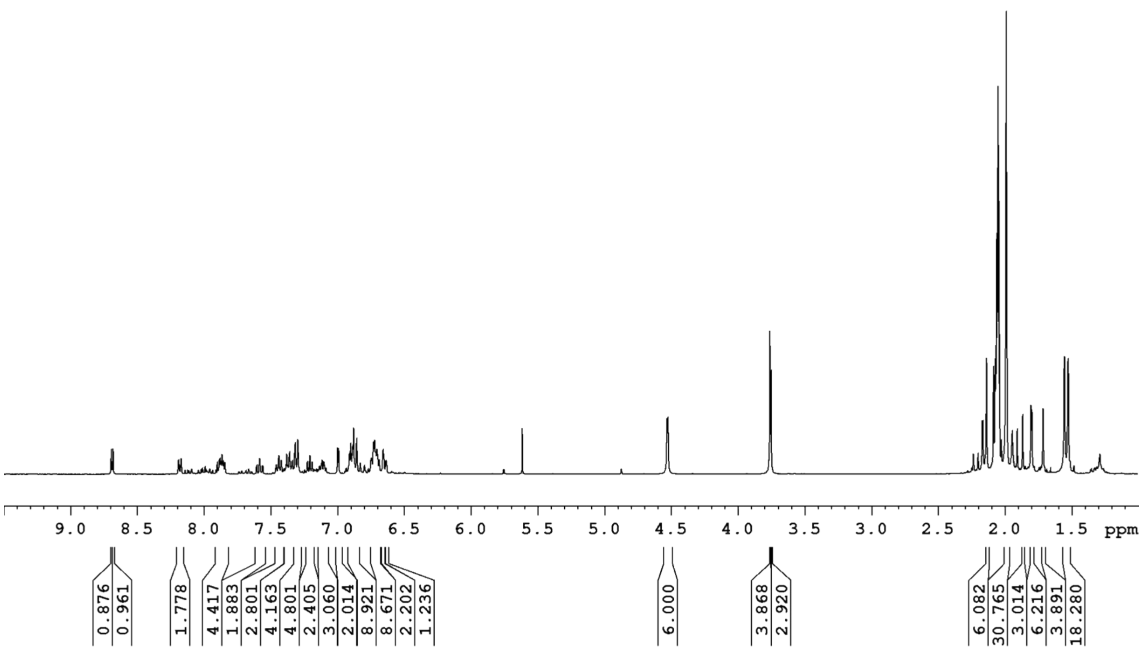


Figure S40. ^{1}H NMR spectrum of **4**.

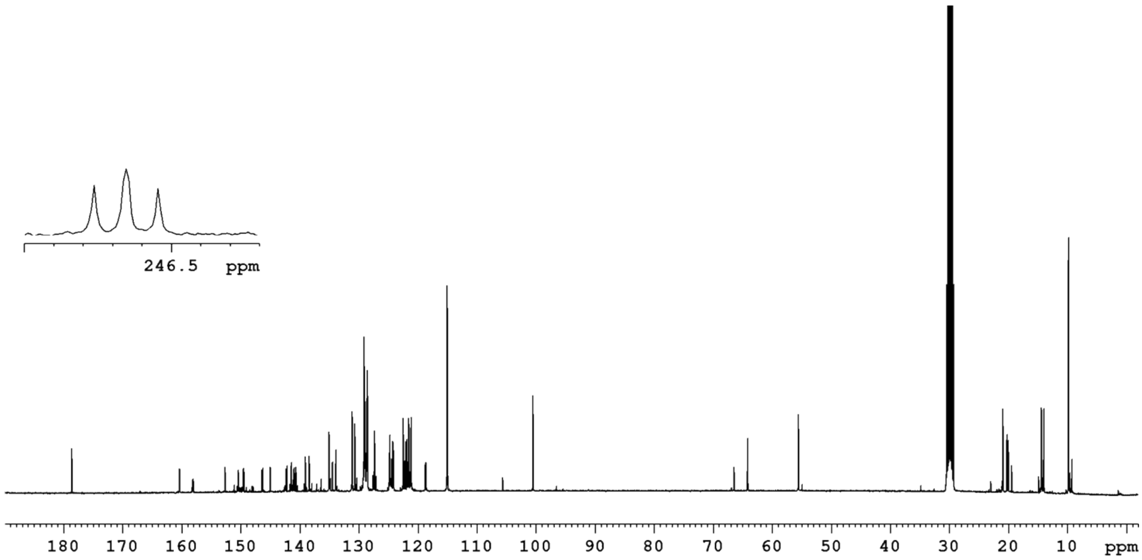


Figure S41. $^{13}C\{^1H\}$ NMR spectrum of **4**.

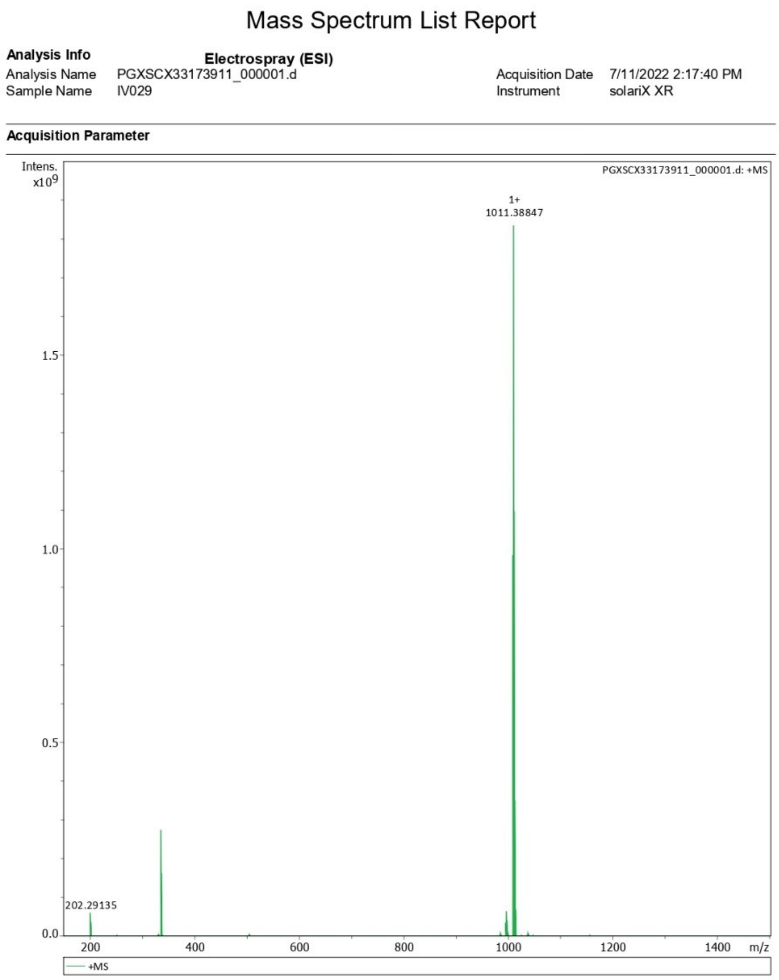


Figure S42. HR-ESI-MS spectrum of **4**.

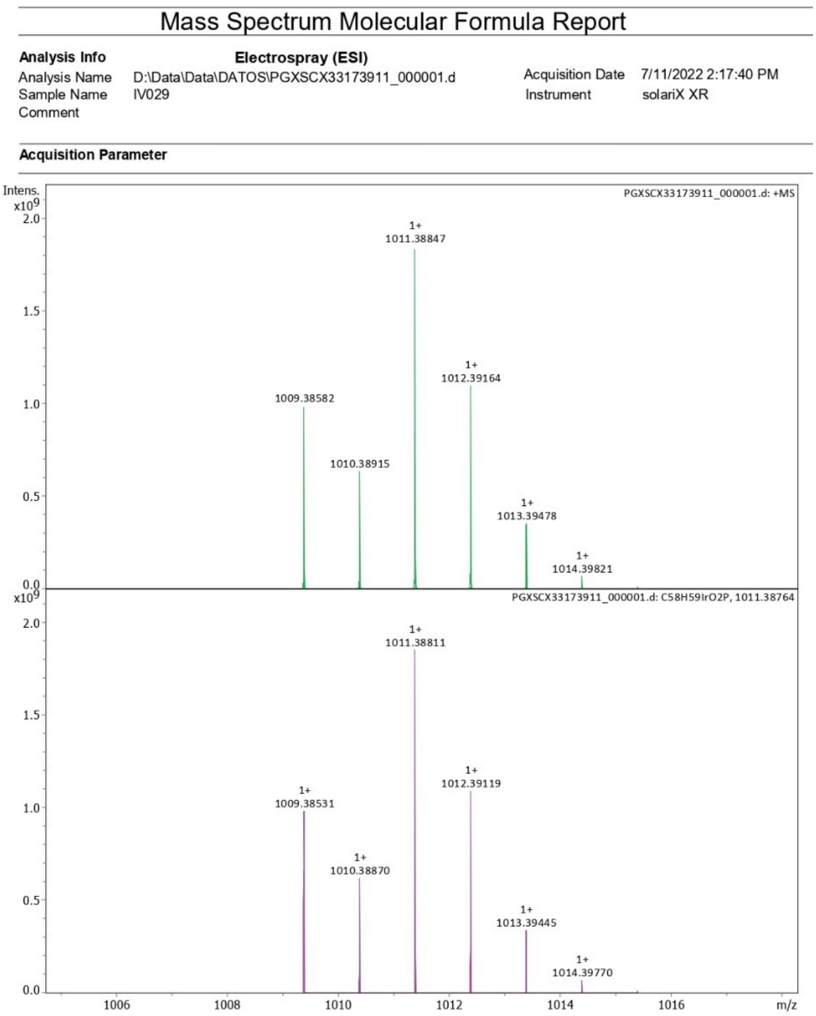


Figure S43 Comparison between experimental (top) and theoretical (bottom) HR-ESI-MS spectra of **4**.

X-ray Diffraction Analysis

Methodology

Crystallographic data for complexes **2** and **3** was collected on a Bruker D8 Venture Photon 100 CMOS diffractometer at 100 K using Mo-Kα radiation (λ = 0.71073 Å). The frames were integrated with the Bruker SAINT[3] software package and the data were corrected for absorption using the program SADABS-2016/2.[4] The structures were solved by direct methods using the program SHELXL-2019/2.[5] All non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least-squares calculations on F^2 using the program SHELXL-2019/2.[6] Hydrogen atoms were inserted at calculated positions and were constrained with isotropic thermal parameters. In both cases disorder solvent molecules were present. Disorder water solvent molecules were not modelled and the disordered density was taken into account using the SQUEEZE/PLATON procedure.[7]

CCDC 2215145 and 2215146 contain the supplementary crystallographic data for **2** and **3**, respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/data_request/cif.

Both crystals show disorder at the iridium centers which was refined with an occupancy of 86% for Ir(1A) and 90% for Ir(2A) in complex **2** and 88% for Ir(1A) in complex **3**.

Table S1. Crystal data and structure refinement for complexes **2** and **3**.

Complex	**3**	**2**
Empirical formula	$C_{67}H_{77}F_6IrO_2P_2$	$C_{77}H_{90}F_{12}Ir_2O_2P_4$
Formula weight	1282.42	1783.76
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
Unit cell dimensions	a = 11.9712(7) Å	a = 10.1340(12) Å
	b = 16.5219(10) Å	b = 18.628(2) Å
	c = 18.1008(9) Å	c = 20.622(2) Å
	α= 95.576(2)°	α= 75.284(4)°
	β= 107.732(2)°	β= 85.701(4)°
	γ = 111.124(2)°	γ = 83.585(4)°
Volume	3093.4(3) Å^3	3737.2(8) Å^3
Z	2	2
Density (calculated)	1.377 Mg/m^3	1.585 Mg/m^3
Absorption coefficient	2.270 mm^{-1}	3.717 mm^{-1}
F(000)	1312	1780
Crystal size	0.284 × 0.237 × 0.042 mm^3	0.207 × 0.066 × 0.027 mm^3
Theta range for data collection	1.959 to 28.330°	2.025 to 28.388°
Index ranges	-15<=h<=15, -22<=k<=22, -24<=l<=24	-13<=h<=13, -24<=k<=24, -27<=l<=27
Reflections collected	180956	198286
Independent reflections	15374 [R(int) = 0.0403]	18637 [R(int) = 0.0663]
Completeness to theta = 25.242°	99.9 %	99.9 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	15374 / 0 / 720	18637 / 0 / 874
Goodness-of-fit on F^2	1.134	1.122
Final R indices [I>2sigma(I)]	R_1 = 0.0364, wR_2 = 0.0928	R_1 = 0.0594, wR_2 = 0.1190
R indices (all data)	R_1 = 0.0382, wR_2 = 0.0937	R_1 = 0.0736, wR_2 = 0.1246
Largest diff. peak and hole	1.296 and -1.494 e.Å^{-3}	1.576 and -2.141 e.Å^{-3}

Analysis

Adequate crystals for X-ray diffraction analysis of the spirobifluorene metallaromatic complexes **2** and **3** were obtained by the recrystallization of the most pure fractions after the column chromatography from a CH_2Cl_2:hexane (1:4 v/v) mixture yielding colourless monocrystals. The asymmetric unit of the metallaromatic complex **3** contain the iridium cation complex, a hexafluorophosphate anion and a hexane solvent molecule (Figure S43). Whereas complex **2**, apart from the diiridium cation complex, presents two hexafluorophosphane anions (Figure S42). In both cases, the cation consists of the pentamethylcyclopentadiene ligand η^5-coordinated to the iridium atom and a trimethylphosphane ligand. In addition, the metal atom forms part of a benzene ring which shares a side with a spirobifluorene leading to the iridaaromatic spirobifluorene moiety. There, the iridium atom, considering the one with a higher occupancy, is displaced from the plane form by the 5 carbon atoms by 0.494 and 0.398 Å (for each iridium atom) in case of complex **2** and 0.401 Å in case of complex **3**. When considering the diiridium complex **2**, both iridium atoms are part of the same spirobifluorine moiety leading to the bimetallic complex. Note that, the coordination sphere presents a "three-ledge piano stool" structure in an octahedral arrangement. Selected bond lengths and angles are listed in Tables S2 and S3.

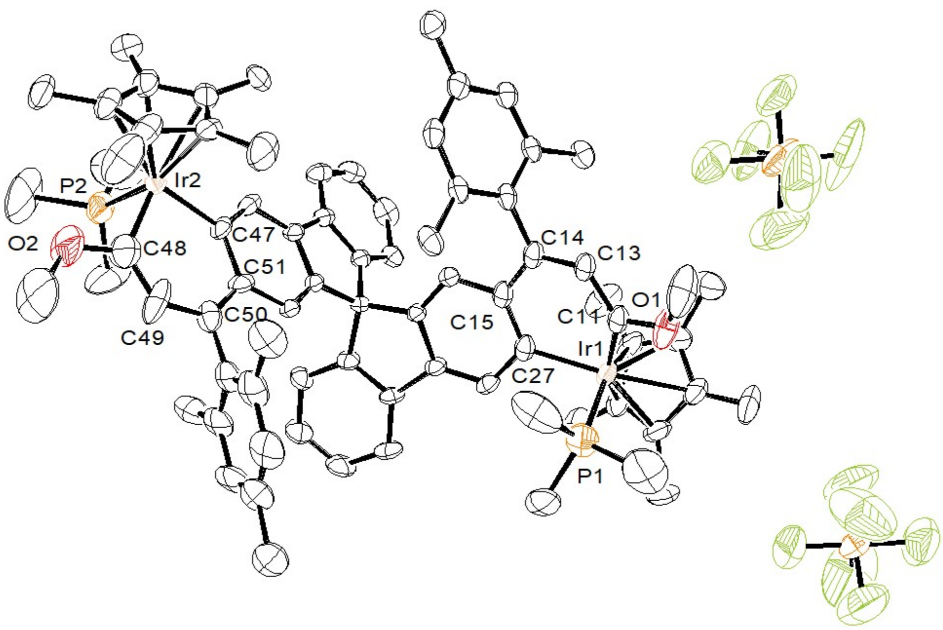


Figure S44. ORTEP representation of complex **2** with thermal ellipsoids drawn at 50% probability level. All hydrogen atoms have been omitted and only Ir(1A) and Ir(2A) (86% and 90% of occupancy, respectively) are shown for clarity.

