SUPPORTING INFORMATION

Highly Linearized Twisted Iridium(III) complexes

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S1. Synthesis

General details. NMR spectra were recorded in deuterated solvent solutions on a Varian VNMRS-600 spectrometer and referenced against solvent resonances (^{1}H, ^{13}C). ESMS data were recorded on a TQD mass spectrometer (Waters Ltd, UK) in either acetonitrile or methanol, GCMS data were recorded on Trace GCMS (ThermoFinnigan) GCMS recorded in DCM, ASAP data were recorded on a Xevo QTOF (Waters) high resolution, accurate mass tandem mass spectrometer equipped with Atmospheric Pressure Gas Chromatography (APGC) and Atmospheric Solids Analysis Probe (ASAP). MALDI data were recorded on a Bruker Autoflex II ToF/FoF spectrometer. Microanalyses were performed by Elemental Analysis Service, London Metropolitan University, UK or Elemental Microanalysis service, Durham University, UK.

Analytical grades of solvents were used. 4-((triisopropylsily)ethynyl)pyridine,[14] 1-(tert-butyl)-4-((4-iodophenyl)ethynyl)benzene[15] and 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine [16], 4-(4-iodo-2,3,5,6-tetramethylphenyl)pyridine,[17] were synthesised according to literature methods. All other chemicals were sourced from standard suppliers.

1-bromo-4-iodo-2,3,5,6-tetramethylbenzene. Bromodurene (5 g, 23.6 mmol), iodine (3.594 g, 14.16 mmol) and periodic acid (1.614 g, 7.08 mmol) were dissolved with the solution of concentrated sulphuric acid (2.5 mL), water (12.5 mL) and glacial acetic acid (75 mL) in a two-necks round-bottomed flask. The solution was heated at 40 ^{o}C for 12 hours with continuous stirring. Water (50 mL) was added and the mixture was extracted into dichloromethane (50 mL). The organic layer was washed with water (50 mL) to remove

inorganics. The solution was dried over magnesium sulphate, filtered and evaporated to dryness. Recrystallization of the crude material in acetone afforded the product as white crystals. Yield: 3.7 g (46 %). **^{1}H NMR** (700 MHz; $CDCl_3$): δ_H 2.58 (s, 6H, H_b), 2.51 (s, 6H, H_a). **^{13}C{^{1}H} NMR** (176 MHz; $CDCl_3$): δ_C 138.5, 134.2, 129.6, 110.3, 28.8, 23.0 ppm. **ES-MS**: m/z 337.917 $[M]^+$. **Anal. Calc.** for $C_{10}H_{12}BrI$: C, 35.43; H, 3.57 %. **Found:** C, 35.39; H, 3.43 %.

4-(2,3,5,6-tetramethylphenyl)pyridine. DMF (dry, 150mL) was added to 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (5.0 g, 24.3 mmol), 3-bromo-1,2,4,5-tetramethylbenzene (5.32 g, 25 mmol) and K_2CO_3 (6.9 g, 50 mmol). The solution was degassed by three freeze-pump-thaw cycles before $Pd(PPh_3)_4$ (1.39 g, 1.2 mmol) was added. The solution was heated to 110 °C for 16 hours. Once cooled, the solution was poured into water and extracted with dichloromethane (DCM). The organic layer was collected and dried over magnesium sulfate before the solvent was removed. The product was purified via column chromatography on silica gel eluted with a solvent gradient from neat DCM to neat diethylether (Et_2O), to give a colourless oil that solidified upon standing. Yield: 3.07 g (60 %). **^{1}H NMR** (700 MHz; $CDCl_3$): δ_H 8.66 (d, J^3_{HH} = 6.0 Hz, 2H, H_a), 7.09 (d, J^3_{HH} = 6.0 Hz, 2H, H_b), 7.03 (s, 1H, H_c), 2.27 (s, 6H, H_d), 1.87 (s, 6H, H_e) ppm. **^{13}C{^{1}H} NMR** (176 MHz; $CDCl_3$): δ_C 150.9, 149.7, 139.2, 133.8, 131.1, 130.9, 124.8, 20.0, 17.06 ppm. **ES-MS**: m/z 212.143 $[M+H]^+$. **Anal. Calc.** for $C_{15}H_{17}N$: C, 85.26; H, 8.11; N, 6.63 %. **Found**: C, 85.19; H, 8.23; 6.69 %.

4-(4-bromo-2-methylphenyl)pyridine. DMF (dry, 150mL) was added to 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (5.0 g, 24.3 mmol), 4-bromo-1-iodo-2-

methylbenzene (10.7 mL, 22.12 g, 75 mmol) and K_2CO_3 (6.9 g, 50 mmol). The solution was degassed by three freeze-pump-thaw cycles before $Pd(PPh_3)_4$ (1.39 g, 1.2 mmol) was added. The solution was heated to 110 °C for 16 hours. Once cooled, the solution was poured into water and extracted with dichloromethane (DCM). The organic layer was collected and dried over magnesium sulfate before the solvent was removed. The product was purified via column chromatography on silica gel eluted with a solvent gradient from neat DCM to neat Et_2O, to give a colourless oil. Yield: 3.19 g (53 %). **^{1}H NMR** (700 MHz; $CDCl_3$): δ_H 8.62 (d, J^3_{HH} = 6.0 Hz, 2H, H_a), 7.42 (s, J^4_{HH} = 2.1 Hz, 1H, H_e), 7.36 (dd, J^3_{HH} =7.6 Hz, J^4_{HH} =2.1 Hz, 1H, H_d), 7.18 (d, J^3_{HH} = 6.0 Hz, 2H, H_b), 7.03 (d, J^3_{HH} = 7.6 Hz, 1H, H_c), 2.22 (s, 3H, H_f) ppm. **^{13}C{^{1}H} NMR** (176 MHz; $CDCl_3$): δ_C 149.7, 148.5, 137.9, 137.2, 133.3, 130.7, 129.1, 123.9, 122.3, 20.0 ppm. **ES-MS**: m/z 248.570 $[M+H]^+$. **Anal. Calc.** for $C_{12}H_{10}NBr$: C, 58.09; H, 4.06; N, 5.65 %. **Found**: C, 57.94; H, 4.14; N, 5.59 %.

4-(4-bromo-2,3,5,6-tetramethylphenyl)pyridine. The same procedure as for 4-(4-bromo-2-methylphenyl)pyridine, except 1-bromo-4-iodo-2,3,5,6-tetramethylbenzene was used in place of 4-bromo-1-iodo-2-methylbenzene. Yield: 3.51 g (50 %). **^{1}H NMR** (700 MHz; $CDCl_3$): δ_H 8.66 (d, J^3_{HH} = 6.0 Hz, 2H, H_a), 7.04 (d, J^3_{HH} = 6.0 Hz, 2H, H_b), 2.44 (s, 6H, H_c), 1.93 (s, 6H, H_d) ppm. **^{13}C{^{1}H} NMR** (176 MHz; $CDCl_3$): δ_C 150.4, 150.0, 138.4, 134.2, 132.3, 129.0, 124.5, 116.5, 21.1, 18.9 ppm. **ES-MS**: m/z 290.053 $[M+H]^+$. **Anal. Calc.** for $C_{15}H_{16}BrN$: C, 62.08; H, 5.56; N, 4.83 %. **Found**: C, 62.04; H, 5.48; N, 5.02 %.

S2. NMR spectra of reported compounds

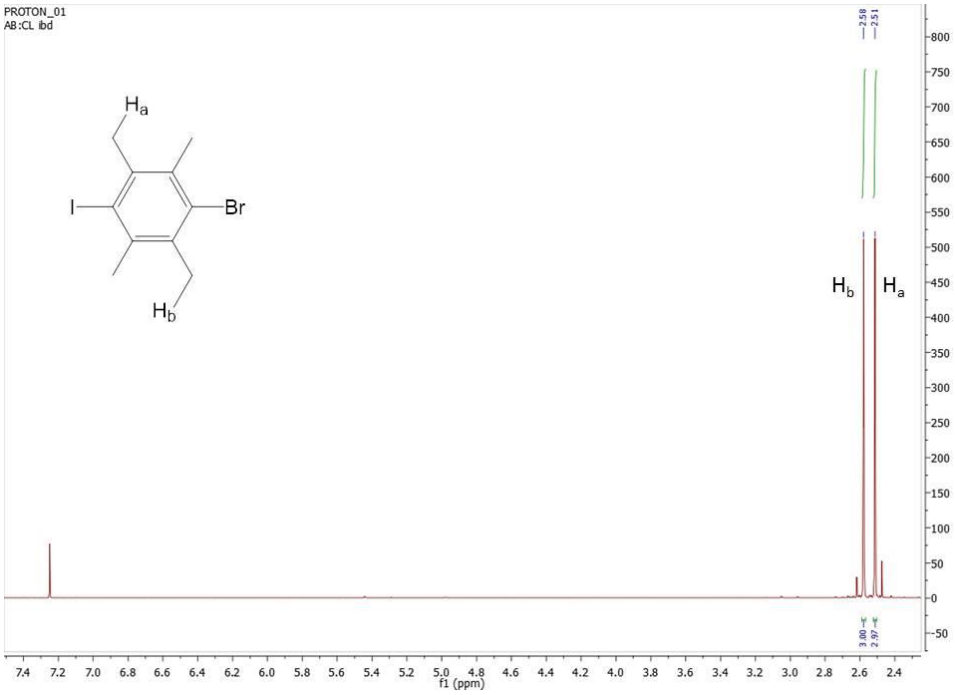

Figure S1. ^{1}H NMR spectrum of 1-bromo-4-iodo-2,3,5,6-tetramethylbenzene recorded in $CDCl_3$.

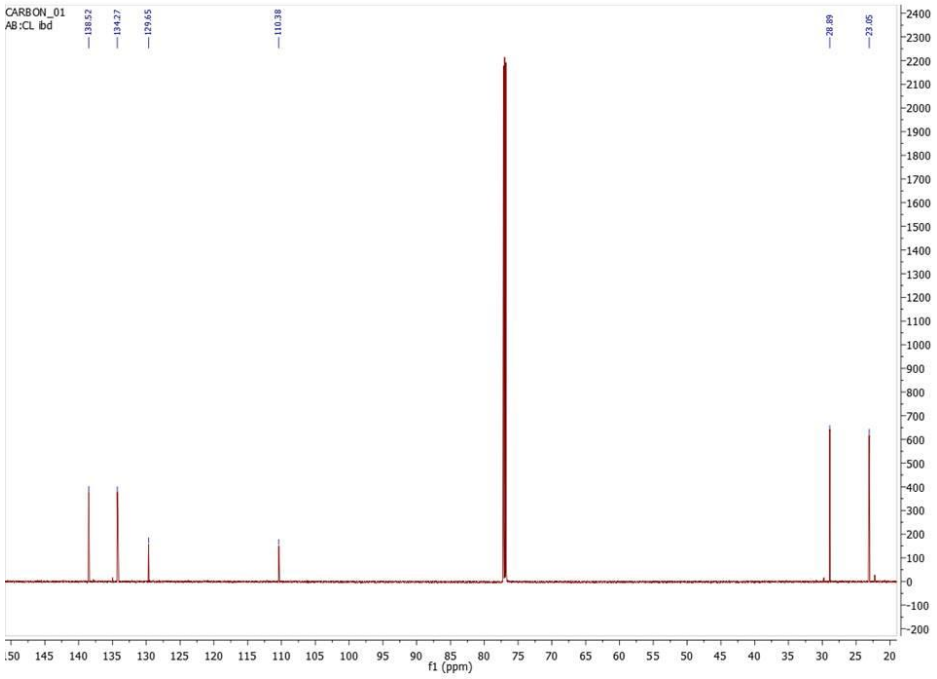

Figure S2. ^{13}C NMR spectrum of 1-bromo-4-iodo-2,3,5,6-tetramethylbenzene recorded in $CDCl_3$.

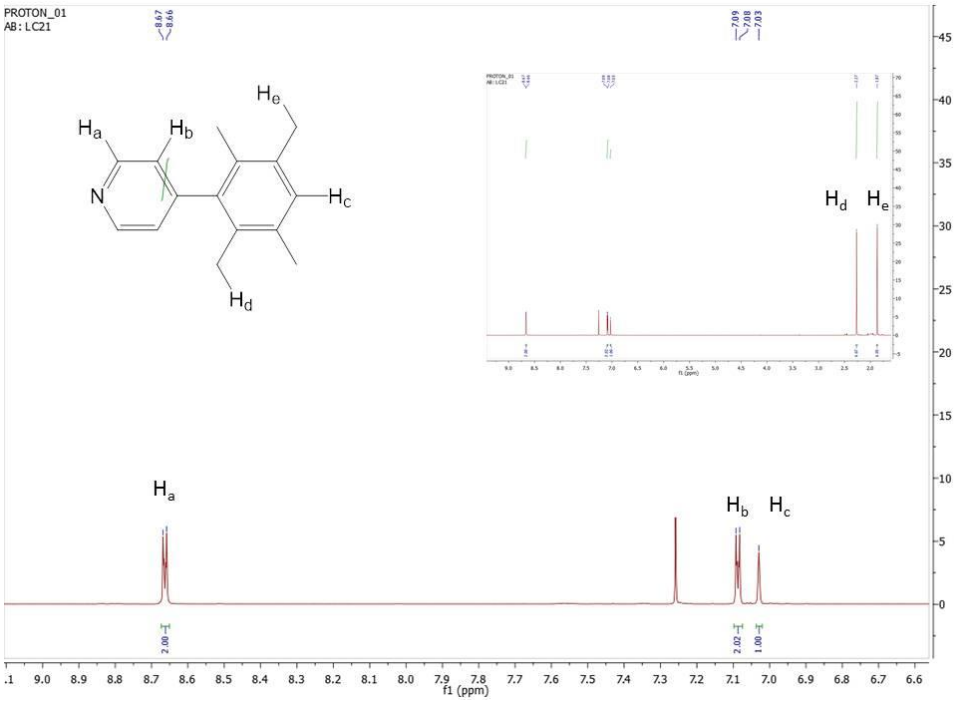

Figure S3. ^{1}H NMR spectrum of 4-(2,3,5,6-tetramethylphenyl)pyridine recorded in $CDCl_3$.