Table S2. Selected bond lengths (Å) and angles (°) for complex **2**

Ir(1A)-P(1)	2.282(2)	C(48)-C(49)	1.354(17)	C(13)-C(11)-Ir(1A)	126.9(5)
Ir(1B)-P(1)	2.165(7)	C(13)-C(14)	1.366(11)	C(13)-C(11)-Ir(1B)	129.4(6)
Ir(2A)-P(2)	2.280(2)	C(49)-C(50)	1.366(13)	C(49)-C(48)-Ir(2A)	124.0(8)
Ir(2B)-P(2)	2.301(9)	C(14)-C(15)	1.461(12)	C(49)-C(48)-Ir(2B)	118.2(10)
Ir(1A)-C(11)	1.984(7)	C(50)-C(51)	1.438(12)	C(14)-C(13)-C(11)	124.7(8)
Ir(1B)-C(11)	1.450(18)	C(15)-C(27)	1.416(11)	C(48)-C(49)-C(50)	126.8(13)
C(48)-Ir(2A)	1.952(9)	C(47)-C(51)	1.443(11)	C(13)-C(14)-C(15)	124.5(8)
C(48)-Ir(2B)	1.812(18)	C(11)-Ir(1A)-C(27)	88.7(3)	C(49)-C(50)-C(51)	126.9(10)
Ir(1A)-C(27)	2.047(6)	C(11)-Ir(1B)-C(27)	102.5(5)	C(27)-C(15)-C(14)	122.4(7)
Ir(1B)-C(27)	2.122(9)	C(48)-Ir(2A)-C(47)	91.5(3)	C(50)-C(51)-C(47)	121.1(7)
C(47)-Ir(2A)	2.056(6)	C(48)-Ir(2B)-C(47)	102.1(12)	C(15)-C(27)-Ir(1)	125.7(6)
C(47)-Ir(2B)	1.881(17)	C(11)-Ir(1A)-P(1)	86.76(19)	C(15)-C(27)-Ir(1)	125.7(6)
O(1)-C(11)	1.335(10)	C(11)-Ir(1B)-P(1)	107.1(9)	C(51)-C(47)-Ir(2)	123.3(6)
O(2)-C(48)	1.354(14)	C(48)-Ir(2A)-P(2)	87.5(3)	C(51)-C(47)-Ir(2)	123.3(6)
C(13)-C(11)	1.448(11)	C(48)-Ir(2B)-P(2)	90.2(5)		

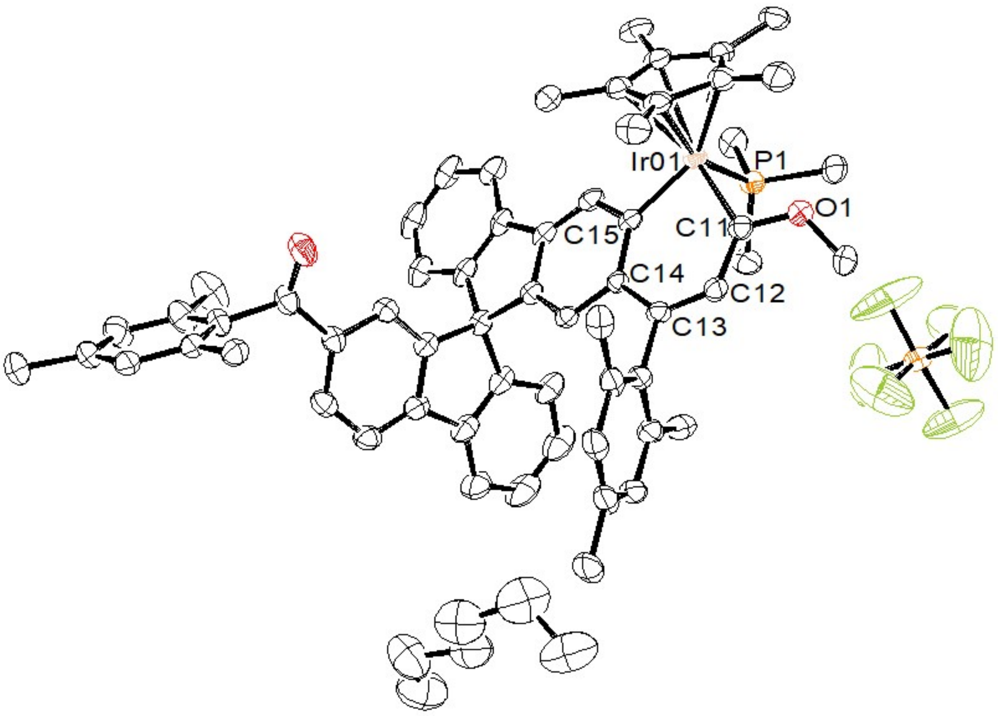


Figure S45. ORTEP representation of complex **3**·Hexane with thermal ellipsoids drawn at 50% probability level. All hydrogen atoms have been omitted and only Ir(1A) (88% of occupancy) is shown for clarity.

Table S3. Selected bond lengths (Å) and angles (°) for complex **3**

Ir(1A)-P(1)	2.183(6)	C(12)-C(13)	1.365(6)	C(12)-C(11)-Ir(1B)	120.1(3)
Ir(1B)-P(1)	2.2901(9)	C(13)-C(14)	1.452(5)	C(13)-C(12)-C(11)	124.9(4)
Ir(1A)-C(11)	1.964(3)	C(14)-C(15)	1.431(5)	C(12)-C(13)-C(14)	125.9(3)
Ir(1B)-C(11)	1.989(6)	C(11)-Ir(1A)-C(15)	89.71(14)	C(15)-C(14)-C(13)	121.6(3)
Ir(1A)-C(15)	2.050(3)	C(11)-Ir(1B)-C(15)	98.0(3)	C(14)-C(15)-Ir(1A)	126.3(3)
Ir(1B)-C(15)	1.757(10)	C(11)-Ir(1A)-P(1)	86.38(10)	C(14)-C(15)-Ir(1B)	127.5(3)
O(1)-C(11)	1.333(5)	C(11)-Ir(1B)-P(1)	88.8(2)		
C(12)-C(11)	1.425(6)	C(12)-C(11)-Ir(1A)	127.4(3)		

UV-Vis spectroscopic studies

Materials and methods

UV/Vis spectra were recorded on a Jasco V-670 spectrophotometer at 298 K using one centimeter quartz cuvette. Solutions were prepared by weighing 25 mg of each compound and dissolved in 25 ml of CH_2Cl_2. The resulting solution was diluted to 10 mL of a 6.0 x 10^{-5} M solution and measured.

Analysis

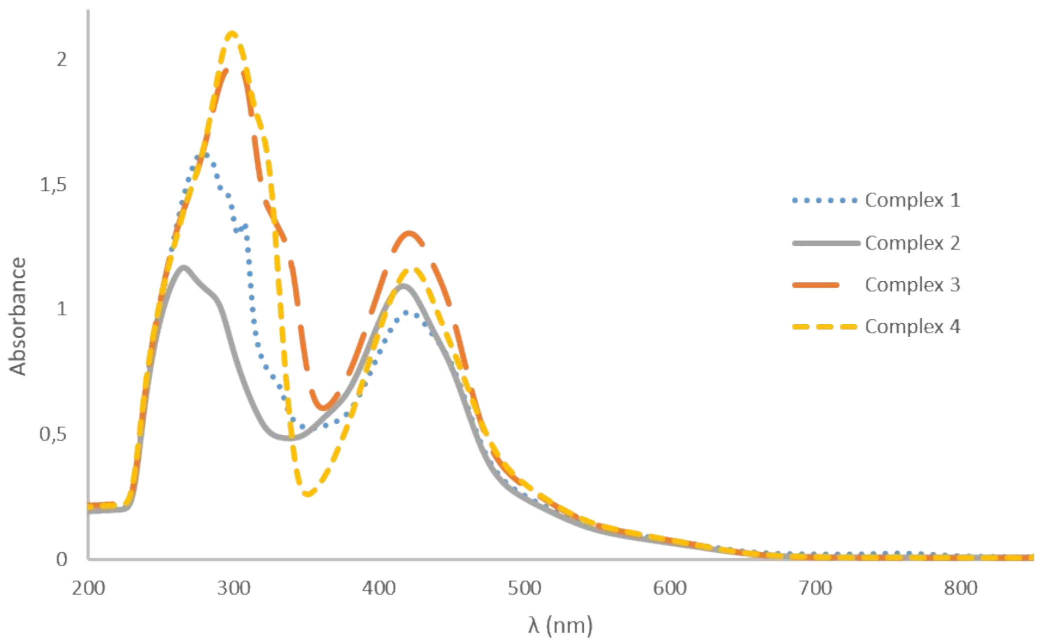


Figure S46. Experimental UV/Vis spectra of the different complexes under study in CH_2Cl_2 at $6 \cdot 10^{-5}$ M.

The UV-Vis data was further used to determine the direct optical gaps through Tauc's plot, a representation of $(\alpha h\nu)^{1/2}$ vs. the photon energy ($h\nu$) where α is the absorption coefficient. A linear fit to the main absorption edge was extrapolated to the x-axis obtaining the optical band gaps for complexes **1**-**4**.

Cyclic voltammetry studies

Methodology

Electrochemical measurements were performed using an Autolab potentiostat/galvanostat (PGSTAT100). A three electrode arrangement was utilized, with a 2 mm diameter glassy carbon electrode (GCE) as a working electrode, a platinum plate as a counter electrode and a Ag/AgCl electrode as a reference electrode. The GCE electrode was polished prior to each experiment using 0.05 μm alumina-water slurry on soft lapping pads.

Ferrocene was used as an internal reference, and the redox potentials presented in this work are related to the standard ferrocene/ferrocenium redox couple (Fc/Fc^+).

Measurements were performed in 10^{-3} $mol \cdot L^{-1}$ solutions of complexes **1**-**4** or the corresponding propargylic alcohols in dichloromethane (DCM) containing tetrabutylammoniumhexafluorophosphate ($TBAPF_6$) 0.1 $mol \cdot L^{-1}$ as supporting electrolyte. Solutions were degassed by passing a stream of nitrogen through the solution for 10 minutes prior to the measurement.

Analysis

The analysis of the propargylic alcohols suggests that the reduction processes observed in the voltammograms can be assigned as metal-based reduction because the propargylic alcohols showed no electrochemical activity in the cathodic potential range. However, the quasi-reversible oxidation might be due to the SBF moiety as it also appeared when the propargylic compounds were measured.

Table S4. Electrochemical data obtained from the cyclic voltammetry measurements

Complex	E_{pc}(V)	E_{pa}(V)	$E_{1/2}$ (V)	ΔE_p (V)[a]	$E_{onset,red}$ (V)	E_{LUMO} (eV)[b]	$E_{onset,oxid}$ (V)	E_{HOMO} (eV)[c]	E_{gap} (eV)
1	-1.51	-1.41	-1.45	0.10	-1.37	-3.73	0.97	-6.07	2.34
	0.94	1.09	1.02	0.15					
2	-1.52	-1.41	-1.46	0.11	-1.40	-3.70	0.93	-6.03	2.33
	-1.61	-1.56	-1.59	0.05					
	0.91	1.11	1.01	0.20					
3	-1.51	-1.40	-1.45	0.11	-1.38	-3.72	0.98	-6.08	2.36
	-1.78	-1.69	-1.74	0.09	-1.74	-3.36			
	0.92	1.07	1.00	0.15					
4	-1.51	-1.40	-1.45	0.12	-1.38	-3.72	0.91	-6.01	2.29
	-1.79	-1.69	-1.74	0.10					
	0.87	1.12	1.00	0.25					

[a]$\Delta E_p = E_{pa}$-E_{pc},; [b]E_{LUMO} (eV) = − ($E_{onset, red}$ + 5.1); [c]E_{HOMO} (eV) = − ($E_{onset, oxid}$ + 5.1)

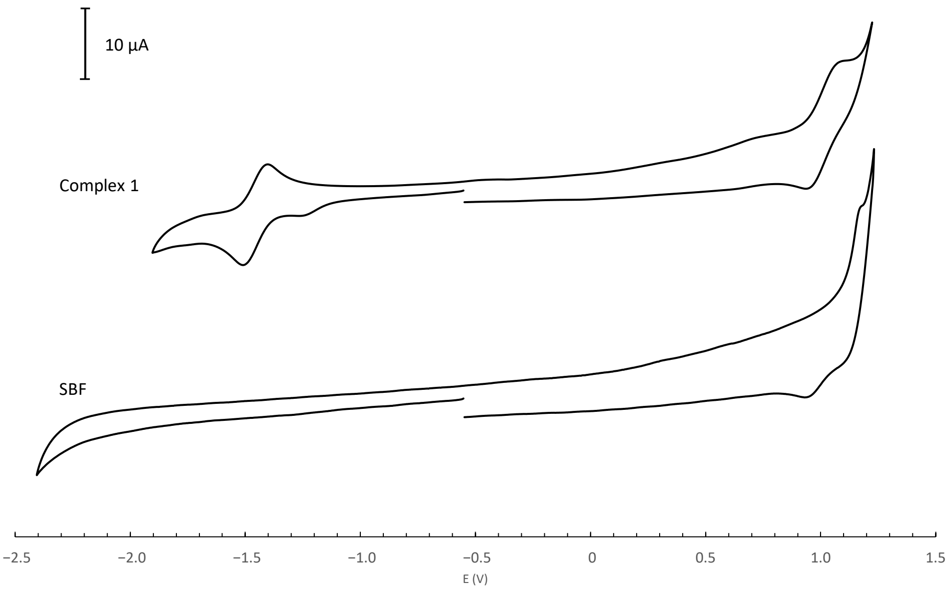


Figure S47. Cyclic voltammograms of 1mM solutions of complex **1** and SBF in CH_2Cl_2, with 0.1 M $TBAPF_6$ as supporting electrolyte. Scan rate: 0.2 V/s

The graphical representation of the peak current vs the $v^{1/2}$ is provided. Note that triangles refer to oxidation waves while squares and circles to reduction waves (at -1.45 V for complexes **1-4** and additonally for -1.59 V for complex **2**).

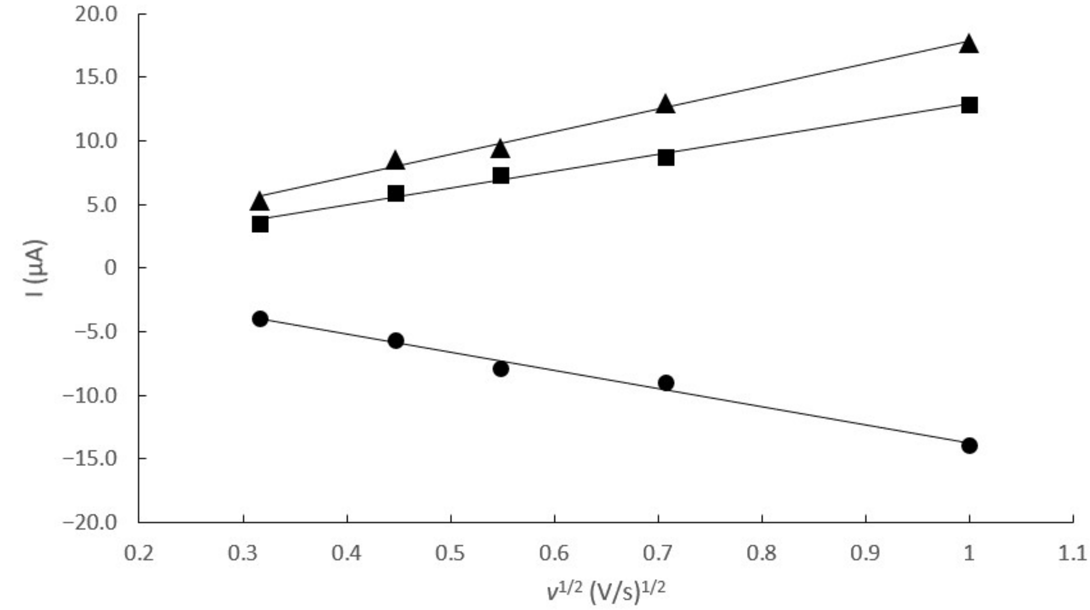


Figure S48. Graphical representation of the peak current vs the $v^{1/2}$ of complex **1**.

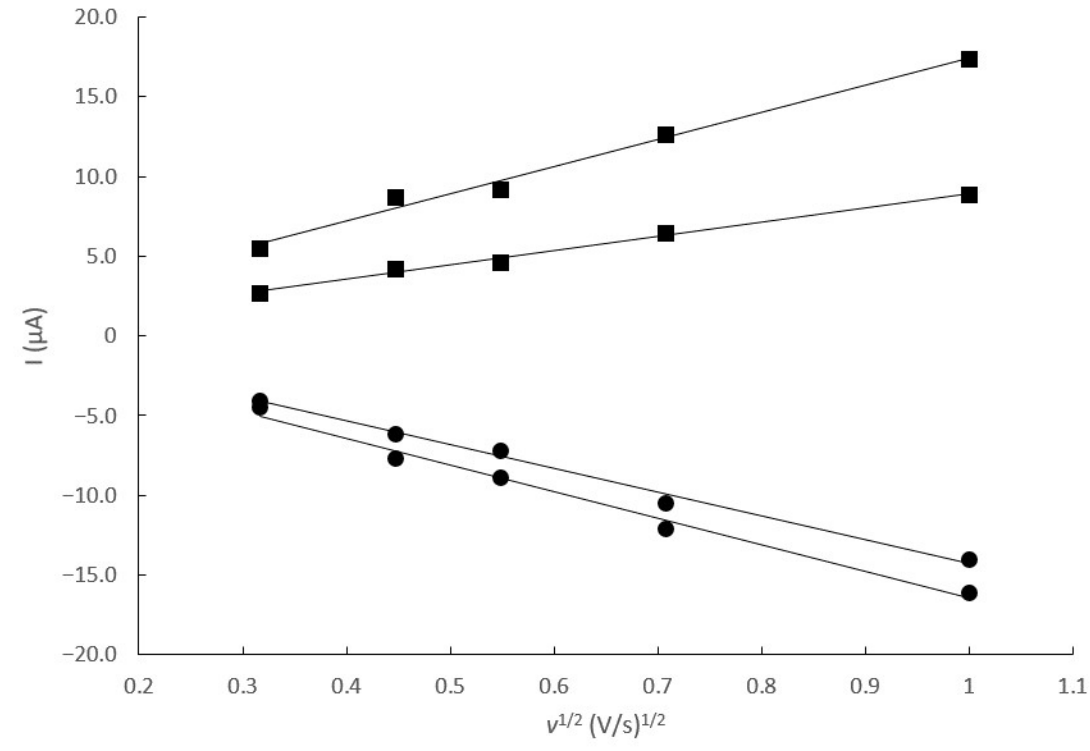


Figure S49. Graphical representation of the peak current vs the $v^{1/2}$ of complex **2**.

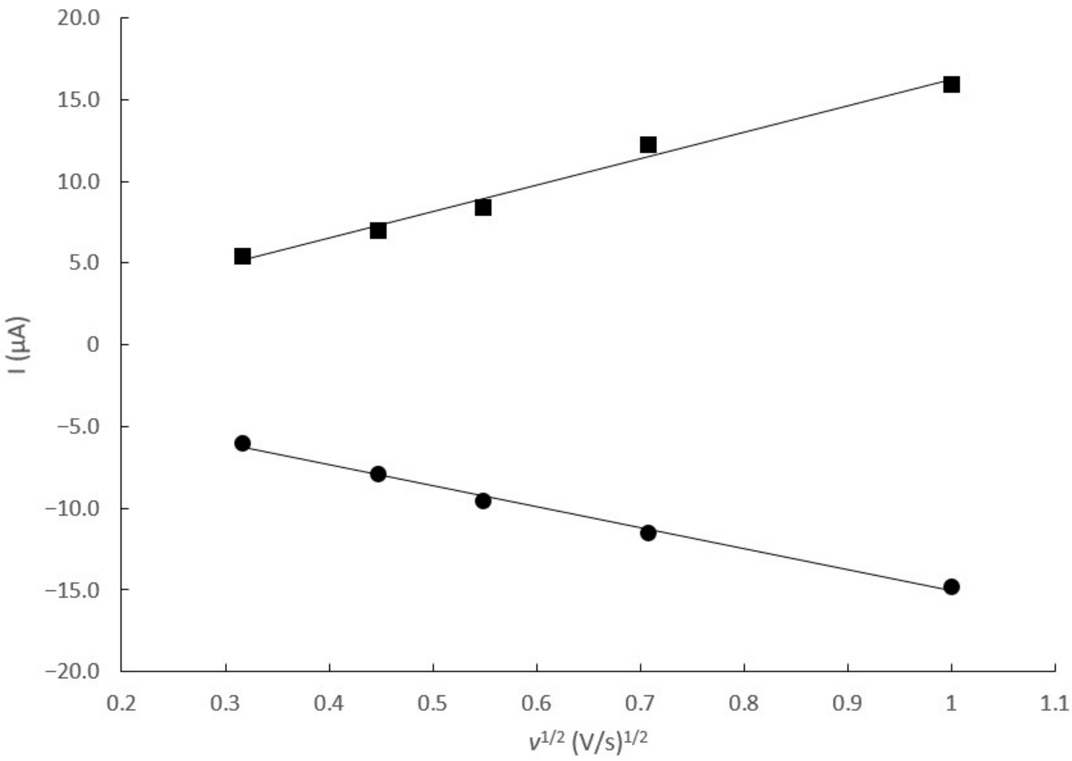


Figure S50. Graphical representation of the peak current vs the $v^{1/2}$ of complex **3**.

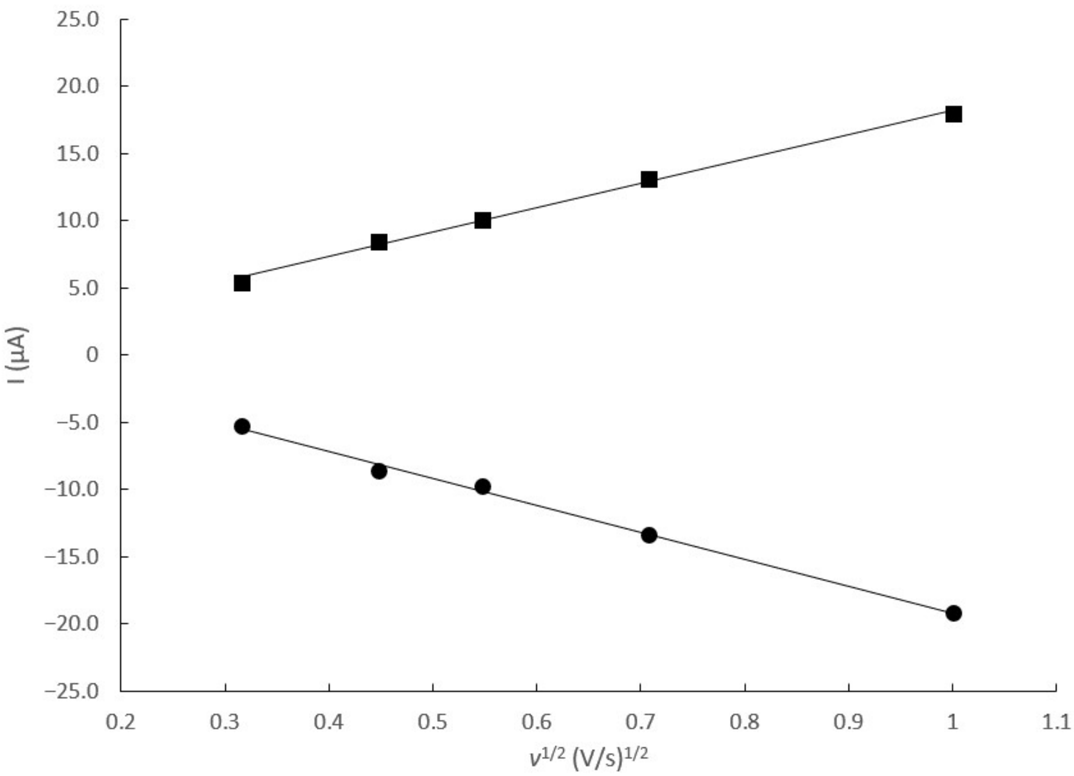


Figure S51. Graphical representation of the peak current vs the $v^{1/2}$ of complex **4**.

Computational Details

General procedures and analysis of the data

Geometry of the studied structures were optimized at B3LYP level of theory in gas phase. 6-31G(d,p) basis set was employed for all atoms except iridium (LANL2DZ was used). Harmonic frequency calculations were performed at the same level to confirm them as local minimums. In order to obtain the UV-Vis spectra, a TD-DFT calculation (cam-B3LYP functional) was performed obtaining the 30 first excited states. Cam-B3LYP method was also employed in order to obtain hyperpolarizabilities.

All calculations were carried out with the GAUSSIAN 09 program package.[8]

Anisotropy of the Current-Induced Density (ACID) Figures and CIV values

In this paper, the anisotropy of the current-induced density (ACID) method for the determination of the aromaticity of the compounds has been chosen. This method, developed by Herges and Geuenich,[9] is based on magnetic properties and allows the visualization of the ring current formed when a magnetic field is applied. It also allows us to give a numerical value to delocalization effects quantify through the CIV (critical isosurface values), value of the isosurface at which the topology of the conjugation changes from cyclic to noncyclic.

The ACID plots of the structures are presented in Figures S52, S53 and S54. The isosurface value is 0.04. The CIV for the cycle with the iridium atom is also shown.

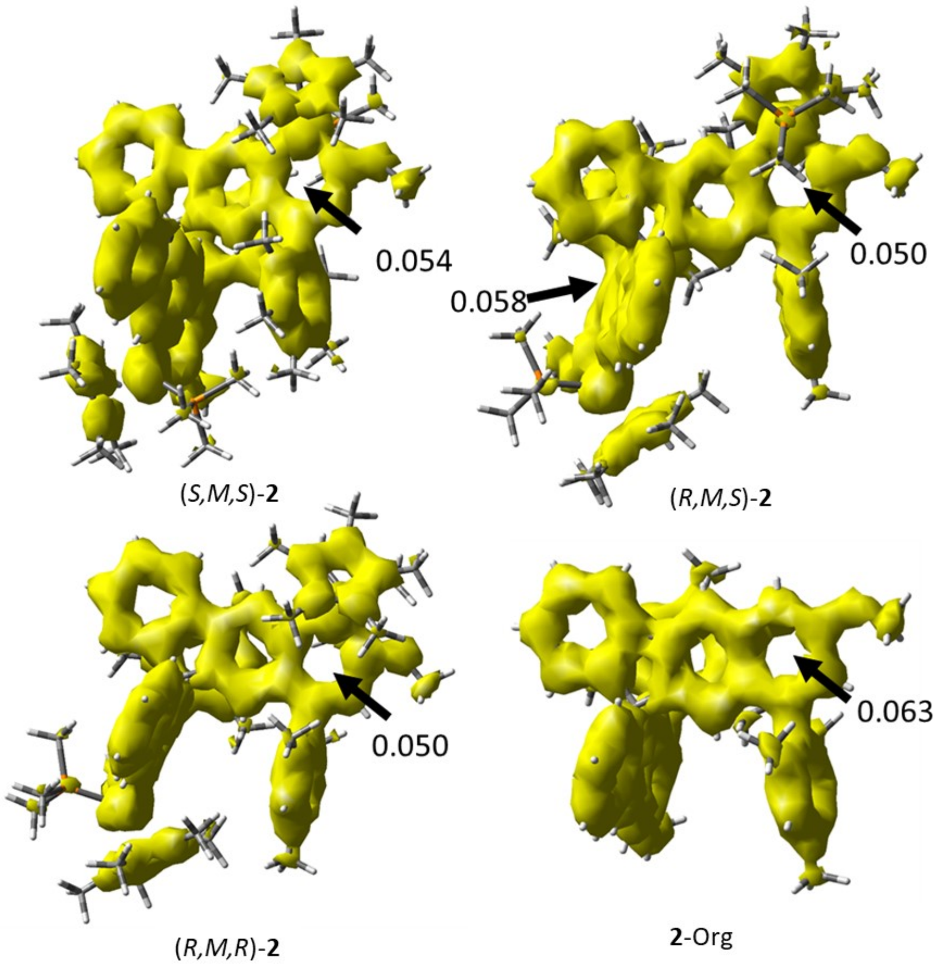


Figure S52. ACID plots for the three diastereoisomers (*S*,*M*,*S*), (*R*,*M*,*S*) and (*R*,*M*,*R*) of complex **2** and the result of exchanging the [IrCp*(PMe_3)] fragments by a CH unit (Org).

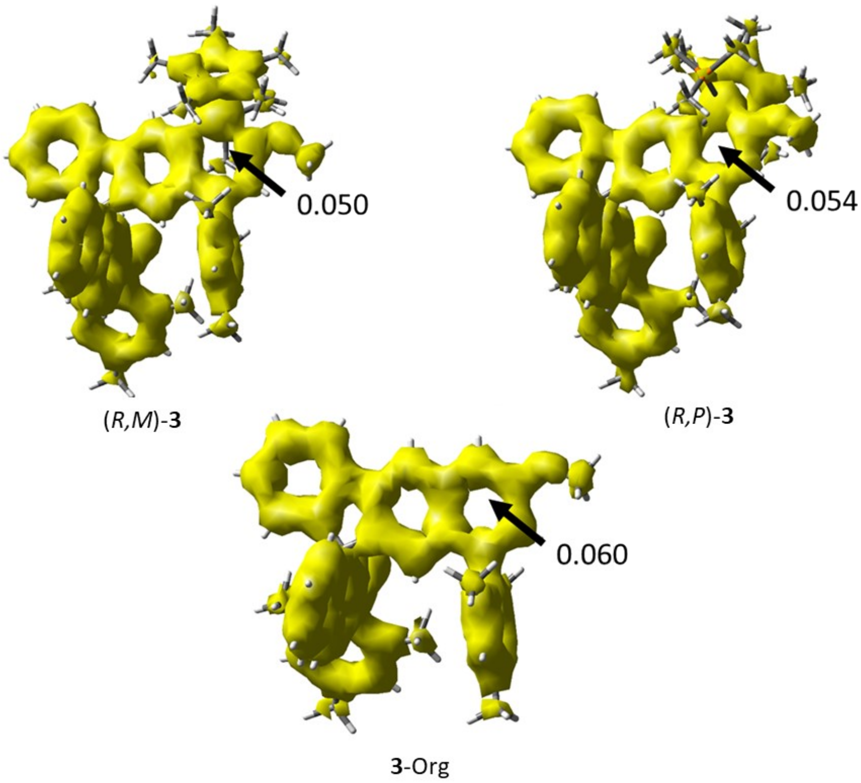


Figure S53. ACID plots for the two diastereoisomers (*R,M*) and (*R,P*) of complex **3** and the result of exchanging the [IrCp*(PMe_3)] fragment by a CH unit (Org).

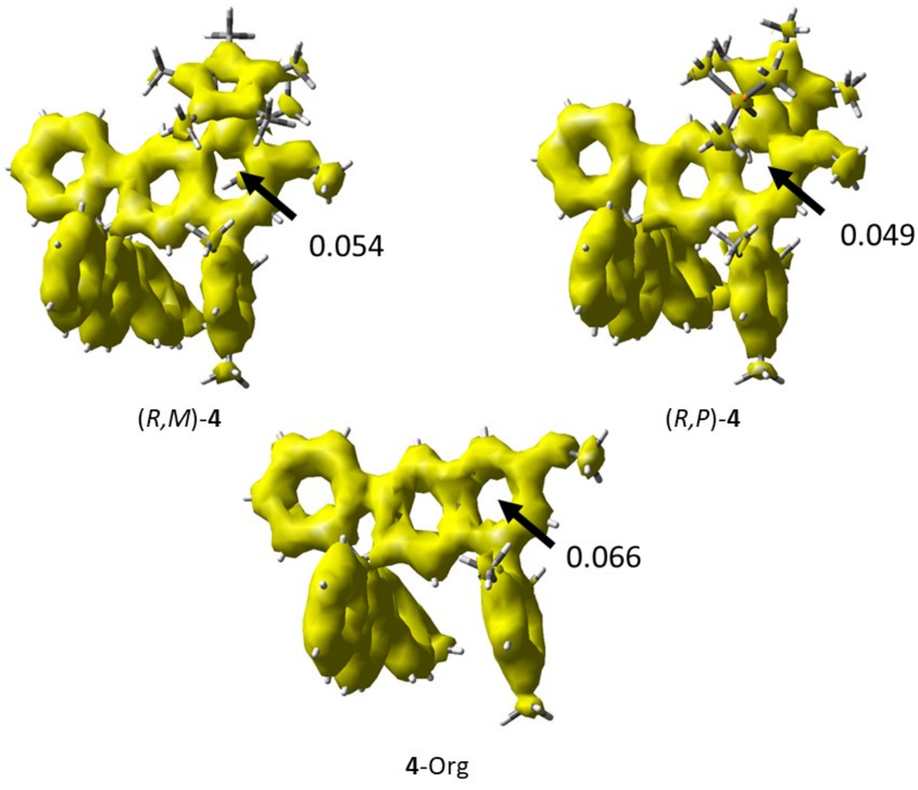


Figure S54. ACID plots for the two diastereoisomers (*R,M*) and (*R,P*) of complex **4** and the result of exchanging the [IrCp*(PMe_3)] fragment by a CH unit (Org).