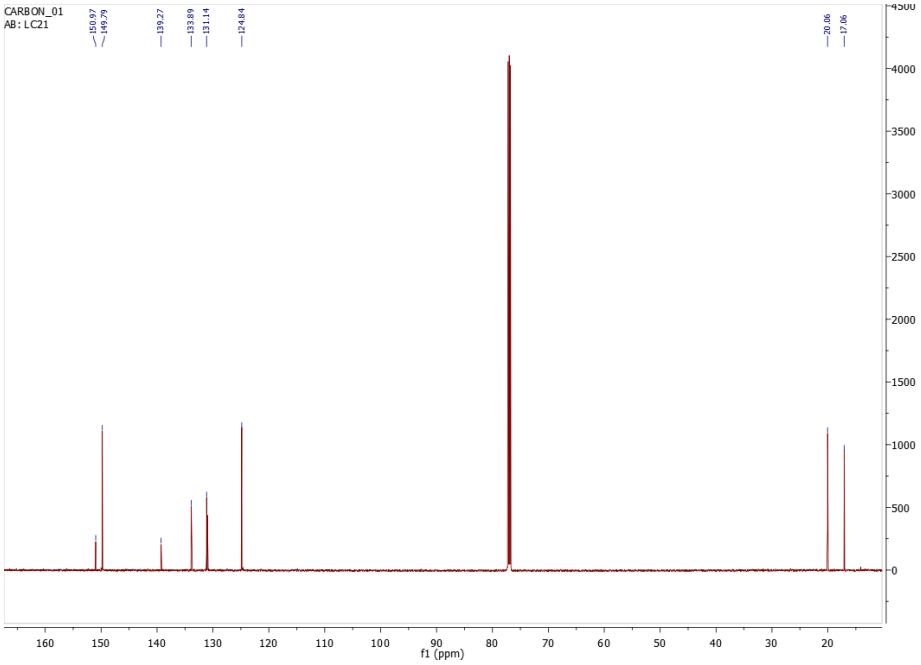

Figure S4. ^{13}C NMR spectrum of 4-(2,3,5,6-tetramethylphenyl)pyridine recorded in $CDCl_3$.

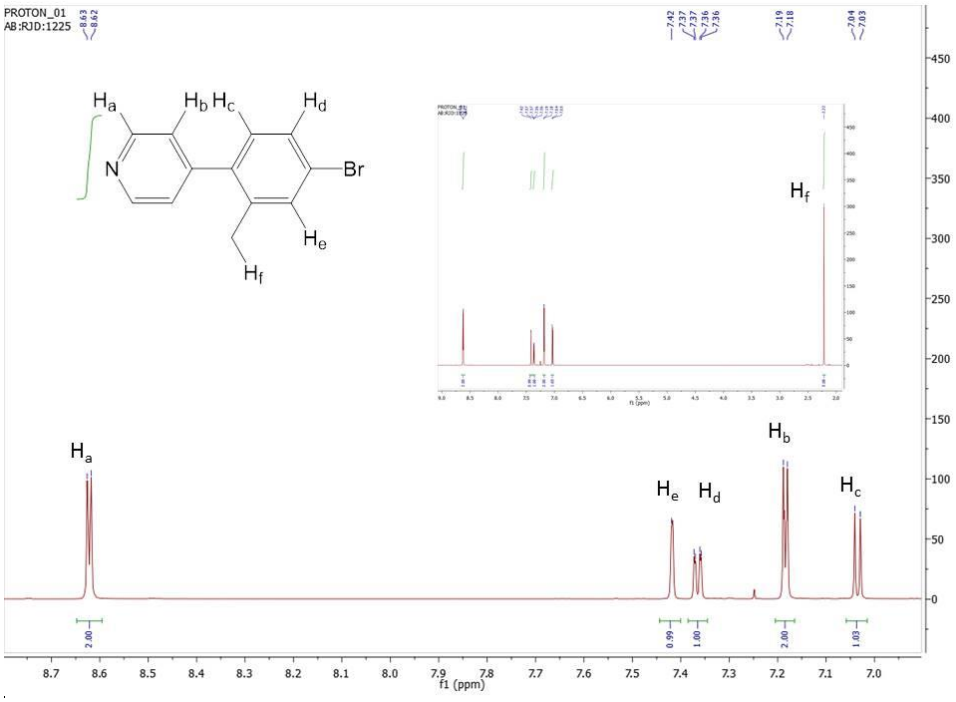

Figure S5. ^{1}H NMR spectrum of 4-(4-bromo-2-methylphenyl)pyridine recorded in $CDCl_3$.

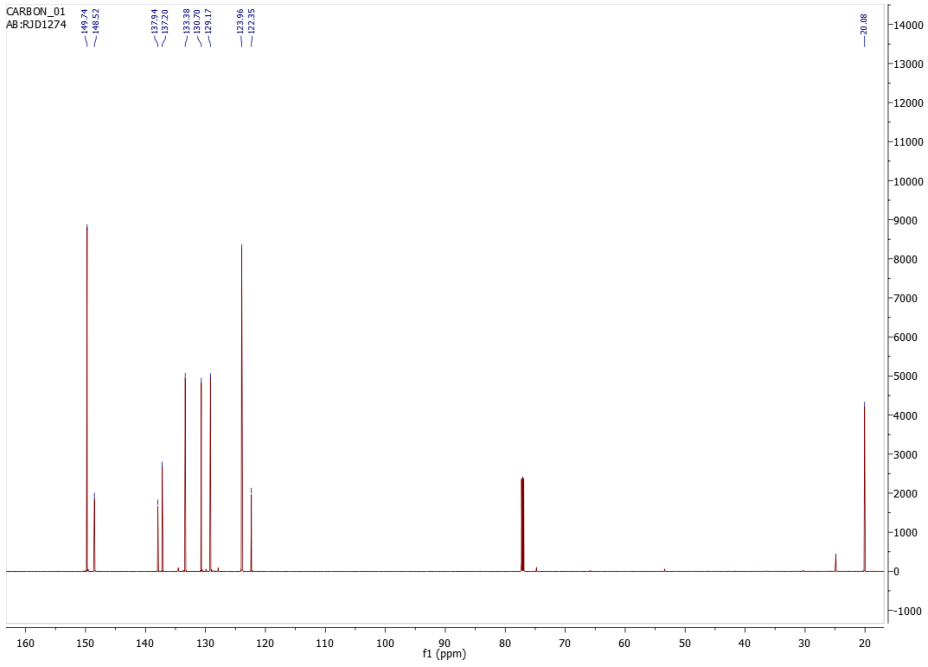

Figure S6. ^{13}C NMR spectrum of 4-(4-bromo-2-methylphenyl)pyridine recorded in $CDCl_3$.

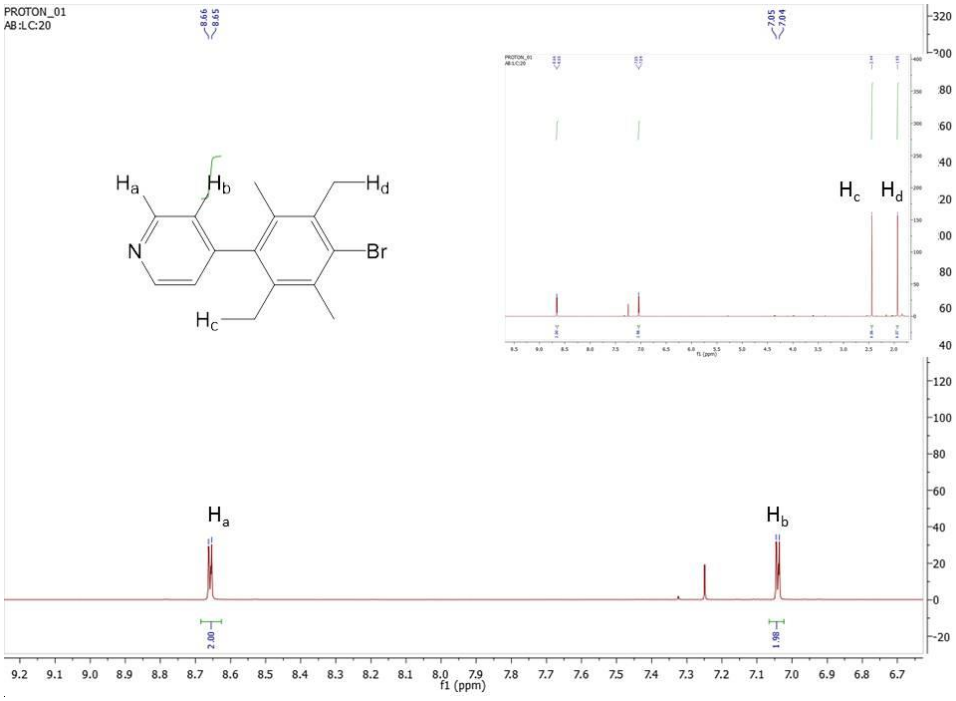

Figure S7. ^{1}H NMR spectrum of 4-(4-bromo-2,3,5,6-tetramethylphenyl)pyridine recorded in $CDCl_3$.

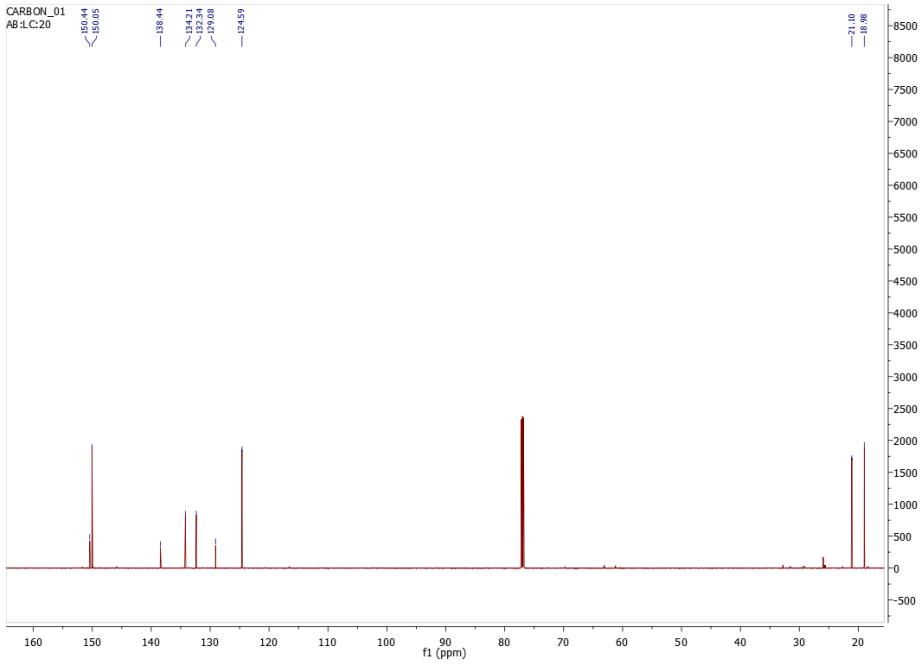

Figure S8. ^{13}C NMR spectrum of 4-(4-bromo-2,3,5,6-tetramethylphenyl)pyridine recorded in $CDCl_3$.