NICS values

In order to compare the ACID results with other method employed to analyzed the aromaticity, nucleus-independent chemical shift (NICS) were calculated for the (*S,M,S*)-**2** and its organic analog. The NICS are defined as the negative of the magnetic shielding[10] and it exhibites negatives values in the center of aromatic rings. They were calculated at B3LYP level and the gauge-independent atomic orbital (GIAO) method[11] were employed. To avoid spurious contributions from the in-plane tensor components that are not related to π effects, as Schleyer has indicated[12], NICS(1) values (1 Å below the plane of the ring) were calculated (Figure S55).

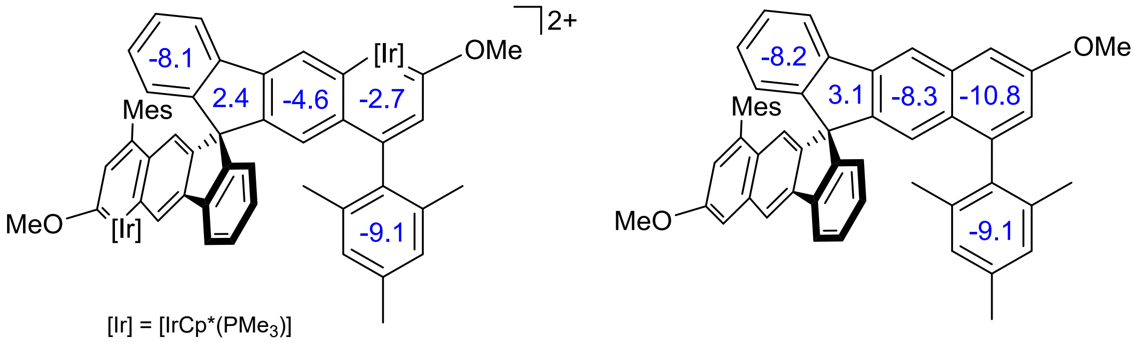


Figure S55. NICS values of the complex (*S,M,S*)-**2** and its organic analog.

Thus, NICS(1) for the iridium cycle of complex (*S,M,S*)-**2** is -2.7 and -10.8 for organic analog which confirm the aromaticity in the diiridium complex **2**.

Hiperpolarizability

The first molecular hyperpolarizabilities were calculated with Gaussian09 employing the finite field method. The first static hyperpolarizability tensor β_{tot} is defined as:

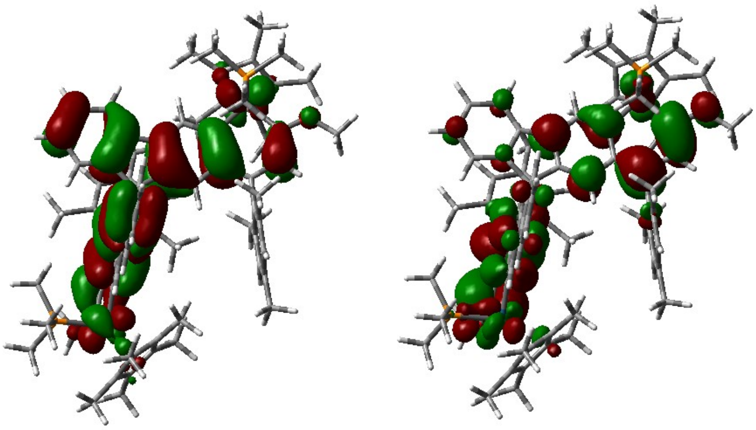
$$\beta_{tot} = \left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2\right]^{1/2}$$

HOMO and LUMO Representations

Complex 2

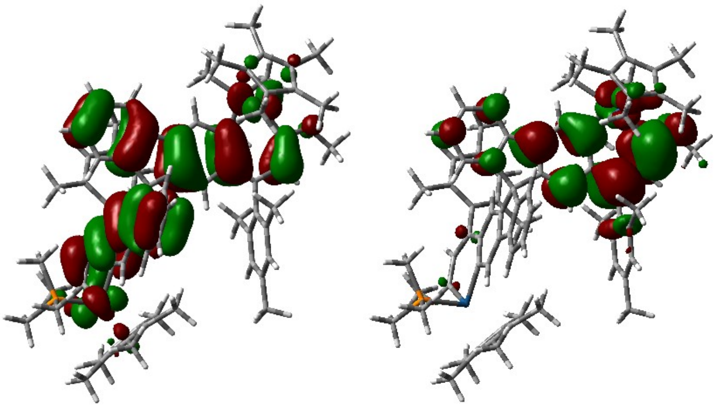
(*R,M,R*)-**2**

HOMO LUMO



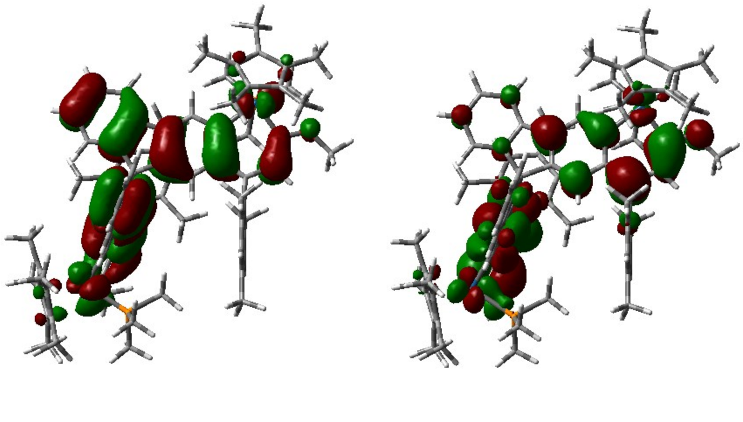
(*R,M,S*)-**2**

HOMO LUMO



(*S,M,S*)-**2**

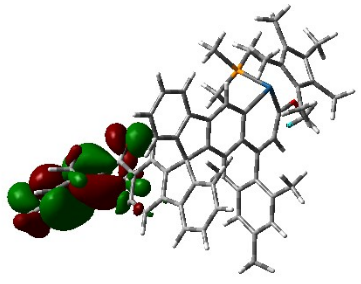
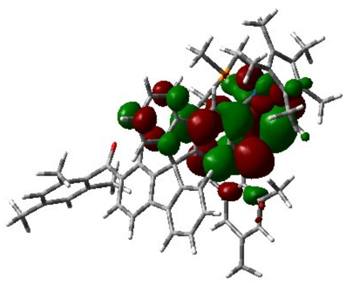
HOMO LUMO



Complex 3

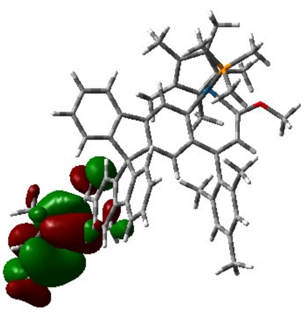
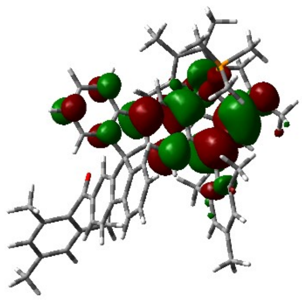
(*R,M*)-**3**

HOMO LUMO

(*R,P*)-**3**

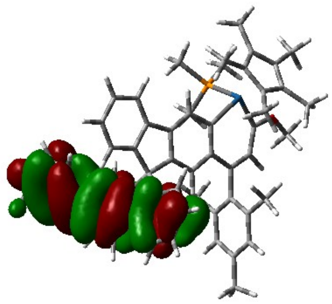
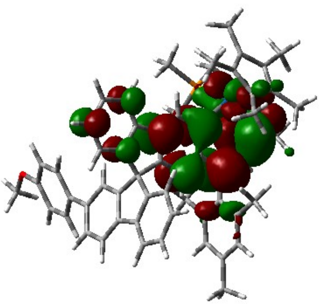
HOMO LUMO

Complex 4

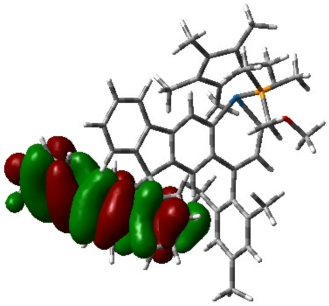
(*R,M*)-**4**

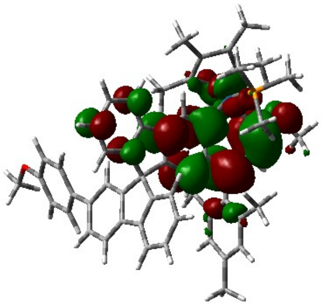
HOMO LUMO

(*R,P*)-**4**

HOMO LUMO





XYZ coordinates

Table S5. Cartesian Coordinates of all optimized structures

Complex (*R,M,R*)-2	**Complex (*R,M,S*)-2**
E=-430.8072897 H	E: -4030.80 63028 H
2 1	2 1
C,0,-0.0555190126,7.3591853555,-0.5728716516	C,0,7.3324123588,1.5900328106,-1.1426767934
C,0,0.8955804264,7.4180090847,-1.6661114012	C,0,6.9577786063,1.036772746,-2.3964749178
C,0,0.7059710654,6.2387564972,-2.4581613765	C,0,5.5296139814,1.2564595527,-2.5648171329
C,0,-0.2981842172,5.4172595178,-1.8221080833	C,0,5.0628654543,2.0140808104,-1.4268408316
C,0,-0.7935180741,6.143545379,-0.6670509792	C,0,6.1558651152,2.1832535116,-0.5214002279
C,0,-0.3340694872,8.4808780329,0.3840957019	C,0,8.7347920579,1.7278571159,-0.6270757225
H,0,-0.8271105847,8.1332933422,1.2945357943	H,0,8.7858757024,1.6793050428,0.4636371024
H,0,-1.0051182054,9.2087885363,-0.0888340366	H,0,9.1401588653,2.7047501945,-0.9194405995
H,0,0.5713437008,9.0238518681,0.666359628	H,0,9.4004583821,0.9668030689,-1.0394727619
C,0,1.7404649134,8.600858531,-2.0458103821	C,0,7.8839662348,0.479898059,-3.4374646547
H,0,1.2240888154,9.2284437137,-2.7828862531	H,0,8.2405417777,1.2829433277,-4.0945178694
H,0,2.6915824331,8.2888868983,-2.4826361463	H,0,7.3871360153,-0.2619757011,-4.0645143284
H,0,1.9632058406,9.2344342929,-1.1843325098	H,0,8.7596471191,0.0030670979,-2.9922181336
C,0,1.3517146958,5.9681692949,-3.7842722196	C,0,4.7567208742,1.0025622517,-3.8276901295
H,0,1.4049598751,4.8990762163,-4.00204888	H,0,3.6907755819,0.8697532581,-3.6302222149
H,0,2.3614540027,6.3802332353,-3.8304105838	H,0,5.1148667554,0.1105398666,-4.3468324296
H,0,0.7660913514,6.4391660234,-4.5831352791	H,0,4.8650035726,1.8480519365,-4.5186333434
C,0,-0.9181658567,4.1749632194,-2.3936959234	C,0,3.6980938276,2.6170538526,-1.2839967092
H,0,-1.2528099999,3.4945002012,-1.6073420943	H,0,3.3806426582,2.6737465857,-0.2412644207
H,0,-0.2168165622,3.6311077132,-3.0303586441	H,0,2.942920282,2.0487105808,-1.8304202658
H,0,-1.7916608841,4.4321954107,-3.0062961124	H,0,3.7032304696,3.6378643759,-1.6860369372
C,0,-2.0132621953,5.7770572671,0.1273772647	C,0,6.1691660105,3.0737315874,0.6892301154
H,0,-2.9146548521,6.1612614408,-0.3669160958	H,0,6.4580588074,4.0955814234,0.4117574488
H,0,-1.993184695,6.2020964083,1.1344974253	H,0,6.8811172568,2.7349215973,1.4456879699
H,0,-2.1284019418,4.6952547941,0.2203893065	H,0,5.1844873645,3.1362390526,1.1588866564
C,0,1.915854509,2.4504062042,0.1930016752	C,0,2.9174397512,-1.4941764606,-0.2635860262
C,0,3.0429349793,2.4101339922,-0.7107461943	C,0,3.1889269642,-2.4842270033,-1.2809042192
C,0,1.2214964754,3.667543578,0.5125252534	C,0,3.8899522502,-0.5201043872,0.1458341387
C,0,3.6326803857,3.5168992571,-1.3022110077	C,0,4.4092930709,-2.6645004065,-1.9135036315
C,0,3.6917086421,1.0946127843,-1.0498643497	C,0,2.1136763516,-3.4503854322,-1.7015849833
Ir,0,1.4952663251,5.4962786746,-0.4025637306	Ir,0,5.6959678282,-0.1450866451,-0.7629374492
C,0,3.1841525277,4.8506732227,-1.1910139431	C,0,5.5597205458,-1.8647144879,-1.7340787496
C,0,3.2438625156,0.3760084579,-2.1782751541	C,0,1.2732801834,-3.1199435209,-2.7850681055
C,0,4.7721060074,0.6096093372,-0.2816952134	C,0,1.9854033963,-4.7009117232,-1.0590061267
C,0,3.8910733808,-0.8164834794,-2.5198646603	C,0,0.3209573833,-4.0529388712,-3.2100234165
C,0,5.3868001319,-0.5872141017,-0.6626523299	C,0,1.0173141487,-5.5990848631,-1.5181353155
C,0,4.9691397131,-1.3136340519,-1.7820944537	C,0,0.1796299318,-5.300989669,-2.5975723298
P,0,2.6768207634,6.2344179357,1.4805547254	P,0,6.77837904,-1.2324108071,1.0074675939
C,0,1.6622893978,6.6041622257,2.9709338755	C,0,7.0281701644,-0.2471502212,2.5423244569
H,0,2.3016370519,6.9677236526,3.7811833927	H,0,7.5477525825,-0.8476049885,3.2952943027
H,0,1.1533543153,5.6952367604,3.2989158292	H,0,6.0603220257,0.0641409929,2.9415085463

H,0,0.914717137,7.3659096127,2.7417349144	H,0,7.6243187589,0.6426807725,2.3300642774
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H,0,4.2240565519,8.0315851532,2.0952372345	H,0,8.9002328377,-2.3818088039,1.4271539602
H,0,2.9596911495,8.6074823544,0.9847645935	H,0,9.1164645804,-0.9720294198,0.3636698058
H,0,4.3037083477,7.6423144086,0.353615508	H,0,8.4210857484,-2.4627359837,-0.2918326278
C,0,3.9397484451,5.0679210187,2.1319981024	C,0,5.9463170776,-2.7477041361,1.6333694512
H,0,4.4168238574,5.4843258765,3.0237950067	H,0,6.5398912037,-3.2053939953,2.4299215615
H,0,4.7024857298,4.8842015181,1.3725074789	H,0,5.8234882511,-3.4654154209,0.8195986835
H,0,3.4642602801,4.1181505637,2.3839436165	H,0,4.9585640003,-2.4891593815,2.0193724184
C,0,0.2083891587,3.5817017273,1.4885307739	C,0,3.5420849495,0.3110417679,1.2301078432
H,0,4.5083024604,3.3094653083,-1.908029131	H,0,4.45415587,-3.4961418367,-2.6086741214
O,0,3.9199579681,5.8212399283,-1.7576930945	O,0,6.6916655391,-2.2336192652,-2.3516223975
C,0,5.1537221451,5.5567538757,-2.4676187509	C,0,6.7860176901,-3.4122139971,-3.1864884369
H,0,5.5215318799,6.5361664712,-2.7707591208	H,0,7.8254003687,-3.4468222772,-3.5102256716
H,0,4.9707008643,4.9408321144,-3.351967062	H,0,6.1309954187,-3.3273190667,-4.0575825343
H,0,5.8844092101,5.0717637733,-1.8152384774	H,0,6.5426526664,-4.3144511299,-2.6193396395
C,0,5.6831590145,-2.5779512529,-2.1963211724	C,0,-0.8237646011,-6.3110361496,-3.1005236331
C,0,2.0905256808,0.8719759708,-3.0222305978	C,0,1.3859734116,-1.7875235111,-3.4923352615
H,0,3.5481810356,-1.3640926306,-3.3949271562	H,0,-0.3196511078,-3.7982229102,-4.0514396228
C,0,5.2646342194,1.3467618815,0.9434908368	C,0,2.864773587,-5.0820835086,0.1108160736
C,0,-0.1403518549,2.374606711,2.0942175363	C,0,2.3015178771,0.2266501055,1.8611216076
C,0,0.5299505903,1.1805261057,1.7458937782	C,0,1.3376584063,-0.7088727349,1.4204561097
C,0,1.5372670741,1.2193692201,0.8135145621	C,0,1.6415055972,-1.5512857243,0.3791513128
C,0,0.0000000000,0.0000000000,2.5671812973	C,0,0.0746025425,-0.6352952,2.2855424015
C,0,-1.0772067383,0.6922185897,3.4116543309	C,0,0.4593158531,0.4768651127,3.2700499036
C,0,-1.1404380076,2.0693495693,3.1187539585	C,0,1.7533805702,0.9648412932,2.9999404901
C,0,-2.0542927648,2.8955495148,3.7815974164	C,0,2.3060721779,1.9845950959,3.7821315725
C,0,-2.8987634387,2.3322542112,4.7377145542	C,0,1.5540707741,2.5072469377,4.8336366726
C,0,-1.9185965123,0.134505179,4.367569017	C,0,-0.2867566464,0.9983014132,4.3208436978
C,0,-2.8306326565,0.963329076,5.0292614685	C,0,0.2688048945,2.0172165205,5.1015292169
C,0,1.0772067383,-0.6922185897,3.4116543309	C,0,-0.2759455617,-1.959755623,2.9745470988
C,0,1.1404380076,-2.0693495693,3.1187539585	C,0,-1.5922013612,-2.3570956769,2.6648535417
C,0,-0.5299505903,-1.1805261057,1.7458937782	C,0,-1.2280041154,-0.3456631064,1.5303019175
C,0,0.1403518549,-2.374606711,2.0942175363	C,0,-2.1872723971,-1.3522260007,1.782177742
C,0,2.0542927648,-2.8955495148,3.7815974164	C,0,-2.1213579907,-3.5384139961,3.1955899565
C,0,2.8987634387,-2.3322542112,4.7377145542	C,0,-1.3237914982,-4.313464157,4.0368860806
C,0,2.8306326565,-0.963329076,5.0292614685	C,0,-0.016810406,-3.913553759,4.3458088627
C,0,1.9185965123,-0.134505179,4.367569017	C,0,0.5150733579,-2.7330738222,3.8165680609
H,0,-3.4910998309,0.5428970469,5.7815459206	H,0,-0.3002493472,2.4314429926,5.9282303829
H,0,6.5667960979,-2.3480769859,-2.8037196381	H,0,-0.3428587764,-7.0511643532,-3.7511690658
H,0,5.037955785,-3.2262346447,-2.7962396883	H,0,-1.6170914421,-5.8342686195,-3.6832711231
H,0,6.0293219592,-3.146768866,-1.3281447853	H,0,-1.2870102589,-6.8619792292,-2.2762597426
H,0,-3.6128354957,2.9580337312,5.2639551929	H,0,1.9669612608,3.2973844397,5.4529887022
H,0,1.8516442223,0.1566730402,-3.8129871259	H,0,0.6354545352,-1.7014214305,-4.2819345315
H,0,2.3252401297,1.8290298254,-3.502343886	H,0,2.3703951596,-1.657633129,-3.9556432368
H,0,1.1869294979,1.0282594008,-2.4223774031	H,0,1.2462131382,-0.9494798298,-2.7997287688
H,0,6.1202974991,0.8339565781,1.3884147807	H,0,2.5961822524,-6.0690049114,0.4941072911
H,0,4.4843746641,1.4191618787,1.7099487359	H,0,2.772403365,-4.3665303158,0.935399663
H,0,5.577337944,2.3689534401,0.703949753	H,0,3.922906204,-5.1141055442,-0.1726053817
H,0,6.2189239374,-0.9580839906,-0.0688779541	H,0,0.9206915414,-6.5611330029,-1.0204296907
H,0,-1.8656943947,-0.9239713403,4.6056353528	H,0,-1.2806033046,0.6188586442,4.5399212101
H,0,-2.1092680392,3.9575630598,3.5599709011	H,0,3.3034979369,2.3651615433,3.5805154759
H,0,2.0773697346,0.3157518526,0.55241808	H,0,0.9235118313,-2.2935689274,0.0472716176
H,0,2.1092680392,-3.9575630598,3.5599709011	H,0,-3.1357034772,-3.8496785485,2.9627735478
H,0,3.6128354957,-2.9580337312,5.2639551929	H,0,-1.7181492625,-5.2318890357,4.4604442449
C,0,-0.2083891587,-3.5817017273,1.4885307739	C,0,-3.4670807311,-1.2602122074,1.2347986125
C,0,-1.2214964754,-3.667543578,0.5125252534	C,0,-3.8671896487,-0.1660603062,0.4417153033
C,0,-1.915854509,-2.4504062042,0.1930016752	C,0,-2.8656527207,0.8235737876,0.1529562623
C,0,-1.5372670741,-1.2193692201,0.8135145621	C,0,-1.5580175036,0.7133307925,0.7206178647
H,0,-2.0773697346,-0.3157518526,0.55241808	H,0,-0.8274287108,1.4845803728,0.5016566697
H,0,-0.3249388937,4.4805465288,1.7779003063	H,0,4.2604074627,1.0431733298,1.5851068444
H,0,3.4910998309,-0.5428970469,5.7815459206	H,0,0.5875768945,-4.5256014139,5.0083960173
H,0,1.8656943947,0.9239713403,4.6056353528	H,0,1.5259001623,-2.4252305782,4.0681924333
H,0,0.3249388937,-4.4805465288,1.7779003063	H,0,-4.1832715705,-2.0444006316,1.4544250745
Ir,0,-1.4952663251,-5.4962786746,-0.4025637306	Ir,0,-5.8630447871,-0.0564562518,-0.0712392088
C,0,-3.0429349793,-2.4101339922,-0.7107461943	C,0,-3.1090359086,1.9440059481,-0.7267274804
C,0,-3.6326803857,-3.5168992571,-1.3022110077	C,0,-4.2791917744,2.1627831038,-1.4383557823
H,0,-4.5083024604,-3.3094653083,-1.908029131	H,0,-4.2703630253,3.0284109364,-2.0920784143
C,0,-3.1841525277,-4.8506732227,-1.1910139431	C,0,-5.455154104,1.3865920481,-1.3558215704
O,0,-3.9199579681,-5.8212399283,-1.7576930945	P,0,-5.501000668,-1.6427147666,-1.7488386388
C,0,-5.1537221451,-5.5567538757,-2.4676187509	C,0,-6.8494632171,-1.7294986749,-2.9973380126

H,0,-4.9707008643,-4.9408321144,-3.351967062	H,0,-6.5939218843,-2.4295246468,-3.7986051058
H,0,-5.5215318799,-6.5361664712,-2.7707591208	H,0,-7.7771630792,-2.0574325944,-2.5234626339
H,0,-5.8844092101,-5.0717637733,-1.8152384774	H,0,-7.0124128553,-0.7343728637,-3.416571138
C,0,0.7935180741,-6.143545379,-0.6670509792	C,0,-5.3094146283,-3.3842262755,-1.1841494963
C,0,0.0555190126,-7.3591853555,-0.5728716516	H,0,-5.1711879131,-4.0471956958,-2.043778304
C,0,0.2981842172,-5.4172595178,-1.8221080833	H,0,-4.4373141742,-3.4601254854,-0.5309537553
C,0,-0.8955804264,-7.4180090847,-1.6661114012	H,0,-6.1949900785,-3.7031840425,-0.6314016098
C,0,-0.7059710654,-6.2387564972,-2.4581613765	C,0,-3.9954842045,-1.3886556918,-2.7740022601
C,0,-3.6917086421,-1.0946127843,-1.0498643497	H,0,-3.1120019743,-1.4105715822,-2.1330157859
C,0,-4.7721060074,-0.6096093372,-0.2816952134	H,0,-3.9155808332,-2.1738273662,-3.5313359858
C,0,-3.2438625156,-0.3760084579,-2.1782751541	H,0,-4.0422883101,-0.4165588192,-3.2690306272
C,0,-5.3868001319,0.5872141017,-0.6626523299	O,0,-6.4822491954,1.697230009,-2.1648603511
C,0,-3.8910733808,0.8164834794,-2.5198646603	C,0,-6.4332260392,2.7928366577,-3.1097239247
C,0,-4.9691397131,1.3136340519,-1.7820944537	H,0,-5.6240751778,2.6521957558,-3.8311314883
C,0,-2.0905256808,-0.8719759708,-3.0222305978	H,0,-7.3937915644,2.7675188035,-3.6227149844
H,0,-1.8516442223,-0.1566730402,-3.8129871259	H,0,-6.3152288611,3.7488081897,-2.5929394365
H,0,-1.1869294979,-1.0282594008,-2.4223774031	C,0,-6.6457159758,0.6236893122,1.9759657613
H,0,-2.3252401297,-1.8290298254,-3.502343886	C,0,-7.5083681251,1.2006988142,0.9718925575
C,0,-5.6831590145,2.5779512529,-2.1963211724	C,0,-6.8568968308,-0.8107911588,1.9682874717
H,0,-5.037955785,3.2262346447,-2.7962396883	C,0,-8.1987167581,0.1351114759,0.3000105071
H,0,-6.5667960979,2.3480769859,-2.8037196381	C,0,-7.8064282354,-1.1005272746,0.9416157816
H,0,-6.0293219592,3.146768866,-1.3281447853	C,0,-2.0352895277,2.9748074985,-0.9517924539
C,0,-5.2646342194,-1.3467618815,0.9434908368	C,0,-1.9275371551,4.0705833972,-0.0668662059
H,0,-5.577337944,-2.3689534401,0.703949753	C,0,-1.1820336375,2.8800724845,-2.0702357177
H,0,-4.4843746641,-1.4191618787,1.7099487359	C,0,-0.9679090327,5.0536184068,-0.3252944708
H,0,-6.1202974991,-0.8339565781,1.3884147807	C,0,-0.2347077968,3.8876639059,-2.2853540136
C,0,-1.7404649134,-8.600858531,-2.0458103821	C,0,-0.1149117026,4.9876252518,-1.4317683978
H,0,-1.9632058406,-9.2344342929,-1.1843325098	C,0,-1.2677370759,1.7166122177,-3.033365245
H,0,-1.2240888154,-9.2284437137,-2.7828862531	H,0,-0.4681091788,1.767478362,-3.7765005548
H,0,-0.5713437008,-9.0238518681,0.666359628	H,0,-1.1866701362,0.7544574057,-2.5152045628
C,0,0.3340694872,-8.4808780329,0.3840957019	H,0,-2.2196065999,1.7084988504,-3.5765902701
H,0,0.8271105847,-8.1332933422,1.2945357943	C,0,0.8809878222,6.0886233463,-1.7073606255
H,0,1.0051182054,-9.2087885363,-0.0888340366	H,0,1.6781265411,5.752288372,-2.3765942485
H,0,1.993184695,-6.2020964083,1.1344974253	H,0,0.3946366875,6.9464682867,-2.1869209081
C,0,-1.3517146958,-5.9681692949,-3.7842722196	H,0,1.3397632723,6.4556069087,-0.7840942994
H,0,-0.7660913514,-6.4391660234,-4.5831352791	C,0,-2.8260779067,4.1996665715,1.142753672
H,0,-2.6915824331,-8.2888868983,-2.4826361463	H,0,-3.884477967,4.2097302711,0.858769341
H,0,-2.3614540027,-6.3802332353,-3.8304105838	H,0,-2.6873557998,3.3651477712,1.8391172398
C,0,0.9181658567,-4.1749632194,-2.3936959234	H,0,-2.6183225521,5.1250037085,1.6846523111
H,0,1.7916608841,-4.4321954107,-3.0062961124	C,0,-9.3026350393,0.303262793,-0.7048202652
H,0,-1.4049598751,-4.8990762163,-4.00204888	H,0,-9.4649346546,-0.6077160396,-1.2856284954
H,0,0.2168165622,-3.6311077132,-3.0303586441	H,0,-10.250340746,0.542636361,-0.2065460571
C,0,2.0132621953,-5.7770572671,0.1273772647	H,0,-9.0828236577,1.1093195759,-1.4077947302
H,0,2.9146548521,-6.1612614408,-0.3669160958	C,0,-7.7516753421,2.6647320289,0.756009486
H,0,1.2528099999,-3.4945002012,-1.6073420943	H,0,-7.9933709565,2.8816987627,-0.2863014827
H,0,2.1284019418,-4.6952547941,0.2203893065	H,0,-8.6025174145,2.9914795844,1.3660636625
H,0,-3.5481810356,1.3640926306,-3.3949271562	H,0,-6.889217747,3.26971471,1.0441175049
H,0,-6.2189239374,0.9580839906,-0.0688779541	C,0,-8.4370030257,-2.4383223911,0.6892497734
P,0,-2.6768207634,-6.2344179357,1.4805547254	H,0,-9.37693746,-2.5100362346,1.2506937518
C,0,-3.636455497,-7.7798196982,1.2071680217	H,0,-8.6860928897,-2.592057969,-0.3635591163
H,0,-4.2240565519,-8.0315851532,2.0952372345	H,0,-7.8024425751,-3.2630603578,1.0206944003
H,0,-4.3037083477,-7.6423144086,0.353615508	C,0,-6.3601624789,-1.7668982414,3.0140120992
H,0,-2.9596911495,-8.6074823544,0.9847645935	H,0,-7.0595411269,-1.8006783714,3.8589752405
C,0,-3.9397484451,-5.0679210187,2.1319981024	H,0,-6.2682790913,-2.7871160951,2.631238516
H,0,-4.4168238574,-5.4843258765,3.0237950067	H,0,-5.3881001224,-1.4665609359,3.4100024913
H,0,-3.4642602801,-4.1181505637,2.3839436165	C,0,-5.8634146498,1.376562759,3.0125009641
H,0,-4.7024857298,-4.8842015181,1.3725074789	H,0,-6.4636207629,1.5066391691,3.9215674435
C,0,-1.6622893978,-6.6041622257,2.9709338755	H,0,-4.9510818441,0.843559269,3.290115803
H,0,-2.3016370519,-6.9677236526,3.7811833927	H,0,-5.5767953589,2.3699754454,2.6610965635
H,0,-0.914717137,-7.3659096127,2.7417349144	H,0,0.4182331302,3.814164026,-3.1522080872
H,0,-1.1533543153,-5.6952367604,3.2989158292	H,0,-0.8904885655,5.8980462323,0.3555417362
Complex (S,*M*,*S*)-2	**Compound 2-Org**
E=-4030.8054874 H	E=-2196.7336454 H
2 1	0 1
C,0,8.2718987465,0.0832147169,0.21056982	C,0,2.8775868977,0.9898333748,-0.1205578099
C,0,7.7681152301,1.1373310578,1.0703634544	C,0,3.7836027679,0.4750211004,-1.0980700081
C,0,6.8605731544,0.5714365688,2.0123597027	C,0,2.9385696968,2.3911149603,0.2062209109
C,0,6.777861875,-0.8524360129,1.7421101161	C,0,4.6931658492,1.3218388629,-1.7118373235
C,0,7.6929513149,-1.1471660571,0.6636451735	C,0,3.7759901818,-0.9767966348,-1.4781285418
C,0,9.3849613436,0.2097020508,-0.7904933522	C,0,4.7451033068,2.7000681462,-1.3880929338