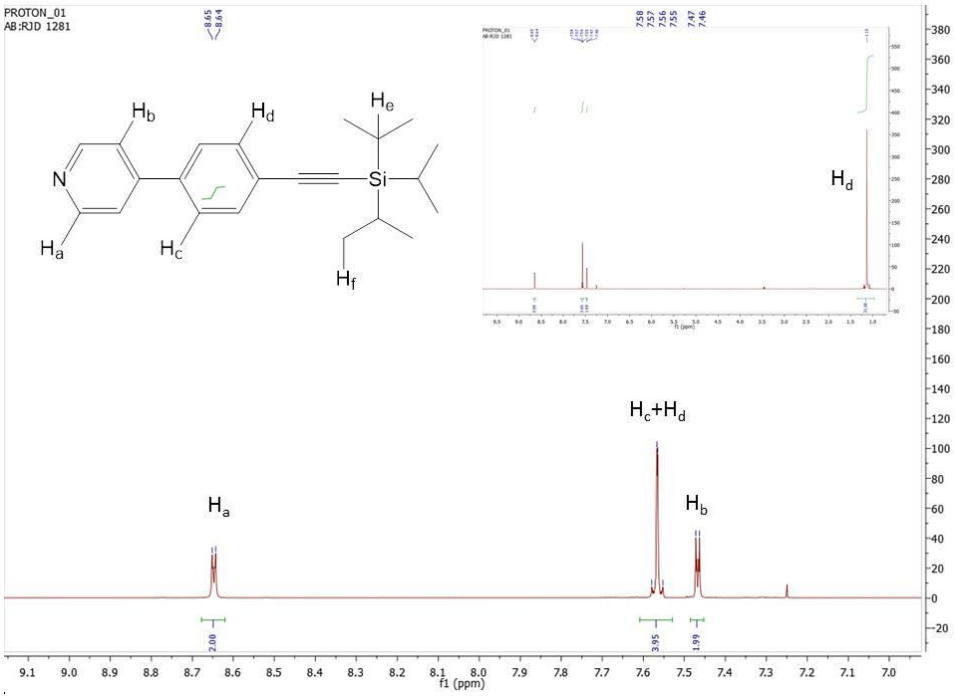

Figure S9. ^{1}H NMR spectrum of 4-(4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

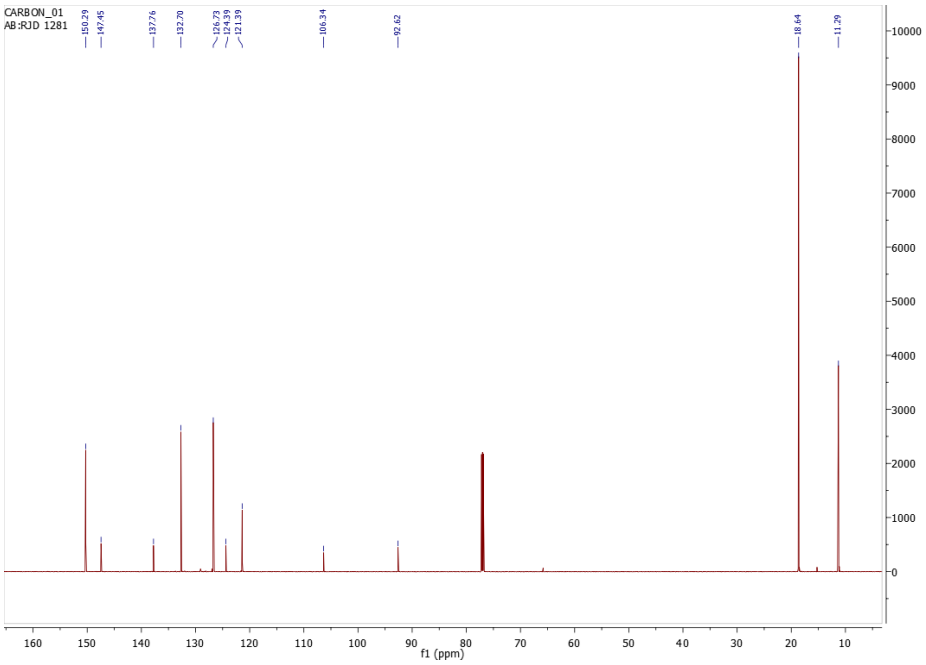

Figure S10. ^{13}C NMR spectrum of 4-(4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

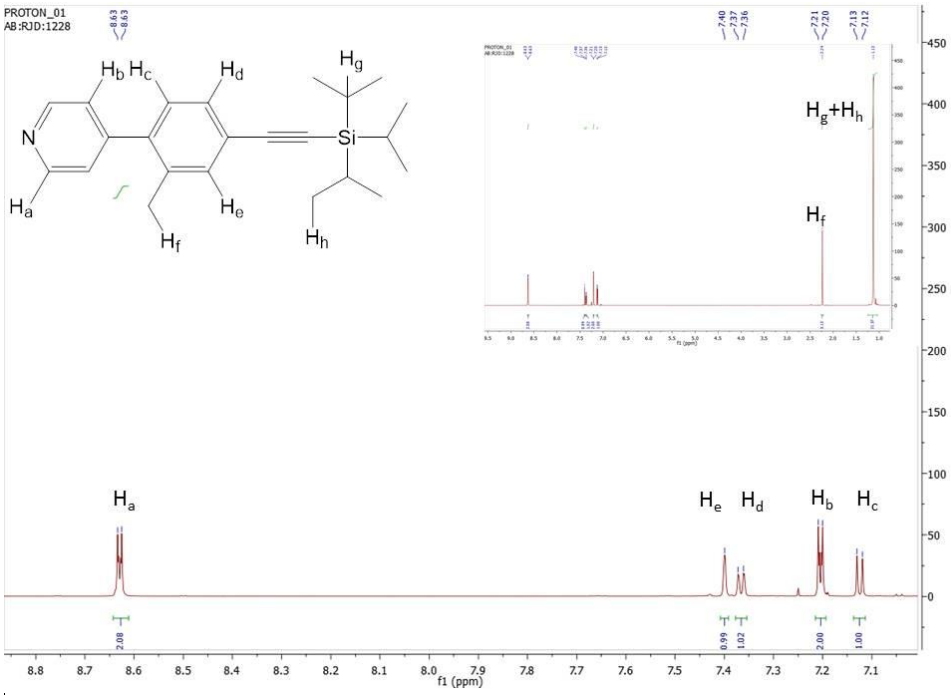

Figure S11. ^{1}H NMR spectrum of 4-(2-methyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

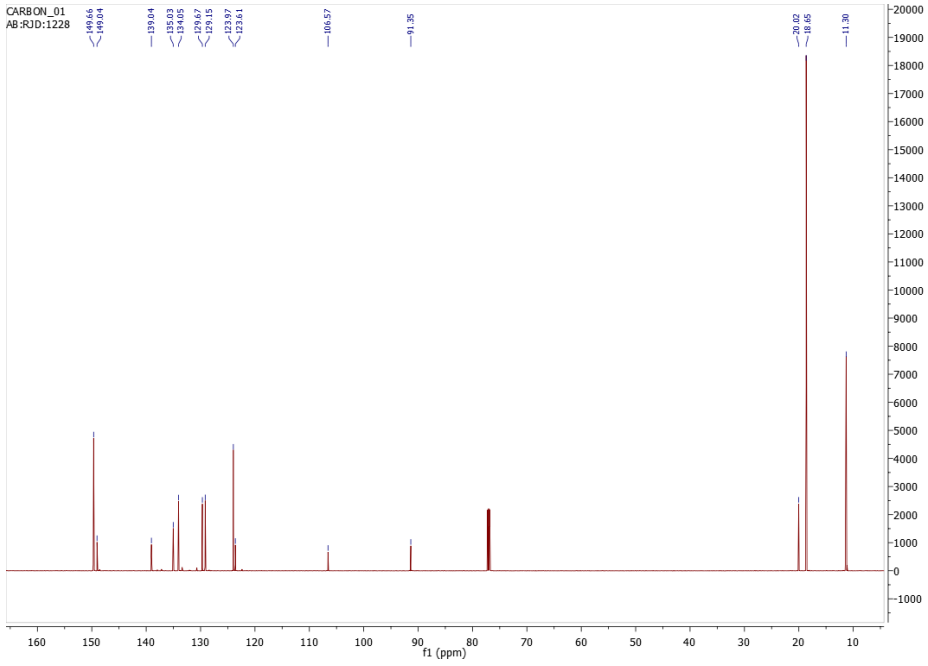

Figure S12. ^{13}C NMR spectrum of 4-(2-methyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

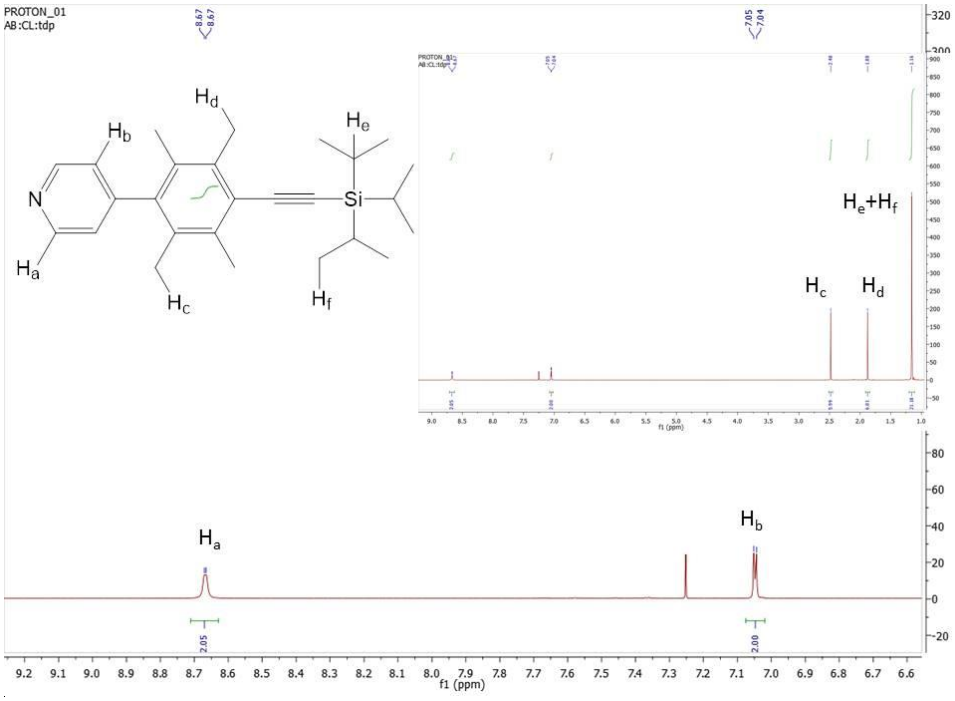

Figure S13. ^{1}H NMR spectrum of 4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

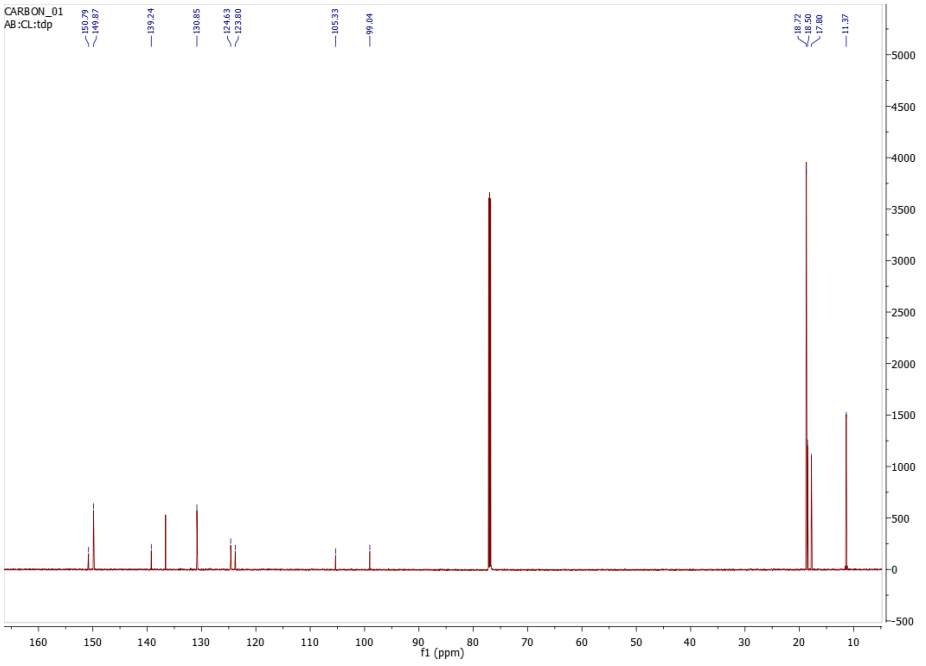

Figure S14. ^{13}C NMR spectrum of 4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine recorded in $CDCl_3$.

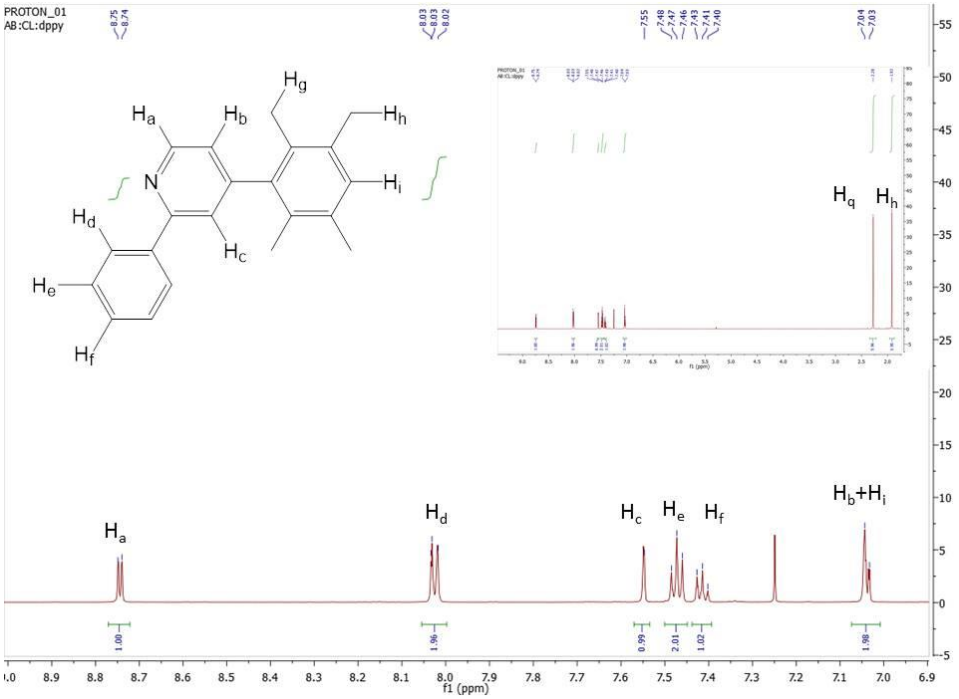

Figure S15. ^{1}H NMR spectrum of **L^{1}H** recorded in $CDCl_3$.