H,0,9.2422278727,-0.4675301029,-1.6352787399	C,0,3.002915864,-1.41640329,-2.5730664608
H,0,10.3516043355,-0.0301657769,-0.3302419191	C,0,4.553021768,-1.9027011005,-0.7507116956
H,0,9.4614906641,1.2244649417,-1.1875546004	C,0,3.0267149705,-2.7700671742,-2.9241092858
C,0,8.2697923373,2.5514135651,1.0789594028	C,0,4.548491479,-3.2470341528,-1.1369284453
H,0,9.1981109403,2.6069680512,1.6611847792	C,0,3.7958463995,-3.7019990279,-2.2225991506
H,0,7.5586563237,3.2387429548,1.5423216363	C,0,2.0483379919,2.9172099951,1.1851291898
H,0,8.5042286222,2.917785702,0.076444408	H,0,5.3703517092,0.9053809573,-2.4482233632
C,0,6.2752853329,1.2591584054,3.2112614422	O,0,5.6203974138,3.5808068689,-1.9614864422
H,0,5.3138492071,0.8289008178,3.4985542972	C,0,6.532137555,3.0999958071,-2.9360813245
H,0,6.1291241811,2.3294722605,3.0428699578	H,0,7.1198414205,3.9648208389,-3.2478642401
H,0,6.9494520231,1.1562668715,4.0709645596	H,0,6.0149860473,2.6845670943,-3.8104932031
C,0,6.0780886371,-1.8570338581,2.610854032	H,0,7.206755909,2.3382210946,-2.5248032543
H,0,5.8700319641,-2.7834863164,2.0714578631	C,0,3.8309155874,-5.1533909691,-2.639987369
H,0,5.1285285431,-1.4681069649,2.9856421657	C,0,2.1464575779,-0.4511760443,-3.3613351446
H,0,6.7001576383,-2.1106867277,3.4782729925	H,0,2.4242774006,-3.1040054627,-3.7661976991
C,0,8.0698005529,-2.5159333563,0.1810978679	C,0,5.3764781925,-1.4661337684,0.4399495741
H,0,8.9417359442,-2.8764553847,0.7402318596	C,0,1.1434583056,2.0893904099,1.8075270749
H,0,8.3379891677,-2.5090356921,-0.877018177	C,0,1.0811570152,0.7006542221,1.4783975795
H,0,7.2637013822,-3.2379295635,0.3291785569	C,0,1.9222620549,0.1624404312,0.5411858879
C,0,2.9927496993,-0.9625344712,-0.0308154922	C,0,0.,0.,2.3107101495
C,0,3.2999525557,-1.9401844185,-1.0497790134	C,0,-0.5341411968,1.1654775488,3.1506541496
C,0,3.9306367143,0.0465112225,0.3790995919	C,0,0.1379542906,2.3627245589,2.8413483603
C,0,4.4705715047,-1.9801995213,-1.7932063761	C,0,-0.1994091767,3.5508404318,3.4952904449
C,0,2.2970996454,-3.0060895422,-1.4017523931	C,0,-1.2100065404,3.5282977032,4.4569146184
Ir,0,5.9245623318,0.128654174,-0.1438823357	C,0,-1.540823017,1.1457475706,4.109742153
C,0,5.5898056464,-1.1381231923,-1.6192913651	C,0,-1.8760889722,2.3355207077,4.7628428994
C,0,1.4334550684,-2.8328654315,-2.5025925617	C,0,0.5341411968,-1.1654775488,3.1506541496
C,0,2.2695523016,-4.2077419449,-0.6595579482	C,0,-0.1379542906,-2.3627245589,2.8413483603
C,0,0.5560788169,-3.86864201,-2.8432455522	C,0,-1.0811570152,-0.7006542221,1.4783975795
C,0,1.3786672503,-5.2150746674,-1.0409013289	C,0,-1.1434583056,-2.0893904099,1.8075270749
C,0,0.517048984,-5.0713794172,-2.1332770294	C,0,0.1994091767,-3.5508404318,3.4952904449
P,0,5.4634174138,1.914684832,-1.5806295677	C,0,1.2100065404,-3.5282977032,4.4569146184
C,0,6.8033200845,2.2777501622,-2.7879445271	C,0,1.8760889722,-2.3355207077,4.7628428994
H,0,6.4982216572,3.0681902284,-3.4804185633	C,0,1.540823017,-1.1457475706,4.109742153
H,0,7.0374800154,1.3696909142,-3.3475405929	H,0,-2.6601064775,2.3343783204,5.5144799931
H,0,7.7045710162,2.5979466942,-2.2607448403	H,0,4.6270355754,-5.3376593634,-3.3725128502
C,0,5.1480535677,3.5405087774,-0.7766087604	H,0,2.887927013,-5.4595990638,-3.1028666325
H,0,4.9695817564,4.3084999779,-1.5354787705	H,0,4.0183847516,-5.8110756226,-1.7858692705
H,0,6.0063189241,3.8364366992,-0.1704450741	H,0,-1.4827370442,4.4442010043,4.9731496085
H,0,4.2690660548,3.4638033092,-0.1328803575	H,0,1.5899911997,-0.9737477219,-4.1438363255
C,0,3.9815050696,1.7045647654,-2.6496000939	H,0,2.7497753393,0.3287844842,-3.8381970522
H,0,3.8434563871,2.5840807666,-3.2850875708	H,0,1.424889486,0.0624624383,-2.7170309751
H,0,3.0985889211,1.5670114336,-2.0222466051	H,0,5.9435392442,-2.3056735174,0.8505569846
H,0,4.1012773142,0.8216511755,-3.2808842078	H,0,4.7426801202,-1.0648631099,1.23829521
C,0,3.4696472331,1.0013796526,1.3066697021	H,0,6.0844431686,-0.6745803763,0.1732112603
H,0,4.5100412611,-2.7493289477,-2.557241998	H,0,5.1474391862,-3.9569209235,-0.570459564
O,0,6.6161631019,-1.2519377302,-2.4790678925	H,0,-2.0585383809,0.2211687916,4.3484403626
C,0,6.6216561713,-2.202153146,-3.5709882868	H,0,0.3149295162,4.4785303798,3.260633771
H,0,7.5624314332,-2.0295928774,-4.0921720491	H,0,1.8772847396,-0.8929505374,0.2914363485
H,0,5.7836150035,-2.0238790243,-4.2498488096	H,0,-0.3149295162,-4.4785303798,3.260633771
H,0,6.5903309487,-3.2280980302,-3.1950457891	H,0,1.4827370442,-4.4442010043,4.9731496085
C,0,-0.4033609097,-6.195226397,-2.5452564357	C,0,-2.0483379919,-2.9172099951,1.1851291898
C,0,1.4341176576,-1.5563512854,-3.3146014969	C,0,-2.9385696968,-2.3911149603,0.2062209109
H,0,-0.1067908042,-3.7325260736,-3.6949062991	C,0,-2.8775868977,-0.9898333748,-0.1205578099
C,0,3.1818674823,-4.4237964007,0.5269860519	C,0,-1.9222620549,-0.1624404312,0.5411858879
C,0,2.1944630967,0.9359699548,1.8679577567	H,0,-1.8772847396,0.8929505374,0.2914363485
C,0,1.2999922144,-0.0933525217,1.4952351347	H,0,2.1026364519,3.9753101871,1.4278627712
C,0,1.6883548558,-1.014766804,0.5533642786	H,0,2.6601064775,-2.3343783204,5.5144799931
C,0,0.0000000000,0.0000000000,2.3020682395	H,0,2.0585383809,-0.2211687916,4.3484403626
C,0,0.2721309508,1.2493825399,3.1509288552	H,0,-2.1026364519,-3.9753101871,1.4278627712
C,0,1.5507248482,1.775277307,2.8792162477	C,0,-3.7836027679,-0.4750211004,-1.0980700081
C,0,2.0084302286,2.9141341851,3.5507335723	C,0,-4.6931658492,-1.3218388629,-1.7118373235
C,0,1.1768981706,3.5176558708,4.4933555274	H,0,-5.3703517092,-0.9053809573,-2.4482233632
C,0,-0.5529686709,1.8513215646,4.0940737461	C,0,-4.7451033068,-2.7000681462,-1.3880929338
C,0,-0.0928900986,2.9899718064,4.7635028248	O,0,-5.6203974138,-3.5808068689,-1.9614864422
C,0,-0.2721309508,-1.2493825399,3.1509288552	C,0,-6.532137555,-3.0999958071,-2.9360813245
C,0,-1.5507248482,-1.775277307,2.8792162477	H,0,-6.0149860473,-2.6845670943,-3.8104932031
C,0,-1.2999922144,0.0933525217,1.4952351347	H,0,-7.1198414205,-3.9648208389,-3.2478642401
C,0,-2.1944630967,-0.9359699548,1.8679577567	H,0,-7.206755909,-2.3382210946,-2.5248032543
C,0,-2.0084302286,-2.9141341851,3.5507335723	C,0,-3.7759901818,0.9767966348,-1.4781285418
C,0,-1.1768981706,-3.5176558708,4.4933555274	C,0,-4.553021768,1.9027011005,-0.7507116956

C,0,0.0928900986,-2.9899718064,4.7635028248 C,0,0.5529686709,-1.8513215646,4.0940737461 H,0,-0.7247448779,3.4690935506,5.5051689227 H,0,0.1405837412,-6.9597922755,-3.1125718131 H,0,-1.2169119762,-5.8361088799,-3.1819210094 H,0,-0.8425117837,-6.694091999,-1.6757238305 H,0,1.5153353687,4.4009051654,5.0260182241 H,0,0.6266533859,-1.5639949287,-4.0509539182 H,0,2.3746206903,-1.4231830638,-3.8613846375 H,0,1.3048923504,-0.6721709865,-2.6804724329 H,0,3.0455954001,-5.4234459078,0.9455454084 H,0,2.9865920237,-3.6973594279,1.3235882834 H,0,4.2363845824,-4.3198239518,0.2475292055 H,0,1.3634959968,-6.1407575913,-0.4703794386 H,0,-1.5351726688,1.4438772684,4.3153938061 H,0,2.9937687264,3.3237532785,3.347460288 H,0,1.0085543915,-1.8006814781,0.2420622844 H,0,-2.9937687264,-3.3237532785,3.347460288 H,0,-1.5153353687,-4.4009051654,5.0260182241 C,0,-3.4696472331,-1.0013796526,1.3066697021 C,0,-3.9306367143,-0.0465112225,0.3790995919 C,0,-2.9927496993,0.9625344712,-0.0308154922 C,0,-1.6883548558,1.014766804,0.5533642786 H,0,-1.0085543915,1.8006814781,0.2420622844 H,0,4.137032048,1.7953336111,1.6239304415 H,0,0.7247448779,-3.4690935506,5.5051689227 H,0,1.5351726688,-1.4438772684,4.3153938061 H,0,-4.137032048,-1.7953336111,1.6239304415 Ir,0,-5.9245623318,-0.128654174,-0.1438823357 C,0,-3.2999525557,1.9401844185,-1.0497790134 C,0,-4.4705715047,1.9801995213,-1.7932063761 H,0,-4.5100412611,2.7493289477,-2.557241998 C,0,-5.5898056464,1.1381231923,-1.6192913651 P,0,-5.4634174138,-1.914684832,-1.5806295677 C,0,-6.8033200845,-2.2777501622,-2.7879445271 H,0,-6.4982216572,-3.0681902284,-3.4804185633 H,0,-7.7045710162,-2.5979466942,-2.2607448403 H,0,-7.0374800154,-1.3696909142,-3.3475405929 C,0,-5.1480535677,-3.5405087774,-0.7766087604 H,0,-4.9695817564,-4.3084999779,-1.5354787705 H,0,-4.2690660548,-3.4638033092,-0.1328803575 H,0,-6.0063189241,-3.8364366992,-0.1704450741 C,0,-3.9815050696,-1.7045647654,-2.6496000939 H,0,-3.0985889211,-1.5670114336,-2.0222466051 H,0,-3.8434563871,-2.5840807666,-3.2850875708 H,0,-4.1012773142,-0.8216511755,-3.2808842078 O,0,-6.6161631019,1.2519377302,-2.4790678925 C,0,-6.6216561713,2.202153146,-3.5709882868 H,0,-5.7836150035,2.0238790243,-4.2498488096 H,0,-7.5624314332,2.0295928774,-4.0921720491 H,0,-6.5903309487,3.2280980302,-3.1950457891 C,0,-6.777861875,0.8524360129,1.7421101161 C,0,-7.6929513149,1.1471660571,0.6636451735 C,0,-6.8605731544,-0.5714365688,2.0123597027 C,0,-8.2718987465,-0.0832147169,0.21056982 C,0,-7.7681152301,-1.1373310578,1.0703634544 C,0,-2.2970996454,3.0060895422,-1.4017523931 C,0,-2.2695523016,4.2077419449,-0.6595579482 C,0,-1.4334550684,2.8328654315,-2.5025925617 C,0,-1.3786672503,5.2150746674,-1.0409013289 C,0,-0.5560788169,3.86864201,-2.8432455522 C,0,-0.517048984,5.0713794172,-2.1332770294 C,0,-1.4341176576,1.5563512854,-3.3146014969 H,0,-0.6266533859,1.5639949287,-4.0509539182 H,0,-1.3048923504,0.6721709865,-2.6804724329 H,0,-2.3746206903,1.4231830638,-3.8613846375 C,0,0.4033609097,6.195226397,-2.5452564357 H,0,1.2169119762,5.8361088799,-3.1819210094 H,0,-0.1405837412,6.9597922755,-3.1125718131 H,0,0.8425117837,6.694091999,-1.6757238305 C,0,-3.1818674823,4.4237964007,0.5269860519	C,0,-3.002915864,1.41640329,-2.5730664608 C,0,-4.548491479,3.2470341528,-1.1369284453 C,0,-3.0267149705,2.7700671742,-2.9241092858 C,0,-3.7958463995,3.7019990279,-2.2225991506 C,0,-2.1464575779,0.4511760443,-3.3613351446 H,0,-1.5899911997,0.9737477219,-4.1438363255 H,0,-1.424889486,-0.0624624383,-2.7170309751 H,0,-2.7497753393,-0.3287844842,-3.8381970522 C,0,-3.8309155874,5.1533909691,-2.639987369 H,0,-2.887927013,5.4595990638,-3.1028666325 H,0,-4.6270355754,5.3376593634,-3.3725128502 H,0,-4.0183847516,5.8110756226,-1.7858692705 C,0,-5.3764781925,1.4661337684,0.4399495741 H,0,-6.0844431686,0.6745803763,0.1732112603 H,0,-4.7426801202,1.0648631099,1.23829521 H,0,-5.9435392442,2.3056735174,0.8505569846 H,0,-5.1474391862,3.9569209235,-0.570459564 H,0,-2.4242774006,3.1040054627,-3.7661976991 C,0,-3.8805747354,-3.2199631712,-0.444307652 C,0,3.8805747354,3.2199631712,-0.444307652 H,0,3.9350512105,4.2776000257,-0.2064327772 H,0,-3.9350512105,-4.2776000257,-0.2064327772

H,0,-4.2363845824,4.3198239518,0.2475292055
H,0,-2.9865920237,3.6973594279,1.3235882834
H,0,-3.0455954001,5.4234459078,0.9455454084
C,0,-9.3849613436,-0.2097020508,-0.7904933522
H,0,-9.4614906641,-1.2244649417,-1.1875546004
H,0,-10.3516043355,0.0301657769,-0.3302419191
H,0,-9.2422278727,0.4675301029,-1.6352787399
C,0,-8.0698005529,2.5159333563,0.1810978679
H,0,-8.3379891677,2.5090356921,-0.877018177
H,0,-8.9417359442,2.8764553847,0.7402318596
H,0,-7.2637013822,3.2379295635,0.3291785569
C,0,-8.2697923373,-2.5514135651,1.0789594028
H,0,-9.1981109403,-2.6069680512,1.6611847792
H,0,-8.5042286222,-2.917785702,0.076444408
H,0,-7.5586563237,-3.2387429548,1.5423216363
C,0,-6.2752853329,-1.2591584054,3.2112614422
H,0,-6.9494520231,-1.1562668715,4.0709645596
H,0,-6.1291241811,-2.3294722605,3.0428699578
H,0,-5.3138492071,-0.8289008178,3.4985542972
C,0,-6.0780886371,1.8570338581,2.610854032
H,0,-6.7001576383,2.1106867277,3.4782729925
H,0,-5.1285285431,1.4681069649,2.9856421657
H,0,-5.8700319641,2.7834863164,2.0714578631
H,0,-1.3634959968,6.1407575913,-0.4703794386
H,0,0.1067908042,3.7325260736,-3.6949062991