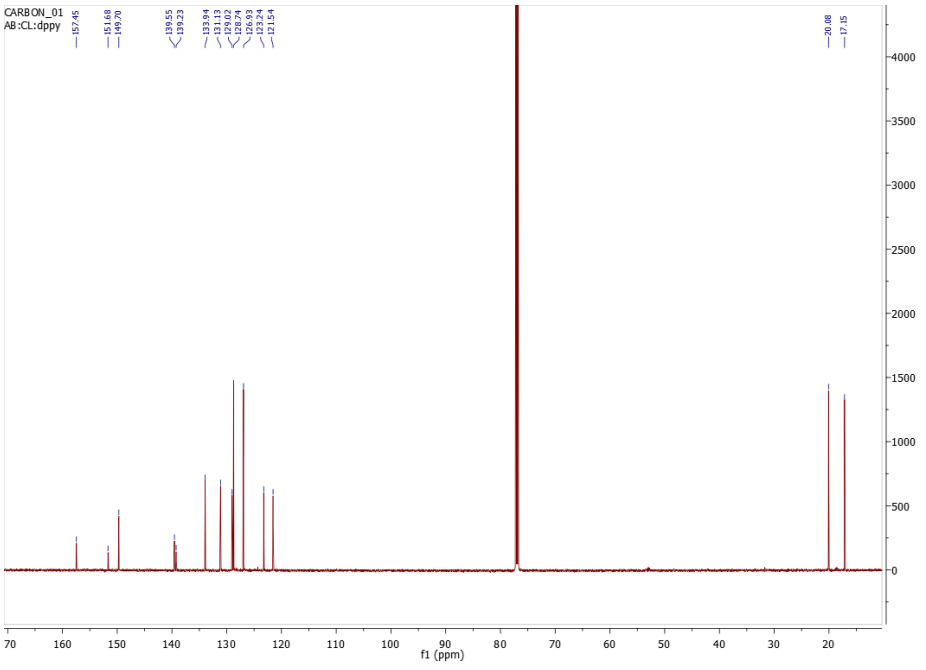

Figure S16. ^{13}C NMR spectrum of **L^{1}H** recorded in $CDCl_3$.

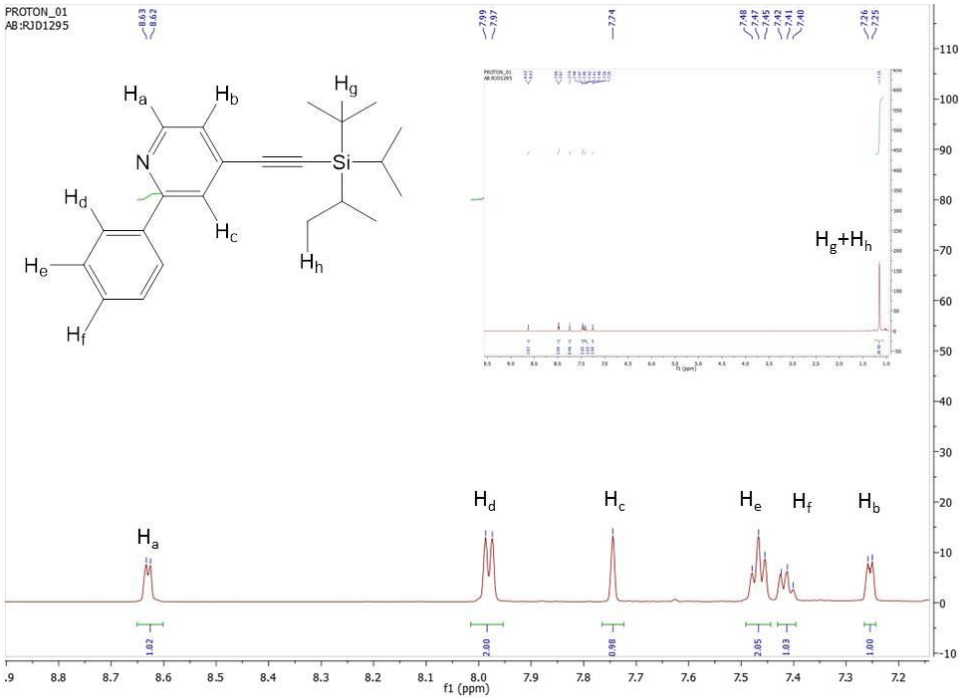

Figure S17. ^{1}H NMR spectrum of **L^{2}H** recorded in $CDCl_3$.

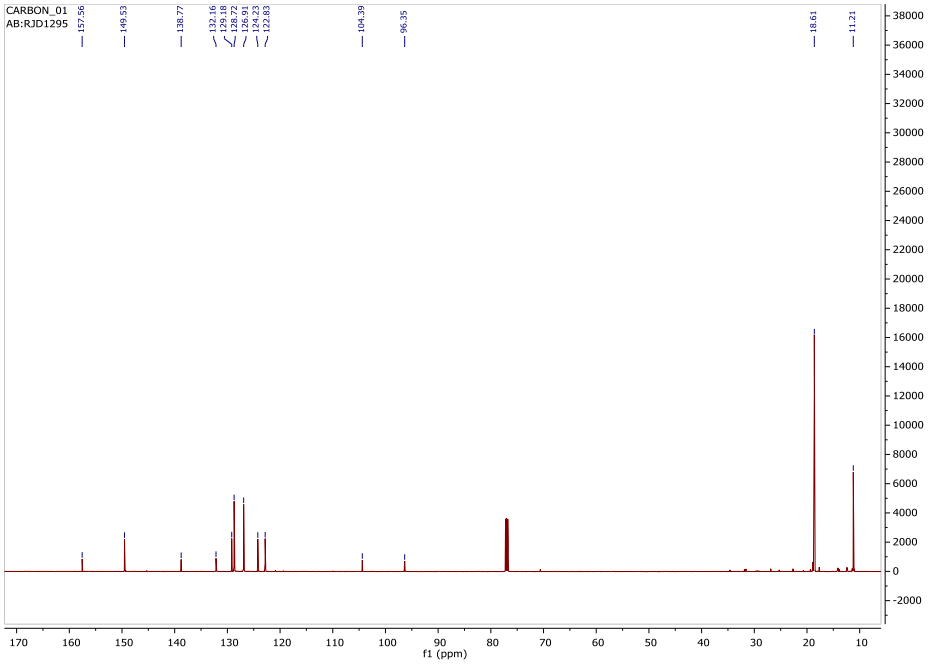

Figure S18. ^{13}C NMR spectrum of **L^{2}H** recorded in $CDCl_3$.

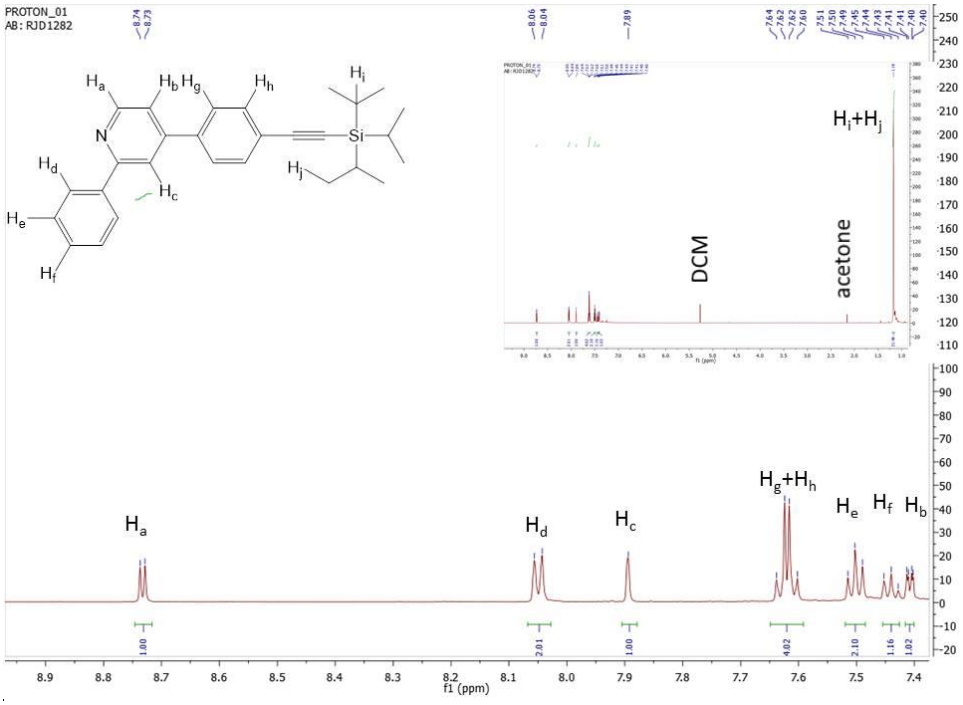

Figure S19. ^{1}H NMR spectrum of **L^{3}H** recorded in $CDCl_3$.

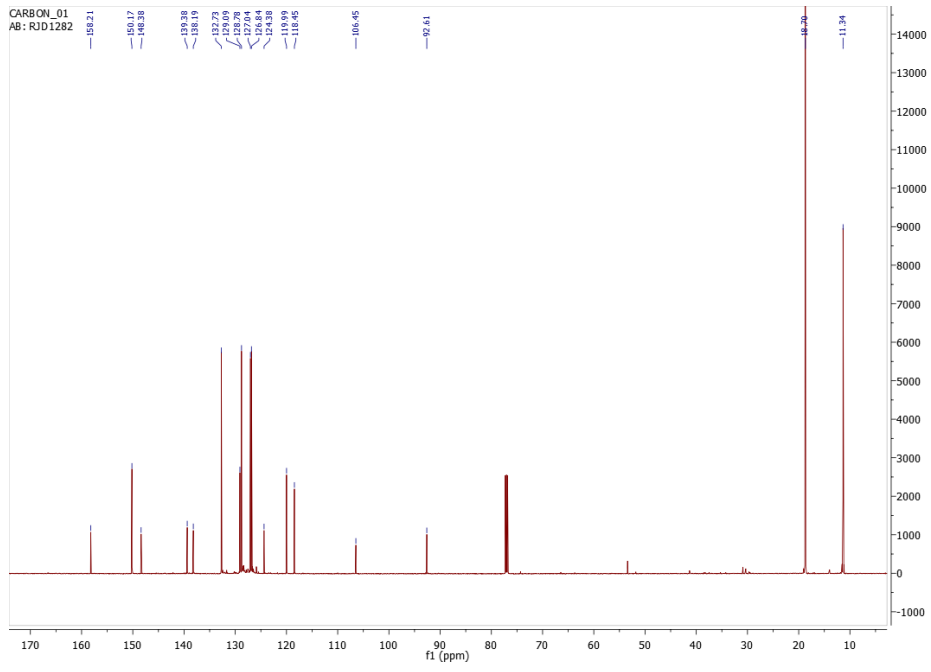

Figure S20. ^{13}C NMR spectrum of **L^{3}H** recorded in $CDCl_3$.

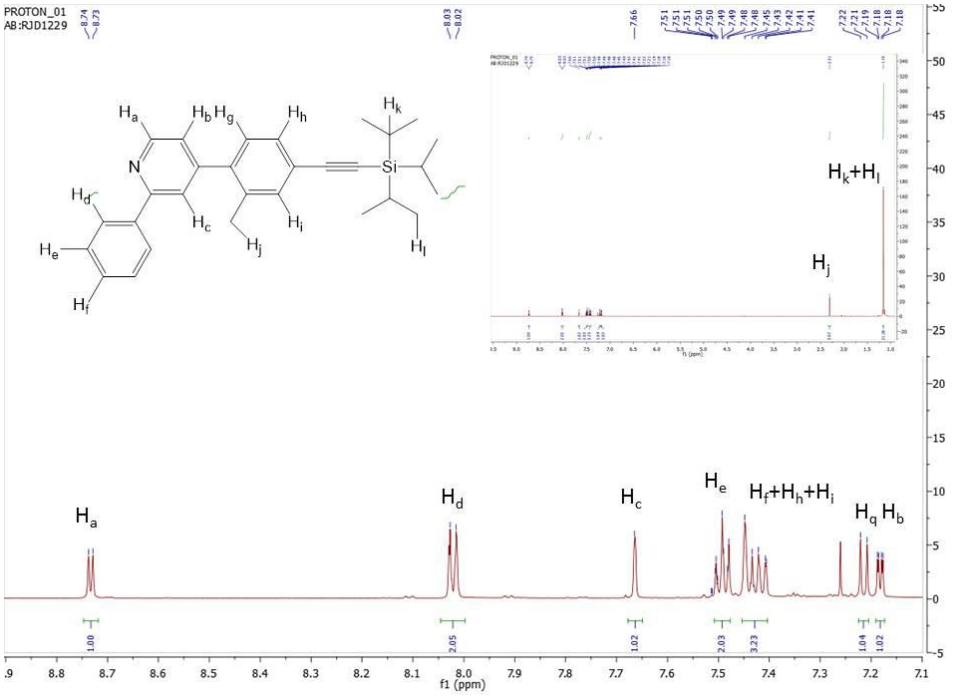

Figure S21. ^{1}H NMR spectrum of **L^{4}H** recorded in $CDCl_3$.

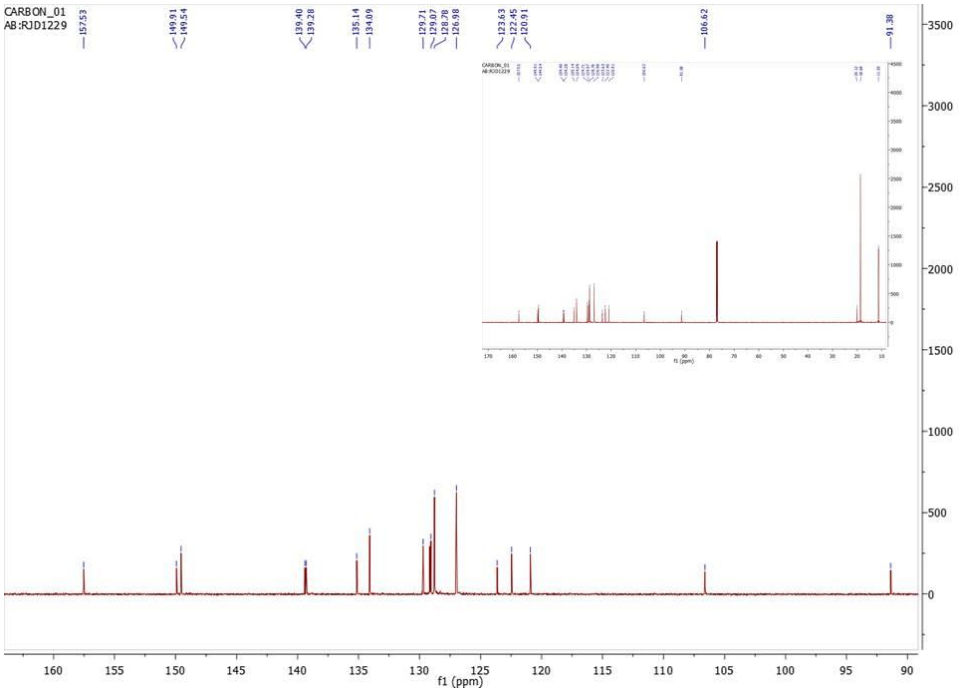

Figure S22. ^{13}C NMR spectrum of **L^{4}H** recorded in $CDCl_3$.

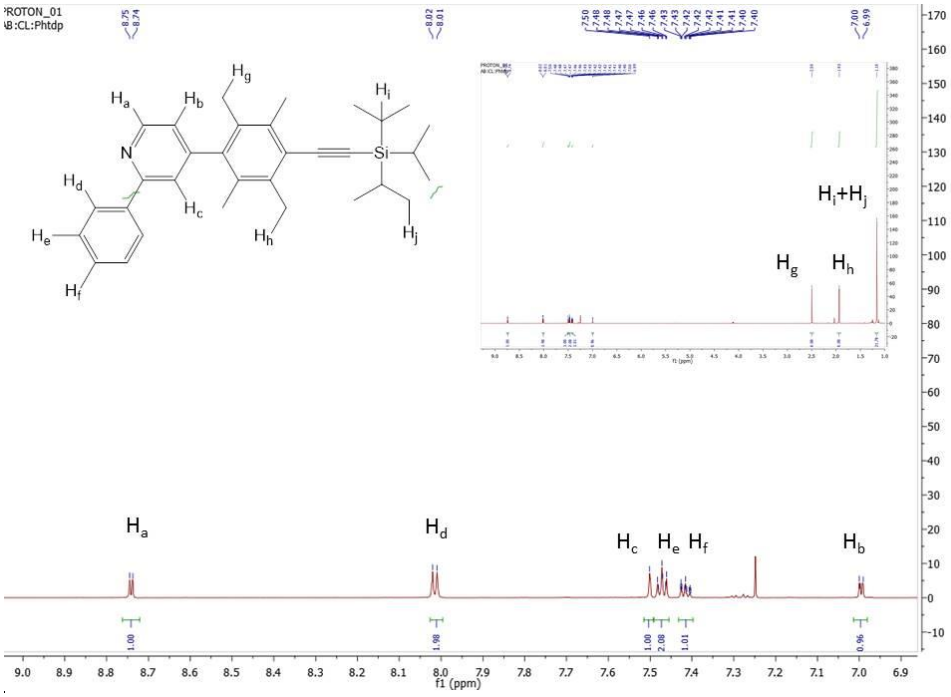

Figure S23. ^{1}H NMR spectrum of **L^{5}H** recorded in $CDCl_3$.

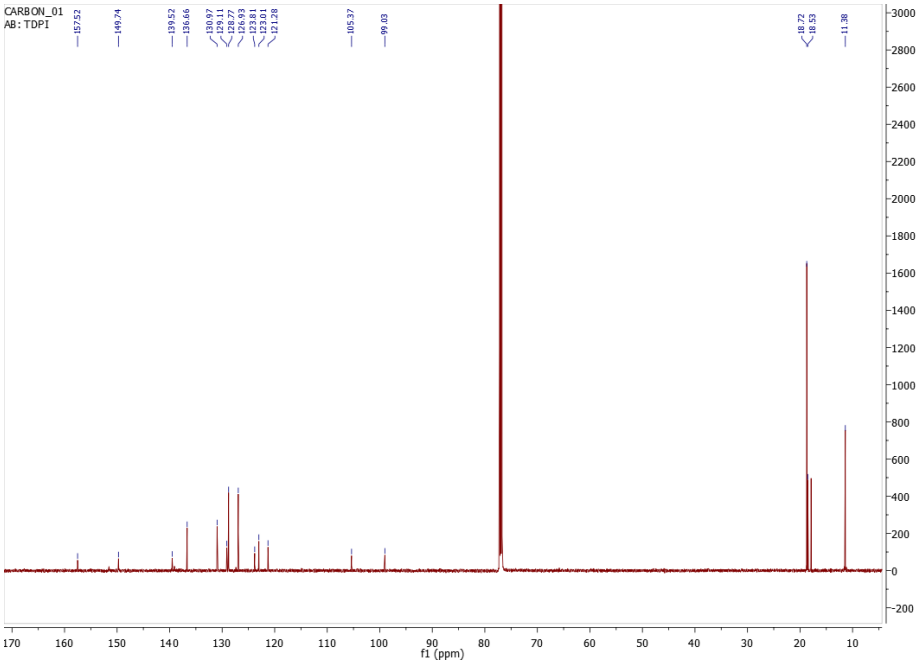

Figure S24. ^{13}C NMR spectrum of **L^{5}H** recorded in $CDCl_3$.

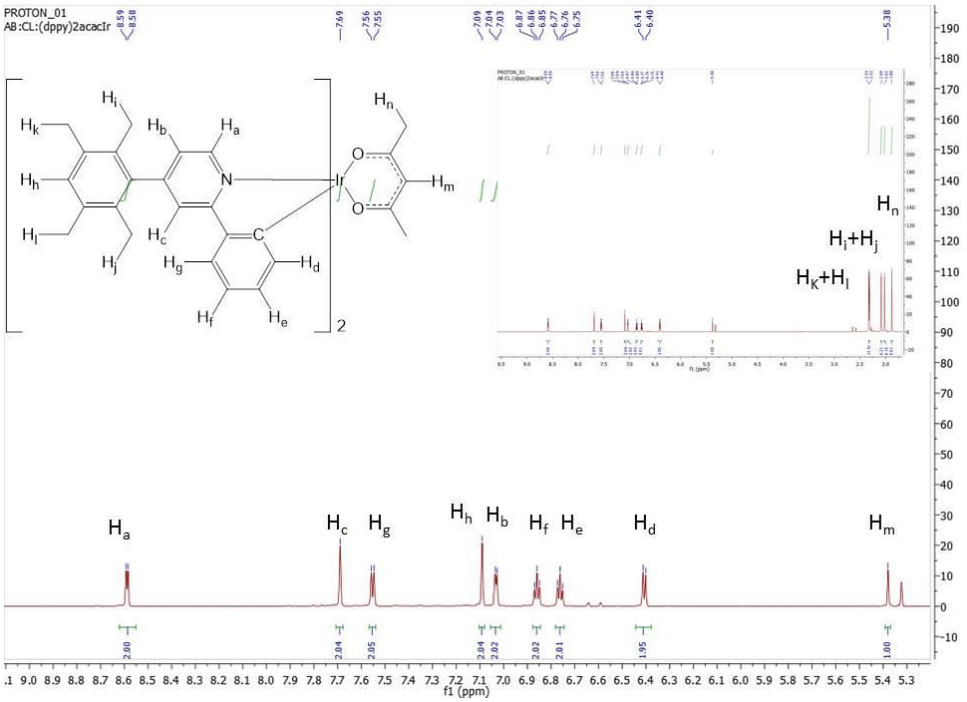

Figure S25. ^{1}H NMR spectrum of **1** recorded in CD_2Cl_2.

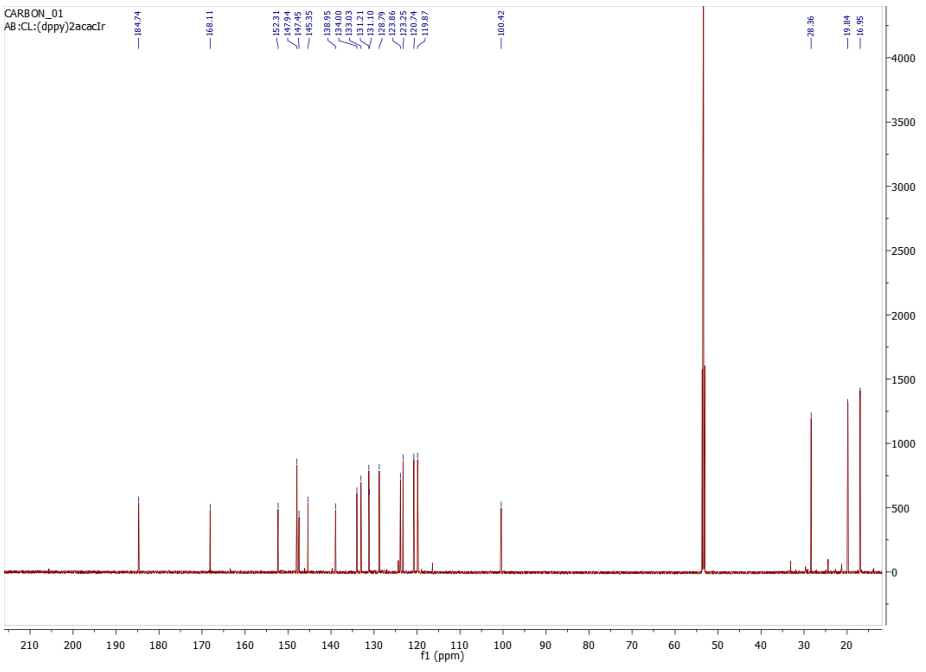

Figure S26. ^{13}C NMR spectrum of **1** recorded in CD_2Cl_2.

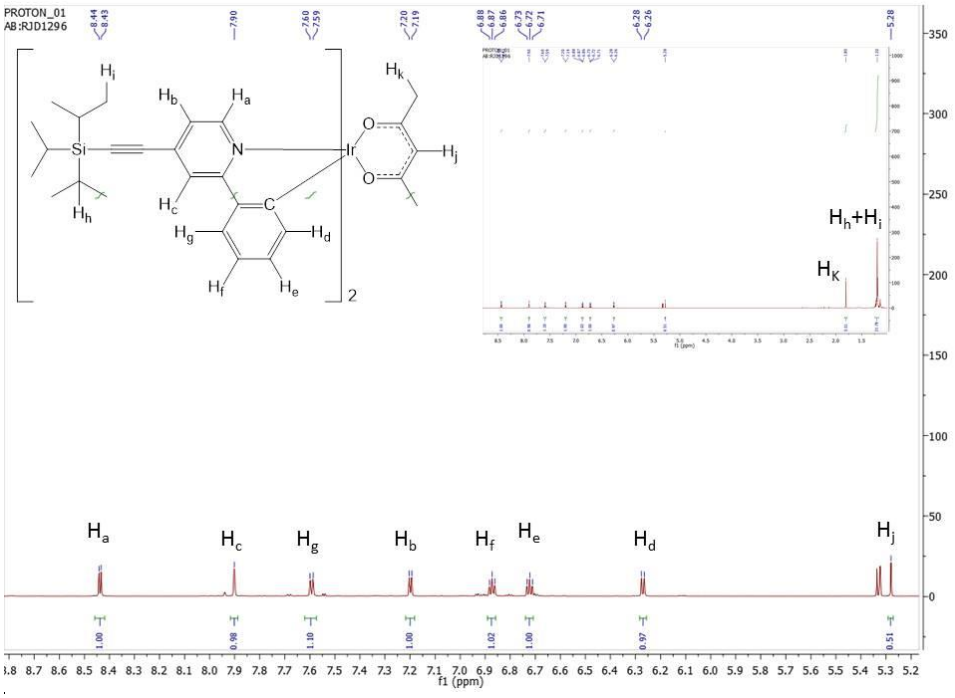

Figure S27. ^{1}H NMR spectrum of **2** recorded in CD_2Cl_2.