Complex (*R,P*)-3
E=-2958.9318586 H
1 1
C,0,4.8630200445,-0.3814218888,-0.7381798844
C,0,4.3865375425,-1.7246939227,-0.4875844177
C,0,3.267291668,-1.985982729,-1.333395373
C,0,3.0263398155,-0.7931390049,-2.1220601032
C,0,4.0428670048,0.1726312832,-1.7781228407
C,0,6.122257292,0.2306342135,-0.193614281
H,0,6.0166637342,1.3097654545,-0.0638835514
H,0,6.9683676522,0.0557632856,-0.870318018
H,0,6.3922213846,-0.1936808824,0.7765119922
C,0,5.0731343427,-2.7310314151,0.3887906889
H,0,5.9023337409,-3.1935637357,-0.1612166056
H,0,4.4016400907,-3.5362653156,0.694645394
H,0,5.5020508469,-2.278536782,1.2864824307
C,0,2.6056032302,-3.3158852814,-1.5509034936
H,0,1.565217184,-3.2053792614,-1.8629557498
H,0,2.6227477644,-3.937829451,-0.6517155018
H,0,3.1257256223,-3.8736326185,-2.3402163294
C,0,2.0527563888,-0.6913687436,-3.2604109751
H,0,1.810879346,0.3477195133,-3.4937541859
H,0,1.1173134687,-1.2079255228,-3.0333701968
H,0,2.473876332,-1.1459094747,-4.1659647389
C,0,4.2854077837,1.4786094788,-2.4747953104
H,0,4.9983032096,1.3346702587,-3.2958698749
H,0,4.709643997,2.221249907,-1.7963475757
H,0,3.3680674922,1.888222269,-2.9033853015
C,0,-0.3880297176,0.6709688289,-0.12449995
C,0,-0.0371402516,2.0696407714,-0.1360467405
C,0,0.5858503605,-0.3746575828,0.0333772665
C,0,1.2356374874,2.5777151561,0.0945113986
C,0,-1.0975237933,3.109530116,-0.3776331763
Ir,0,2.6334259979,-0.1300471776,0.0393983753
C,0,2.4028231584,1.8156718481,0.2886958633
C,0,-1.7660049599,3.7145835277,0.7074898073
C,0,-1.3806633915,3.5110829948,-1.7009231596
C,0,-2.7094054801,4.7134295698,0.4450133335
C,0,-2.3302556509,4.5152899321,-1.9118961321
C,0,-3.0088978934,5.129475809,-0.8551640177
P,0,2.59909292,-0.4145627955,2.359829293
C,0,4.1429440827,0.1388516831,3.1955204991
H,0,4.0498966861,0.0493218511,4.2821411095
H,0,4.3403199194,1.1790872251,2.9280161849
H,0,4.987240539,-0.4676542809,2.8601544705
C,0,2.3749187843,-2.1413069426,2.9565676186

Complex (*R,M*)-3
E=-2958.9314318
1 1
C,0,3.0616212593,-2.950299547,-0.8966737889
C,0,2.6327782817,-2.1014627175,-1.9836827135
C,0,3.7892961024,-1.4943054358,-2.5614934155
C,0,4.9570444199,-2.0359641571,-1.8763230172
C,0,4.5171526537,-2.9399223489,-0.8732874604
C,0,2.1855828086,-3.9015834931,-0.1324985603
H,0,2.5942754439,-4.1205718829,0.8568578014
H,0,2.0956835109,-4.854458978,-0.669135226
H,0,1.1779730964,-3.5029160233,0.0020041379
C,0,1.2234403088,-1.9726511113,-2.4769254727
H,0,1.0246514236,-2.746740312,-3.2284470426
H,0,1.0372610225,-1.0036568019,-2.9429379551
H,0,0.4961860952,-2.0998937908,-1.6728328099
C,0,3.8219169952,-0.6897262992,-3.8303859257
H,0,4.6636132884,0.0067008426,-3.857336337
H,0,2.9044506751,-0.1128890117,-3.9694748959
H,0,3.9219438597,-1.3491281956,-4.7021284546
C,0,6.3792069031,-1.820524522,-2.3052198581
H,0,7.0859327304,-2.0323956817,-1.4998638983
H,0,6.5566559842,-0.802171587,-2.6609924485
H,0,6.6227777657,-2.4937592577,-3.1369001833
C,0,5.3829168663,-3.8420900539,-0.0439348138
H,0,5.5595061423,-4.7876971015,-0.5718567711
H,0,4.9149626745,-4.0821326325,0.9121984289
H,0,6.3552498954,-3.3922047056,0.1678992314
C,0,1.1080428874,0.441862005,1.0530917057
C,0,1.4269072177,-0.185697148,2.3118254058
C,0,1.9831183114,0.3851296299,-0.0845699224
C,0,2.6160214136,-0.8458833459,2.5978714119
C,0,0.4522850451,-0.112818504,3.4558064122
Ir,0,3.6359759508,-0.8218560514,-0.2783263871
C,0,3.6610345759,-1.0894930681,1.6858455826
C,0,-0.546495608,-1.1021155728,3.5820409505
C,0,0.5676815296,0.9082326397,4.4225596965
C,0,-1.4101963306,-1.0502014025,4.6805995074
C,0,-0.322224847,0.9197459226,5.5012609597
C,0,-1.3190753943,-0.0484877414,5.6513000027
P,0,4.9972765815,1.0614000679,-0.0331349145
C,0,4.4384012702,2.2844069711,1.2212623715
H,0,5.1538731373,3.1082827524,1.2971311688
H,0,4.3431696491,1.7987862171,2.1947466734
H,0,3.4609038364,2.6767446903,0.9345468767
C,0,5.2399415727,2.1070566358,-1.5296399464

H,0,2.4024635606,-2.1676396597,4.0501938283	H,0,5.9025634036,2.9474181872,-1.3008296697
H,0,3.1657851148,-2.7842919048,2.5656712436	H,0,4.2761002422,2.4955387538,-1.8657364924
H,0,1.4082929267,-2.5195397612,2.6172812082	H,0,5.6822401186,1.5184787758,-2.3361817233
C,0,1.2813275102,0.4944619706,3.2621390669	C,0,6.716190759,0.6702998563,0.4966663413
H,0,1.3582644389,0.3056182368,4.3366722534	H,0,7.2867941465,1.5871348761,0.6732833707
H,0,0.3020738956,0.1656721928,2.9093828747	H,0,7.2177327049,0.0818299204,-0.274466125
H,0,1.3748186316,1.5665141191,3.0777721021	H,0,6.6793770124,0.0767576736,1.4122317483
C,0,0.0975635169,-1.691523646,0.1264711002	C,0,1.6169724948,1.1427735863,-1.2132512845
H,0,1.3067981558,3.6600101122,0.1087625222	H,0,2.7150406267,-1.1998114103,3.6185127295
O,0,3.5483420579,2.4594671628,0.5856372186	O,0,4.7927835472,-1.6532629188,2.1454123198
C,0,3.6171815561,3.8968101866,0.7210319437	C,0,4.9737715673,-2.0170507598,3.5320076697
H,0,4.6502634272,4.1075066269,0.9957079086	H,0,5.9849210412,-2.4183948376,3.5910275009
H,0,2.9451470121,4.2497995069,1.5078621899	H,0,4.2549287495,-2.7840522996,3.8329809596
H,0,3.3784263494,4.3911577388,-0.2245725081	H,0,4.8818673763,-1.1433524812,4.1830455977
C,0,-4.052442848,6.1897183712,-1.1130896652	C,0,-2.2854435812,0.002094695,6.8102627067
C,0,-1.4969849621,3.2960915959,2.1358193228	C,0,-0.6999020719,-2.2052598395,2.5588171641
H,0,-3.2239988047,5.1776613199,1.2830190442	H,0,-2.1756950134,-1.8164547722,4.7781309263
C,0,-0.6772452204,2.8830361632,-2.8836121443	C,0,1.6214870657,1.9876986697,4.3106429164
C,0,-1.2648580918,-1.9854734703,0.0462433306	C,0,0.4222845358,1.8624651019,-1.2641287132
C,0,-2.2089947626,-0.9488794577,-0.127055339	C,0,-0.4600170515,1.8586297632,-0.1602057236
C,0,-1.7784521523,0.3508560448,-0.2170949533	C,0,-0.1176966135,1.17393979,0.9788011075
C,0,-3.6344900638,-1.5037663418,-0.1184255205	C,0,-1.7295665879,2.6517017187,-0.4757973134
C,0,-3.3622107044,-3.0042127903,0.0270883403	C,0,-1.4176844636,3.1508935894,-1.8898830249
C,0,-1.9790442587,-3.2593090033,0.1276863426	C,0,-0.1653244256,2.6746523682,-2.3292812904
C,0,-1.5051179233,-4.5674101801,0.2768422382	C,0,0.3150229041,3.0032753934,-3.6017454477
C,0,-2.4260542056,-5.6128934869,0.3228582223	C,0,-0.4671832984,3.8109600718,-4.4257930377
C,0,-4.2773331998,-4.0496269014,0.0730749363	C,0,-2.1947792997,3.9560592341,-2.7147344811
C,0,-3.8002319508,-5.3556612794,0.2214226338	C,0,-1.7111755044,4.2834555684,-3.985265139
C,0,-4.4848991908,-1.1423503368,-1.3392130662	C,0,-2.0663456766,3.7663874162,0.5182458034
C,0,-5.6634895458,-0.4774684367,-0.9460740947	C,0,-3.350520409,3.574439168,1.065661687
C,0,-4.4841214615,-0.9282553789,1.0221653827	C,0,-2.9967192671,1.7892124327,-0.4028471872
C,0,-5.6632915391,-0.3425985083,0.5154768279	C,0,-3.9268768631,2.3499611895,0.4973505713
C,0,-6.5951136689,-0.0653170873,-1.9022638852	C,0,-3.8668940626,4.4837439335,1.9922673716
C,0,-6.3358933199,-0.324161347,-3.2494112436	C,0,-3.0888137603,5.5820800494,2.3628765047
C,0,-5.1644907248,-0.9857239481,-3.636665647	C,0,-1.8141460797,5.7710422648,1.8158496408
C,0,-4.2305690967,-1.4008592257,-2.6809885521	C,0,-1.2949717463,4.8622293045,0.8871537632
H,0,-4.5033946637,-6.1822399661,0.2579924575	H,0,-2.3069981408,4.9122307311,-4.6399620317
H,0,-3.8137885772,6.7784352471,-2.0036007386	H,0,-1.8329573263,0.4698436958,7.6892983695
H,0,-4.1449408492,6.8754299818,-0.2661502145	H,0,-2.6242161986,-0.9986523234,7.0932513491
H,0,-5.0387694698,5.7384331008,-1.2768064217	H,0,-3.1771859873,0.5867950661,6.5528803167
H,0,-2.0784574666,-6.6350791734,0.4369035044	H,0,-0.1120460302,4.0774818882,-5.4165093144
H,0,-2.1071237372,3.8761405438,2.8320597894	H,0,-1.496395496,-2.8949177066,2.8476459226
H,0,-0.446980879,3.4429401006,2.4130160901	H,0,0.2221174222,-2.7866901531,2.4474537711
H,0,-1.7279957678,2.23687278,2.2961729582	H,0,-0.9499310468,-1.8041962059,1.5699392663
H,0,-1.0412292434,3.3072257556,-3.8222561004	H,0,1.5056962799,2.7272537401,5.1063286279
H,0,-0.8391849787,1.800068549,-2.9202391915	H,0,1.5574634642,2.5152428128,3.3525120189
H,0,0.406280307,3.0452637228,-2.8421423225	H,0,2.6350122911,1.5764889885,4.3859038546
H,0,-2.5435532042,4.825381059,-2.9322077505	H,0,-0.2321659209,1.7091479339,6.2438015144
H,0,-5.3433001852,-3.8584100128,-0.0058612081	H,0,-3.1592551879,4.3262896278,-2.3803970451
H,0,-0.4404425983,-4.7703307309,0.3527411995	H,0,1.2794652864,2.6398172878,-3.9460695023
H,0,-2.495054363,1.1564365794,-0.3328202838	H,0,-0.7751767972,1.1842221921,1.8411191121
H,0,-7.5069157001,0.4458721493,-1.6071703276	H,0,-4.8566256443,4.3439480976,2.4172951447
H,0,-7.0509352472,-0.0119197832,-4.0045703629	H,0,-3.4771302106,6.2990423589,3.0799868324
C,0,-6.5837498488,0.2451168848,1.3867713578	C,0,-5.1550302858,1.7217391425,0.717574958
C,0,-6.3128230123,0.2468783725,2.7557935921	C,0,-5.4392941528,0.5364793473,0.0378520907
C,0,-5.1309182118,-0.3229922504,3.260756856	C,0,-4.508523185,-0.0297370037,-0.8506791385
C,0,-4.2096278674,-0.9153392537,2.3770864928	C,0,-3.2734051665,0.6088733918,-1.0675187335
H,0,-3.3019086719,-1.3445521518,2.789317975	H,0,-2.5685315755,0.1495206711,-1.7532313991
H,0,0.7972224319,-2.508299928,0.2662873993	H,0,2.2645979661,1.142445029,-2.0844968901
H,0,-4.9810557336,-1.1819480237,-4.6888447801	H,0,-1.2248720394,6.6338091782,2.111979637
H,0,-3.3265152386,-1.9206853379,-2.9859028092	H,0,-0.3084755923,5.0174054037,0.4589103143
H,0,-7.4950608478,0.7007026044,1.0107105857	H,0,-5.8799003488,2.1411484338,1.4090539836
H,0,-7.0149978893,0.7057796481,3.4445188986	H,0,-6.386698041,0.0333178073,0.2028043266
C,0,-4.775400853,-0.2690391249,4.7154654139	C,0,-4.7556214123,-1.3362938731,-1.5425419102
O,0,-3.6331199026,-0.5333319175,5.076651582	O,0,-3.8322501601,-1.9153940491,-2.1049182093
C,0,-5.8208506765,0.1526160065,5.7186689983	C,0,-6.1356205488,-1.9461468488,-1.5037305611
C,0,-5.6607726849,1.3805886061,6.3944182068	C,0,-6.3349837214,-3.1340189145,-0.7696730817
C,0,-6.9043935419,-0.6956200387,6.0230239355	C,0,-7.1914669606,-1.3752592211,-2.2422863006
C,0,-6.614495887,1.7545492196,7.3438723903	C,0,-7.6061580783,-3.7130673686,-0.7609581397
C,0,-7.8242149886,-0.2867596687,6.9950473922	C,0,-8.4426304128,-2.0012016286,-2.2177610368
C,0,-7.7026014697,0.9345603275,7.66279763	C,0,-8.6738496988,-3.1657149865,-1.4808195415