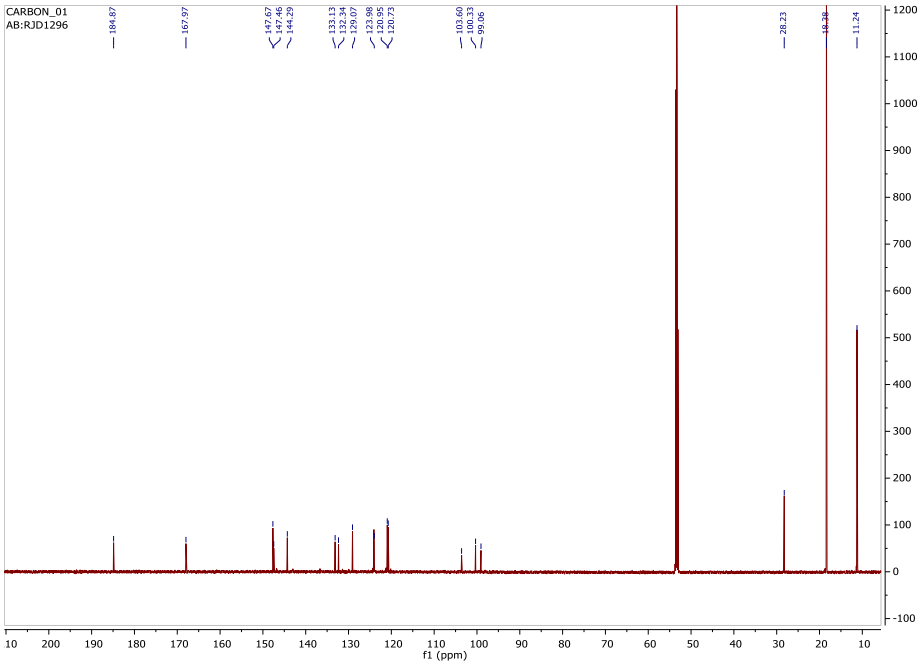

Figure S28. ^{13}C NMR spectrum of **2** recorded in CD_2Cl_2.

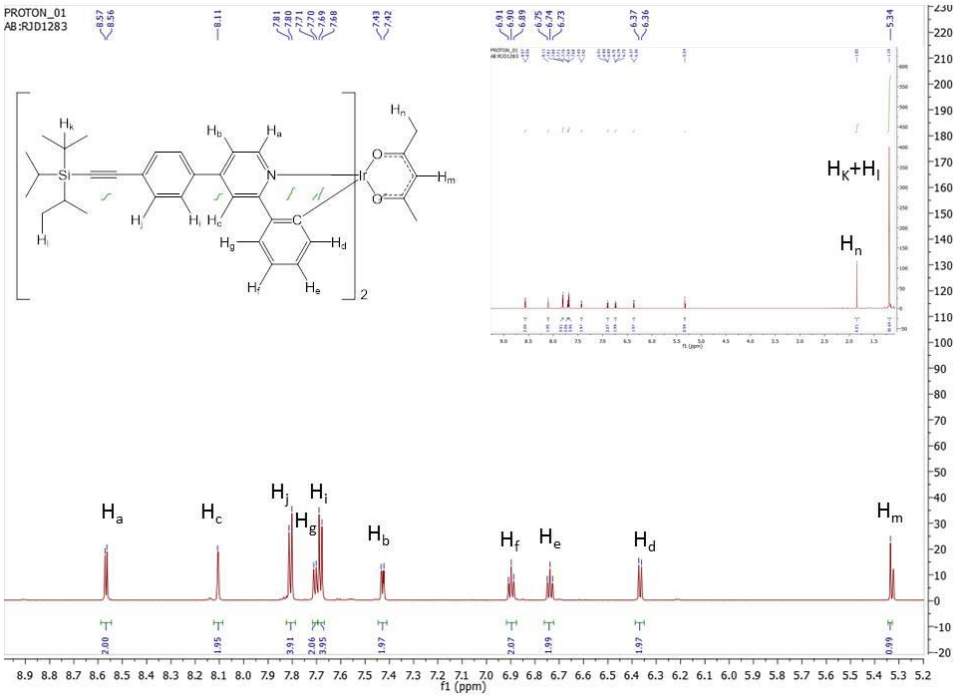

Figure S29. ^{1}H NMR spectrum of **3** recorded in CD_2Cl_2.

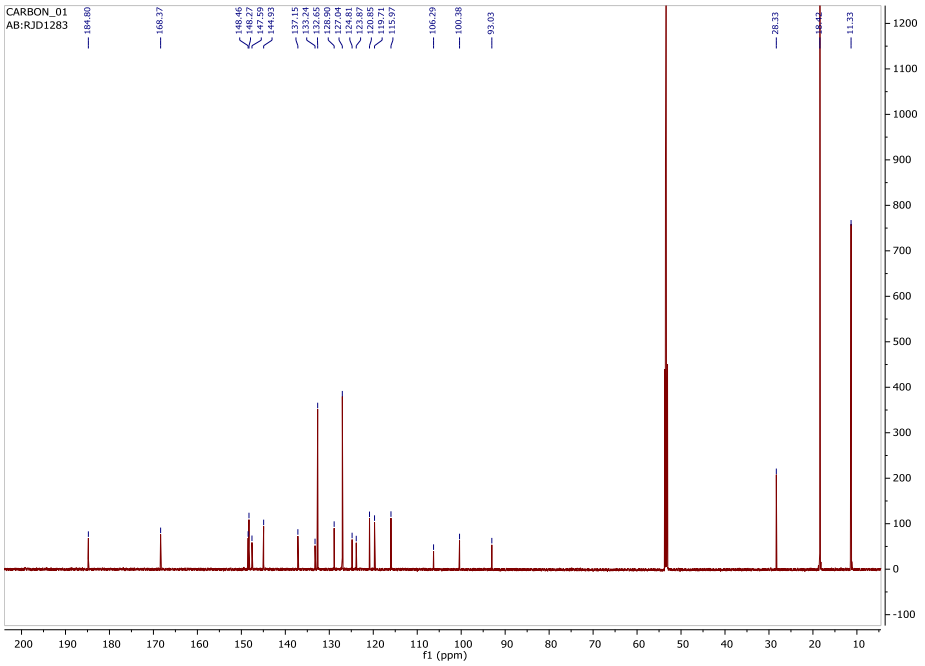

Figure S30. ^{13}C NMR spectrum of **3** recorded in CD_2Cl_2.

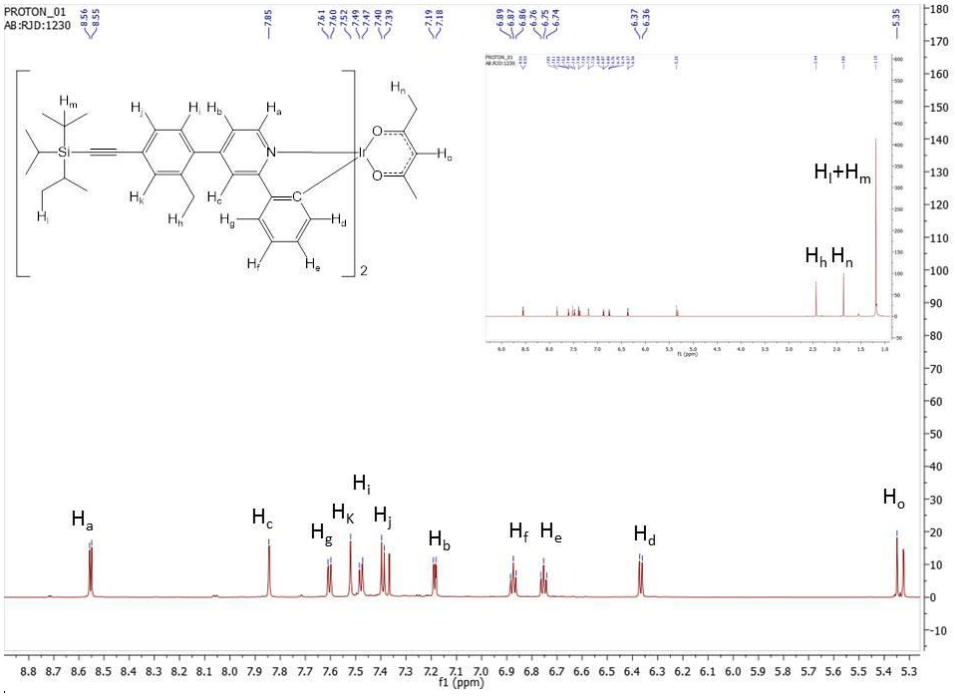

Figure S31. ^{1}H NMR spectrum of **4** recorded in CD_2Cl_2.

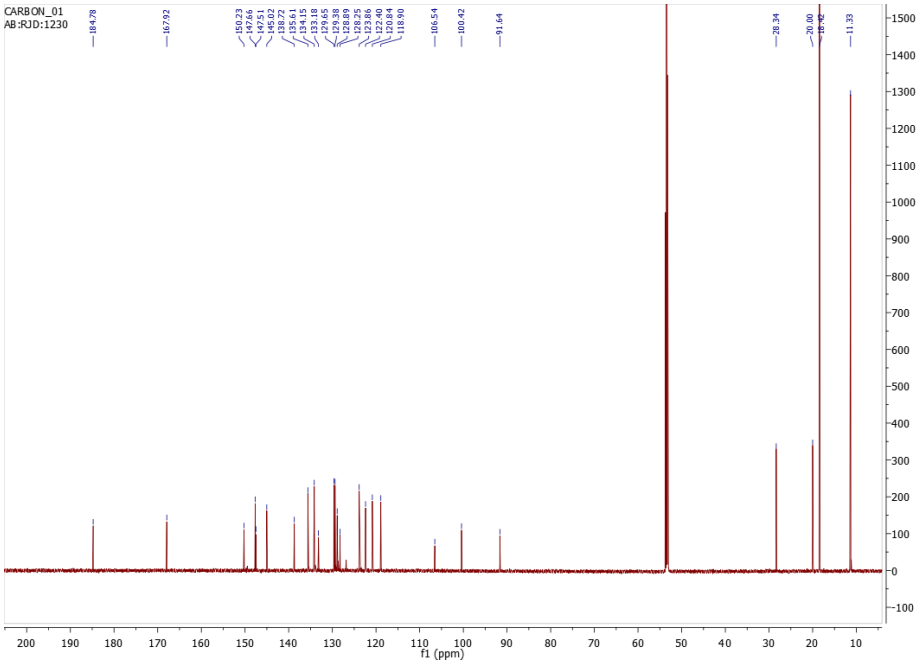

Figure S32. ^{13}C NMR spectrum of **4** recorded in CD_2Cl_2.

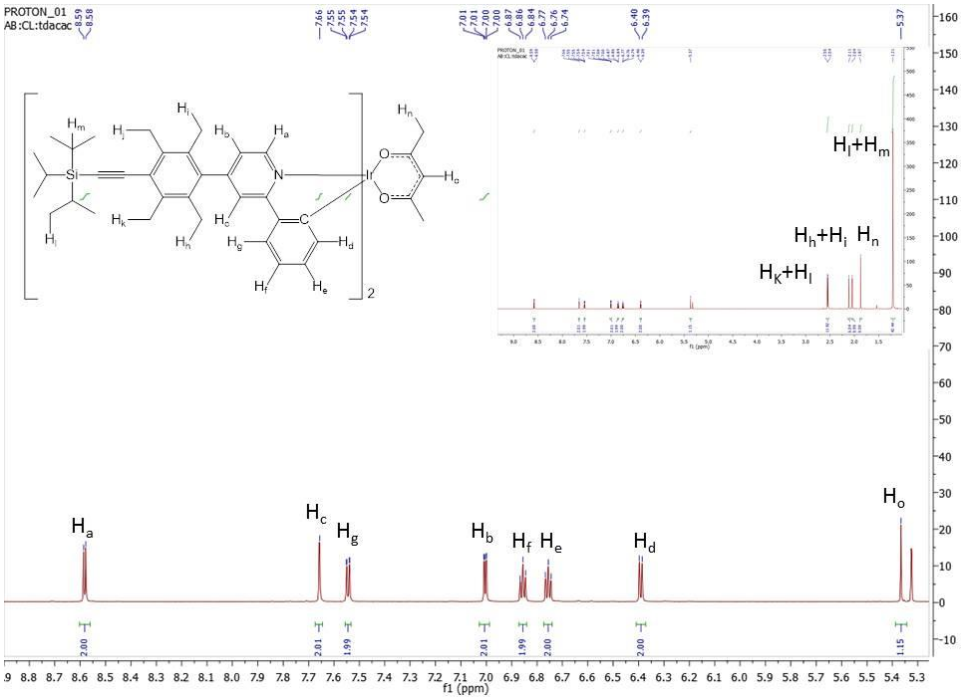

Figure S33. ^{1}H NMR spectrum of **5** recorded in CD_2Cl_2.

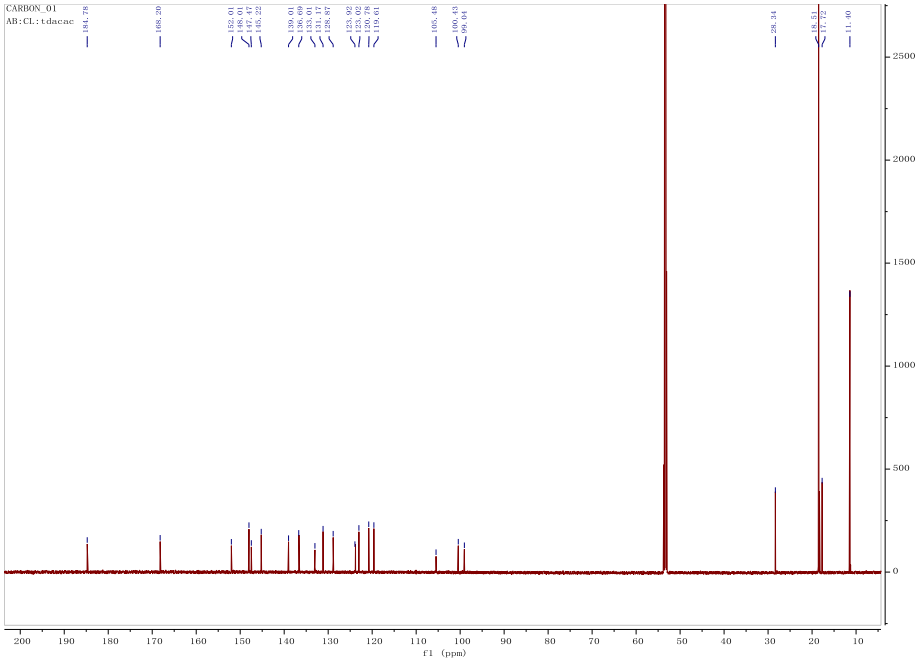

Figure S34. ^{13}C NMR spectrum of **5** recorded in CD_2Cl_2.

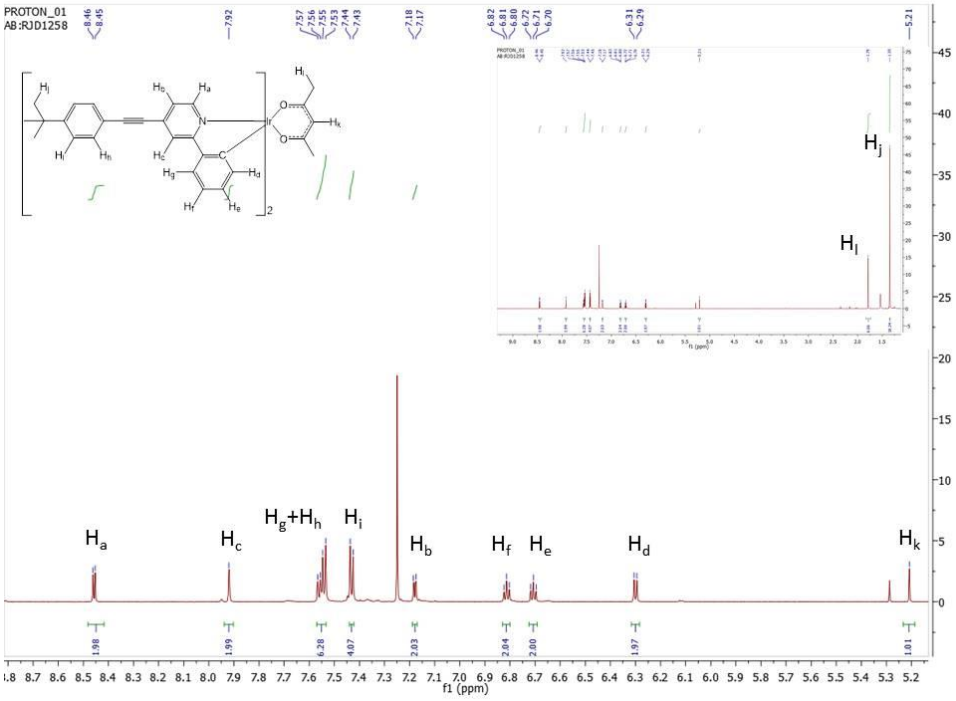

Figure S35. ^{1}H NMR spectrum of **6** recorded in $CDCl_3$.

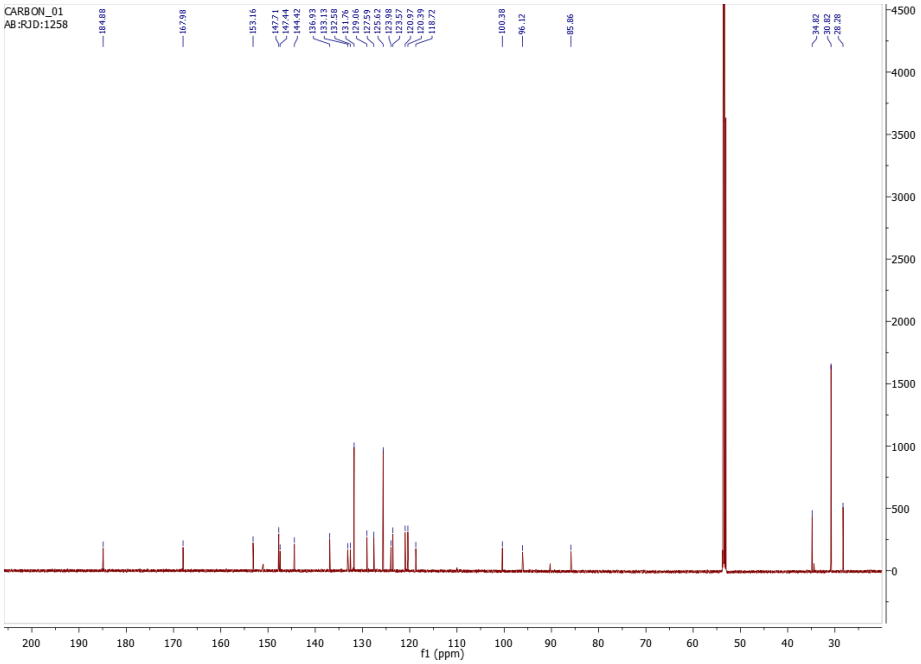

Figure S36. ^{13}C NMR spectrum of **6** recorded in CD_2Cl_2.

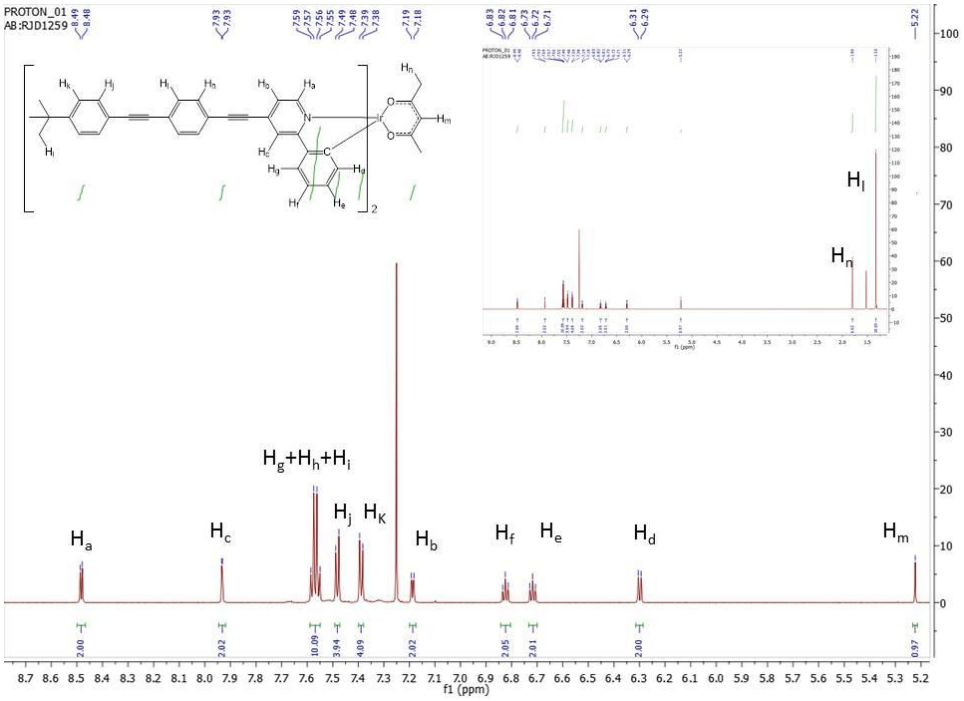

Figure S37. ^{1}H NMR spectrum of **7** recorded in $CDCl_3$.

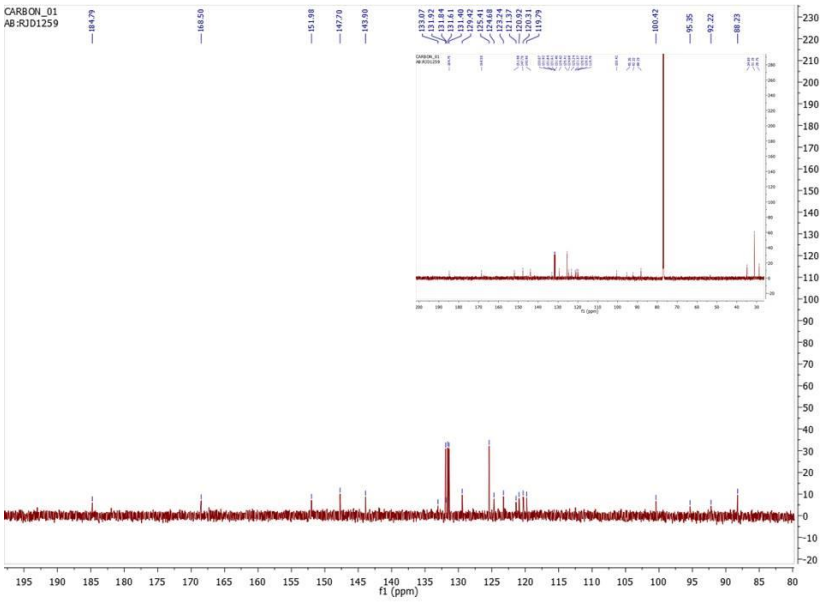

Figure S38. ^{13}C NMR spectrum of **7** recorded in $CDCl_3$.

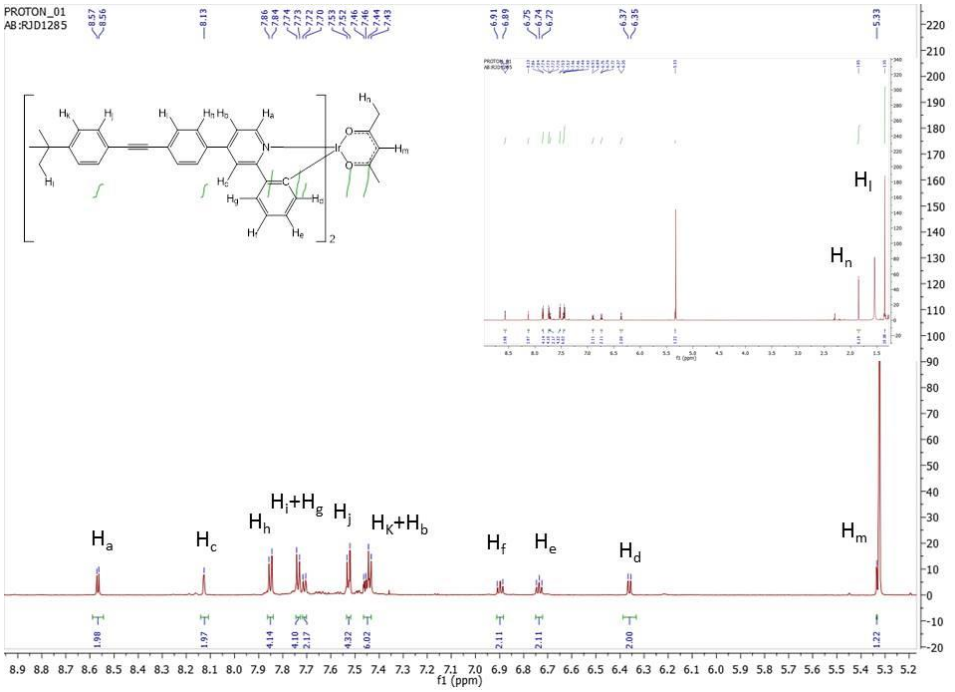

Figure S39. ^{1}H NMR spectrum of **8** recorded in CD_2Cl_2.

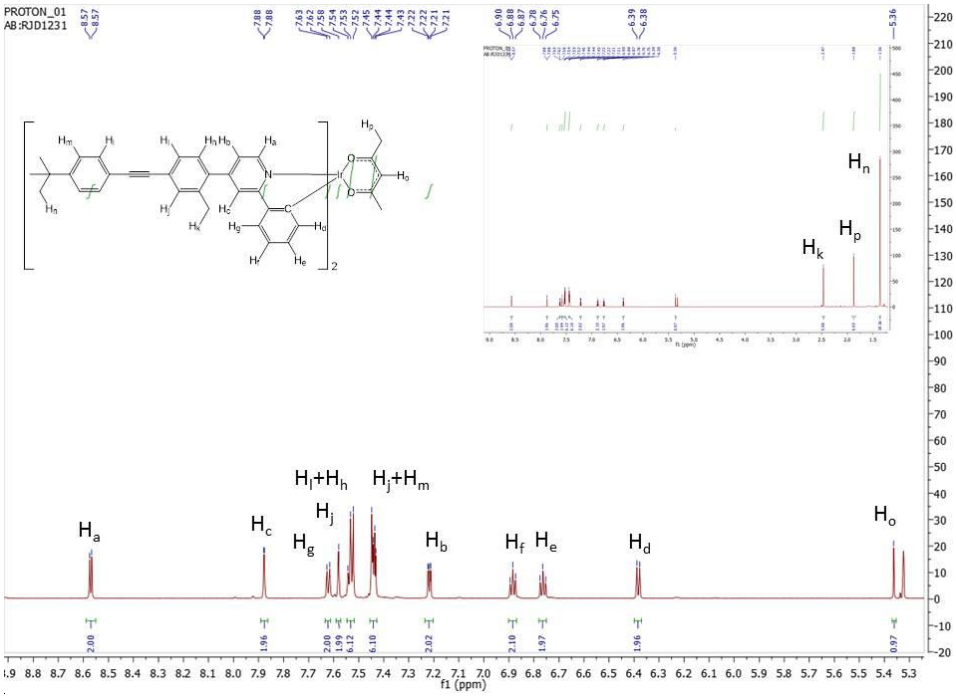

Figure S40. ^{1}H NMR spectrum of **10** recorded in CD_2Cl_2.