H,0,-6.5011561102,2.7088469741,7.8535743082 H,0,-8.6553375723,-0.9448368296,7.2384788214 C,0,-7.0799216347,-2.0402905225,5.3491705432 H,0,-7.4106037437,-1.9370928394,4.3096278461 H,0,-6.1457281143,-2.6112719403,5.3346013801 H,0,-7.8273226102,-2.6391856164,5.8756222195 C,0,-8.6961130362,1.3440994133,8.7237170147 H,0,-9.6629250048,0.8538458777,8.5785322046 H,0,-8.3382546199,1.0710067121,9.7241743829 H,0,-8.8593645531,2.4261238277,8.7233202407 C,0,-4.4864186697,2.2901953181,6.1060768937 H,0,-3.5432551026,1.8114339964,6.3855955938 H,0,-4.4154867671,2.5375718786,5.0401320863 H,0,-4.5765678576,3.2271852389,6.6613498376	H,0,-7.7652976082,-4.6202505513,-0.1821632024 H,0,-9.256069393,-1.567545259,-2.795155195 C,0,-6.9973544696,-0.127001088,-3.0771781905 H,0,-6.8917112673,0.769042891,-2.455397155 H,0,-6.1000990584,-0.1932235907,-3.7013888798 H,0,-7.8524027304,0.0293329521,-3.7396520459 C,0,-10.0272339934,-3.8355955338,-1.4884598538 H,0,-10.8270135268,-3.1216495993,-1.7050299694 H,0,-10.0736355607,-4.6199434128,-2.254119405 H,0,-10.2450095287,-4.3097142313,-0.5266272564 C,0,-5.2054511214,-3.7806940334,0.0019393981 H,0,-4.4156561656,-4.1222182358,-0.6737788687 H,0,-4.7417215782,-3.0811678028,0.7075469397 H,0,-5.5675796474,-4.6397588124,0.5722578159
Compound 3-Org E=-2041.8902002 0 1 C,0,0.9127705453,0.3229245171,0.9921708754 C,0,1.2878146613,-0.2647110412,2.2391804629 C,0,1.8092725431,0.1970982608,-0.1277719987 C,0,2.4942442741,-0.9375443609,2.3508517005 C,0,0.3961465142,-0.1698040437,3.4425428516 C,0,3.372036145,-1.057007621,1.2451007299 C,0,-0.5642730782,-1.1728137203,3.6909782016 C,0,0.5328913221,0.9098038937,4.3402310691 C,0,-1.3648073297,-1.079881048,4.834287522 C,0,-0.2884467831,0.9631872185,5.4710936184 C,0,-1.2452441793,-0.0198499815,5.7366458643 C,0,1.448316825,0.7765409072,-1.3774971408 H,0,2.7549641213,-1.3744143393,3.3076332233 O,0,4.5728742813,-1.7078570783,1.2981021953 C,0,4.9708264165,-2.309276723,2.5200598473 H,0,5.9430159037,-2.7647880671,2.3258485473 H,0,4.2676020219,-3.0886621143,2.8400344881 H,0,5.0760215104,-1.5700852073,3.324438043 C,0,-2.1434554033,0.0760906605,6.9474664318 C,0,-0.7392529326,-2.338377536,2.7436818882 H,0,-2.1009097368,-1.8583884102,5.0231797189 C,0,1.5480318554,2.003744556,4.0965339838 C,0,0.2549937689,1.4478865568,-1.5053320545 C,0,-0.6319301905,1.5721552823,-0.3925143937 C,0,-0.3162975563,1.0268871176,0.8232733367 C,0,-1.8841469267,2.362822916,-0.7917852283 C,0,-1.5920588684,2.6658730853,-2.2664175075 C,0,-0.3514465011,2.1276268136,-2.6560427296 C,0,0.1074462374,2.2910259417,-3.96577658 C,0,-0.6830460997,2.9945043152,-4.875072241 C,0,-2.3777909422,3.3672621048,-3.1739586691 C,0,-1.9160464993,3.5291694322,-4.4835871582 C,0,-2.1203101745,3.6182076685,0.0528964748 C,0,-3.3886272845,3.5807957528,0.6632929864 C,0,-3.1969696575,1.6038068128,-0.5717647946 C,0,-4.0571446293,2.3337362395,0.2769160398 C,0,-3.813392177,4.6308382601,1.4814097668 C,0,-2.9582623419,5.7150846061,1.6814111456 C,0,-1.6977628647,5.7497779933,1.0732054789 C,0,-1.2709666003,4.6998901279,0.2539901937 H,0,-2.5196691957,4.0739066802,-5.2035208155 H,0,-1.6468772454,0.5919362331,7.7749138261 H,0,-2.4485622259,-0.9140085737,7.299434167 H,0,-3.0593001023,0.6358261128,6.7192258109 H,0,-0.3391729768,3.1280900428,-5.8965717706 H,0,-1.5263712877,-3.0110174243,3.0942708908 H,0,0.1833158309,-2.9196338818,2.6425409931 H,0,-1.0075532851,-1.9999595891,1.7371501536 H,0,1.5127044195,2.7526185478,4.8920974988 H,0,1.3654354428,2.5132705785,3.1442429457 H,0,2.5674532968,1.6065454305,4.0488212364 H,0,-0.1758655892,1.7960913773,6.1618933812 H,0,-3.3348998806,3.7830209287,-2.872335568 H,0,1.0631694005,1.8769697235,-4.2742088968	**Complex (*R*,*P*)-4** E=-2842.1773131 H 1 1 C,0,4.8622172687,-0.2997382739,-0.9111525898 C,0,4.4292619393,-1.6643062349,-0.7063449163 C,0,3.2632415047,-1.9057663878,-1.4943196583 C,0,2.9503987338,-0.6786312,-2.200106464 C,0,3.965765738,0.2911473465,-1.8653409065 C,0,6.1386887625,0.3141661635,-0.4106525369 H,0,6.0115232843,1.3777012739,-0.1978186341 H,0,6.9406950821,0.2138802951,-1.1529893329 H,0,6.4863388446,-0.1668372271,0.5068503672 C,0,5.188400024,-2.7019770336,0.067879886 H,0,5.9804879638,-3.1253450976,-0.5625121807 H,0,4.5497833617,-3.5311003504,0.3806161697 H,0,5.6763811752,-2.2877718659,0.9537539772 C,0,2.618322566,-3.2382895048,-1.7444265294 H,0,1.5598679021,-3.137141485,-1.9920659513 H,0,2.6994811667,-3.9049514812,-0.8814628837 H,0,3.1044811045,-3.7423511662,-2.5895395886 C,0,1.9012955639,-0.5351258656,-3.264193459 H,0,1.6166019576,0.508801869,-3.4117262454 H,0,0.9972103893,-1.0935514733,-3.0109639545 H,0,2.273129666,-0.9177657095,-4.2229359944 C,0,4.137975933,1.6387436657,-2.501154306 H,0,4.8076247159,1.558272083,-3.366159093 H,0,4.5815915517,2.3551723814,-1.8069195393 H,0,3.188796709,2.0458245253,-2.8565650017 C,0,-0.3519997344,0.6269756778,0.0381586634 C,0,-0.0169682063,2.0270390697,0.1069065623 C,0,0.6384328322,-0.4138449064,0.0980047109 C,0,1.2603246171,2.5371625691,0.312806045 C,0,-1.0978671218,3.0667708271,-0.0154057199 Ir,0,2.6821177529,-0.1428217376,0.0167440377 C,0,2.4438192928,1.7820129601,0.3962130095 C,0,-1.7282945038,3.5804195173,1.1371795796 C,0,-1.4392432987,3.5609289657,-1.2927960158 C,0,-2.6919816554,4.5831427413,0.9880292008 C,0,-2.4074293983,4.5647591458,-1.3902718752 C,0,-3.048814315,5.0899197251,-0.2645209643 P,0,2.7802882765,-0.566929604,2.3099945682 C,0,4.3634368812,-0.0517843266,3.0953659346 H,0,4.3325065256,-0.2149580785,4.1769948447 H,0,4.5357799897,1.0066164143,2.8885249104 H,0,5.1931203234,-0.6233720299,2.6734882051 C,0,2.5984929097,-2.3292734947,2.8094745951 H,0,2.6931513983,-2.426939581,3.8953020929 H,0,3.3663077686,-2.9391135951,2.3296600568 H,0,1.6150211179,-2.6921677453,2.5033756254 C,0,1.5102770639,0.2744223535,3.3385606869 H,0,1.643196084,0.0161339083,4.3930618179 H,0,0.5148239465,-0.033246773,3.0129881469 H,0,1.5938487223,1.3566621158,3.2204027125 C,0,0.1686175094,-1.739812436,0.1271584815 H,0,1.3192479334,3.6170224595,0.3967866931 O,0,3.59770438,2.4224072705,0.6693453308 C,0,3.6585852643,3.8500341328,0.8856423347

H,0,-0.9892205212,1.1201015602,1.6698636139	H,0,4.7035323086,4.059298007,1.1124634825
H,0,-4.7906125371,4.6068280251,1.9553069884	H,0,3.0297217998,4.1467132472,1.729428208
H,0,-3.2726145368,6.5395378419,2.3145598776	H,0,3.3594169777,4.3957057684,-0.0134205169
C,0,-5.3151760068,1.8275748918,0.6112126277	C,0,-4.1137571021,6.1513932408,-0.4013045392
C,0,-5.7053263798,0.5941852612,0.0919413968	C,0,-1.3973687173,3.0598891808,2.5180917147
C,0,-4.8519407881,-0.1366840446,-0.7539077528	H,0,-3.1771614531,4.9766258157,1.8781612761
C,0,-3.5833537146,0.3784921047,-1.0840064273	C,0,-0.7814865463,3.0284743233,-2.5464536166
H,0,-2.9401415557,-0.2043678759,-1.7352438417	C,0,-1.1920594939,-2.0466909956,0.0529164697
H,0,2.1298253844,0.6756523254,-2.2180961106	C,0,-2.152515164,-1.0145353556,-0.0408312681
H,0,-1.0444485023,6.6013107007,1.239285021	C,0,-1.7403273898,0.2942393512,-0.0460061068
H,0,-0.2925515505,4.7301105029,-0.2164416286	C,0,-3.568832985,-1.5899590812,-0.0989816425
H,0,-5.9825155962,2.3807665528,1.265619523	C,0,-3.2747395654,-3.0906501055,-0.0404926603
H,0,-6.6787053781,0.1855776668,0.343292101	C,0,-1.8881787837,-3.3329026174,0.0508495289
C,0,-5.2436786508,-1.4678306126,-1.309282358	C,0,-1.3957519915,-4.6412455516,0.1192866346
O,0,-4.4600503716,-2.1254467713,-1.983120989	C,0,-2.3017591041,-5.7002480516,0.0952241237
C,0,-6.627202315,-2.0107159877,-1.0151186302	C,0,-4.1746822801,-4.1502709636,-0.064188447
C,0,-6.7881637907,-2.9626417623,0.0092450598	C,0,-3.6793753471,-5.4560129144,0.0042268955
C,0,-7.7225904371,-1.6138674069,-1.8041883696	C,0,-4.3654094173,-1.1586612721,-1.3364542224
C,0,-8.0615384475,-3.4896569066,0.2424923672	C,0,-5.5518018119,-0.5010651337,-0.9562959288
C,0,-8.9775674052,-2.1722605198,-1.5401735266	C,0,-4.477712509,-1.0955156905,1.0343991876
C,0,-9.1692278288,-3.1099339016,-0.5217594361	C,0,-5.6184592339,-0.4608313845,0.5095720705
H,0,-8.1894343746,-4.2187803526,1.0397356811	C,0,-6.4322051629,-0.021406886,-1.9289184693
H,0,-9.8256175924,-1.8672062642,-2.1494743495	C,0,-6.1154080095,-0.2075545677,-3.2765529837
C,0,-7.5545945902,-0.6169324375,-2.9294296507	C,0,-4.9372299275,-0.8636546166,-3.6499832116
H,0,-7.2306145741,0.3622605735,-2.5593300566	C,0,-4.0528707429,-1.3447542216,-2.6774376443
H,0,-6.7988543686,-0.9532659153,-3.647300078	H,0,-4.3708197261,-6.2930735341,-0.0138830774
H,0,-8.4939100279,-0.4762146482,-3.4701585915	H,0,-3.9138396352,6.8124642048,-1.2496218717
C,0,-10.5281702859,-3.7213587088,-0.2742823791	H,0,-4.1850019755,6.7662676558,0.5003130347
H,0,-11.333034279,-3.0456748945,-0.578571654	H,0,-5.0993912872,5.6994152926,-0.5670660802
H,0,-10.6529449439,-4.6522612473,-0.8415118362	H,0,-1.9402388095,-6.7227375628,0.1463334161
H,0,-10.6712417964,-3.9653798032,0.7828099452	H,0,-1.9810260615,3.5814102546,3.2801131264
C,0,-5.6090259783,-3.4152797902,0.8409106072	H,0,-0.3371795304,3.1936135236,2.7612426629
H,0,-4.8508218249,-3.8978923559,0.2159569226	H,0,-1.617357159,1.9899176404,2.6069984371
H,0,-5.119662195,-2.5719134593,1.3417614101	H,0,-1.1788215464,3.5252559372,-3.4345607421
H,0,-5.9219683938,-4.1260460643,1.6099038276	H,0,-0.9492958075,1.9518961713,-2.662211706
C,0,3.029956393,-0.4972777783,0.0291063514	H,0,0.3033151125,3.1864285183,-2.5324417839
H,0,3.7131139699,-0.5991807526,-0.8080951577	H,0,-2.6663438123,4.945630757,-2.3754482053
	H,0,-5.2428476165,-3.9687030835,-0.1348354941
	H,0,-0.3285220678,-4.8335917824,0.1879207767
	H,0,-2.4698657017,1.0948231827,-0.0979979598
	H,0,-7.3507112922,0.4850782486,-1.6464876143
	H,0,-6.7926769324,0.1575134609,-4.042997171
	C,0,-6.5737953125,0.0690079657,1.3794314953
	C,0,-6.378725599,-0.0457983107,2.7548215974
	C,0,-5.238980692,-0.6765706527,3.2939662137
	C,0,-4.2821252665,-1.2032269623,2.4028680659
	H,0,-3.3864581143,-1.6776261402,2.7939142092
	H,0,0.8821133204,-2.5539220674,0.1947492806
	H,0,-4.7094993903,-1.0045300656,-4.7023901183
	H,0,-3.1421681599,-1.8603437239,-2.9703689594
	H,0,-7.46850969,0.5523045522,0.9972028303
	H,0,-7.1386624267,0.3344571702,3.4303230784
	C,0,-5.0517710146,-0.7896276945,4.7604059084
	C,0,-4.4564360078,-1.9308236313,5.3344170145
	C,0,-5.4608395178,0.2305712285,5.6312375736
	C,0,-4.2801769273,-2.0437876824,6.7054202862
	H,0,-4.1579243323,-2.7572185964,4.6959578054
	C,0,-5.2924530758,0.1323518054,7.0133148818
	H,0,-5.9019069618,1.1360308675,5.2246889655
	C,0,-4.6979831166,-1.0115539044,7.5603443052
	H,0,-3.8375541091,-2.9315649855,7.145331032
	H,0,-5.6187338729,0.9488398232,7.646469138
	O,0,-4.4823492061,-1.2178151512,8.8883878197
	C,0,-4.9326165972,-0.2322952999,9.8075779489
	H,0,-4.6842652737,-0.6109156391,10.7998154055
	H,0,-4.4258968657,0.728586451,9.6510700962
	H,0,-6.0172575343,-0.0825698681,9.7387757079
Complex (*R,M*)-4	**Compound 4-Org**
E=-2842.1772421 H	E=-1925.1333126 H
1 1	0 1
C,0,-3.0725933912,-2.8305051691,-0.8876165088	C,0,-0.4297511121,0.8039858282,-0.6866135365

C,0,-2.5026738727,-2.7852790197,0.4377719932	C,0,-0.8650414392,1.0398761265,-2.0267798094
C,0,-3.5528924806,-2.5043829634,1.3684861831	C,0,-1.2700192011,0.0236300935,0.1846147624
C,0,-4.7969026725,-2.4475408207,0.6163409353	C,0,-2.0741907479,0.5211402992,-2.4623407802
C,0,-4.5113864201,-2.6605706429,-0.7598284165	C,0,-0.0349872941,1.8446352631,-2.9836633311
C,0,-2.3552068894,-3.2555573667,-2.1370908929	C,0,-2.8960325877,-0.2455749338,-1.5997821858
H,0,-2.8239139464,-2.8389471895,-3.0317407596	C,0,0.9149643602,1.2040795056,-3.8066108986
H,0,-2.3733182685,-4.3481697362,-2.2360905726	C,0,-0.2199794933,3.2399000465,-3.078997741
H,0,-1.3093379351,-2.9413053953,-2.1298922226	C,0,1.6563568601,1.9693205196,-4.7128353186
C,0,-1.0769775898,-3.0949451992,0.781970475	C,0,0.542893671,3.9664815795,-3.998951768
H,0,-0.9778151537,-4.160982573,1.0213748258	C,0,1.488023032,3.3518307656,-4.8242977481
H,0,-0.7308712906,-2.5255345734,1.6465646041	C,0,-0.8493451734,-0.219905053,1.5230351364
H,0,-0.4038945583,-2.8782002889,-0.0498354414	H,0,-2.3809679332,0.7148507005,-3.48343462
C,0,-3.4455763156,-2.5662758854,2.8663037281	O,0,-4.0969398584,-0.7809421456,-1.9754205744
H,0,-4.1569244387,-1.899848729,3.3609735319	C,0,-4.5561156284,-0.5650525436,-3.3002489454
H,0,-2.4431850513,-2.3028868811,3.2118753813	H,0,-5.5173333425,-1.0765527663,-3.370296327
H,0,-3.65222638,-3.5824399468,3.2263712175	H,0,-3.8701300158,-0.9884479676,-4.0450053346
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