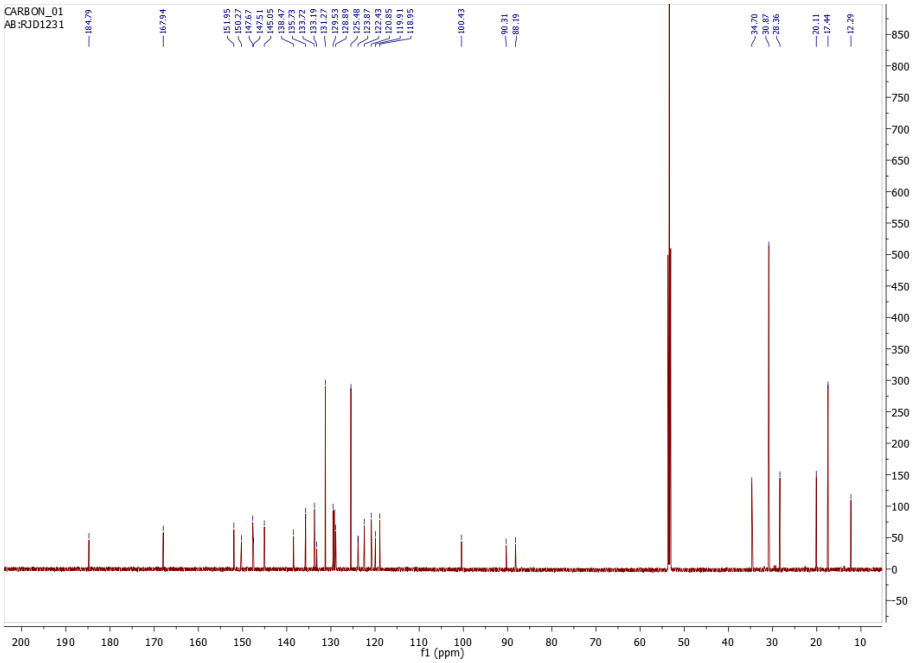

Figure S41. ^{13}C NMR spectrum of **10** recorded in CD_2Cl_2.

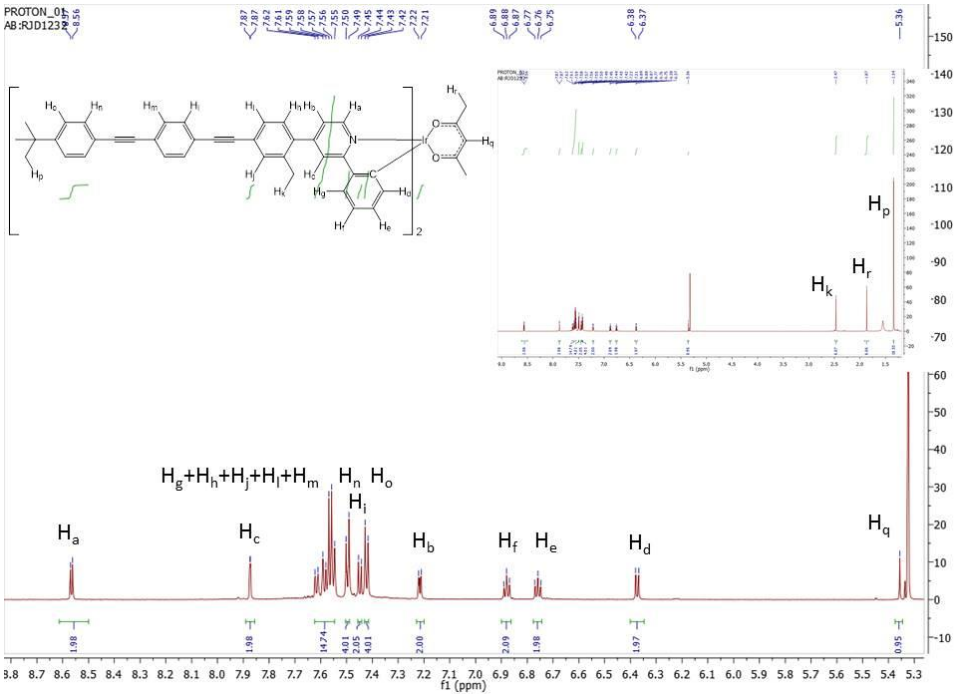

Figure S42. ^{1}H NMR spectrum of **11** recorded in CD_2Cl_2.

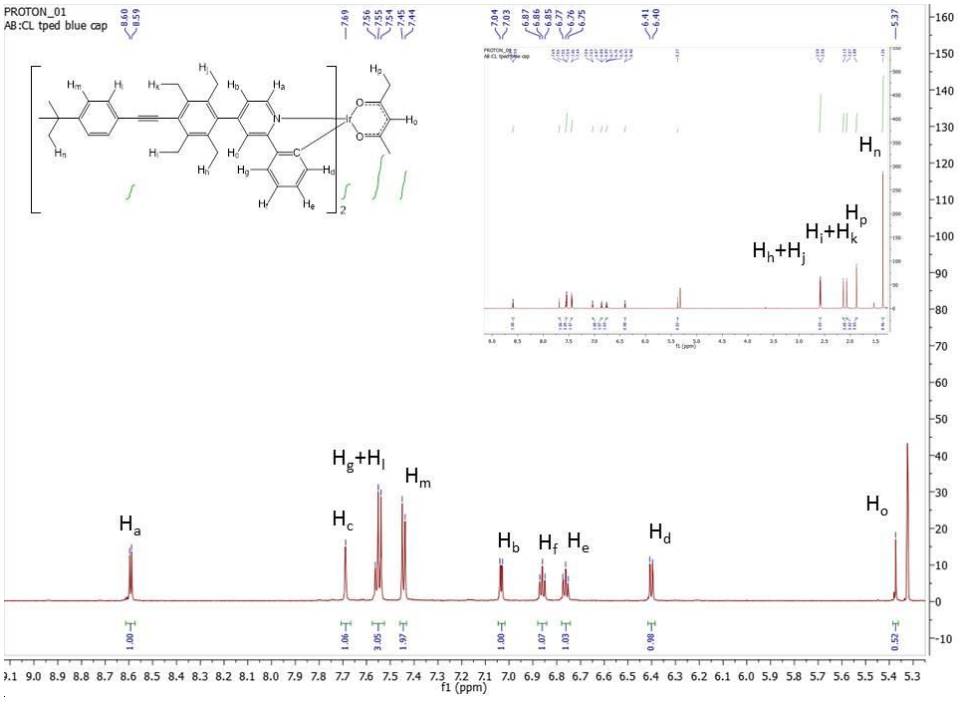

Figure S43. ^{1}H NMR spectrum of **12** recorded in CD_2Cl_2.

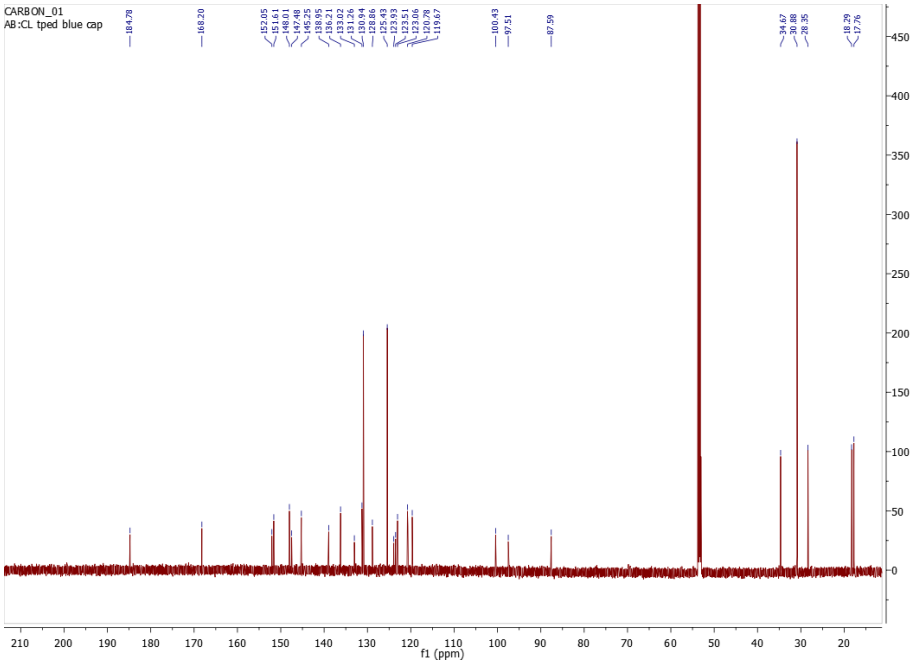

Figure S44. ^{13}C NMR spectrum of **12** recorded in CD_2Cl_2.

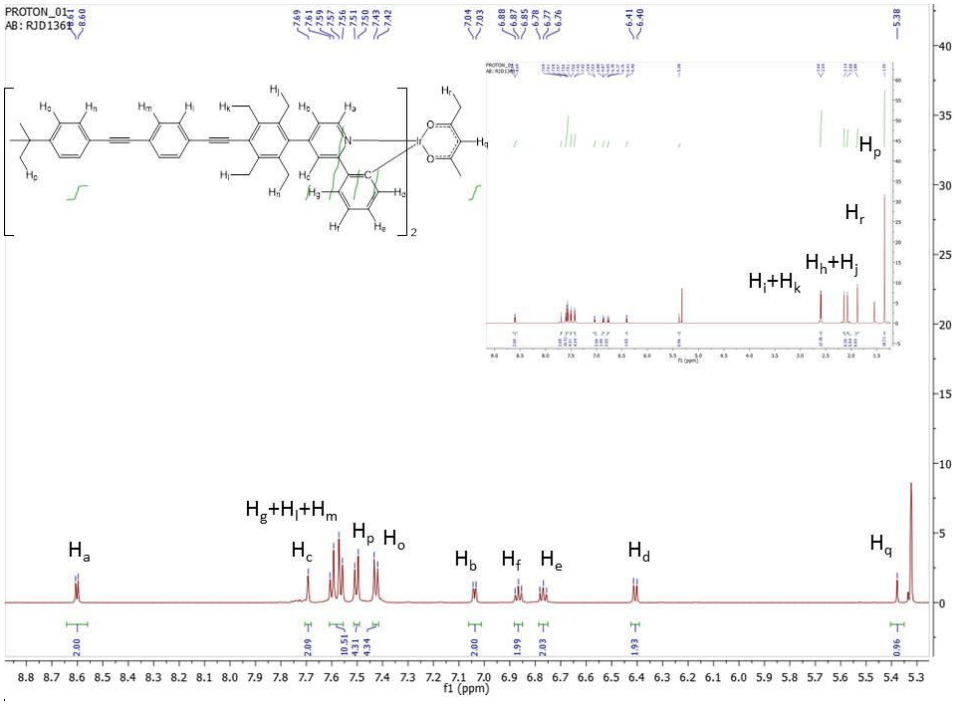

Figure S45. ^{1}H NMR spectrum of **13** recorded in CD_2Cl_2.

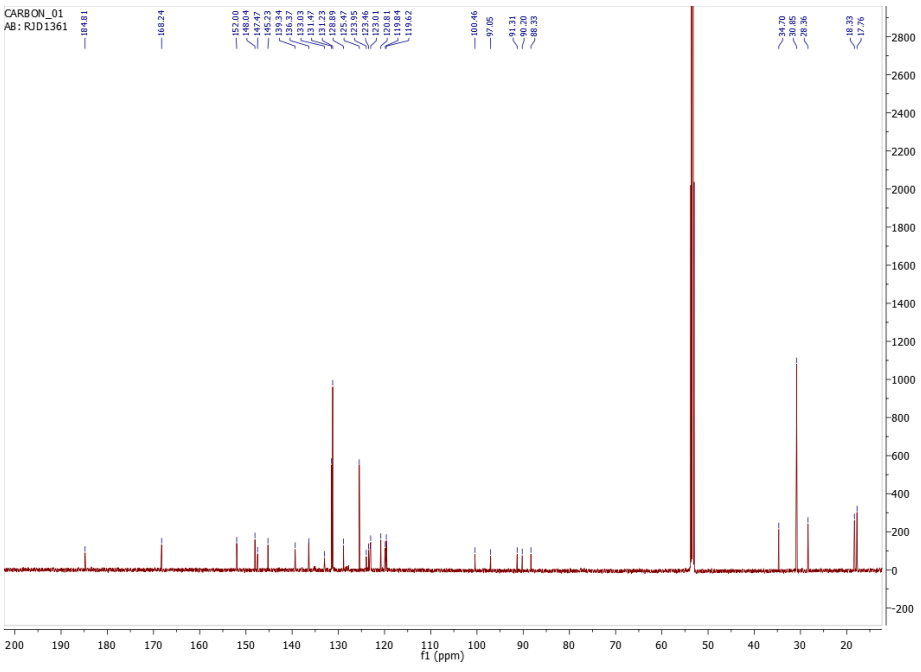

Figure S46. ^{13}C NMR spectrum of **13** recorded in CD_2Cl_2.

S3. Crystallographic data

Table S1. Crystal and Refinement Data for **4-(2,3,5,6-tetramethylphenyl)pyridine**, **4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine**, and **L^1H**.

Name	4-(2,3,5,6-tetramethylphenyl)pyridine	4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl) ethynyl) phenyl)pyridine	L^1H
Identification code	14srv267	15srv083	14srv269
Empirical formula	$C_{15}H_{17}N$	$C_{26}H_{37}NSi$	$C_{21}H_{21}N$
Formula weight	211.30	391.66	287.39
Temperature (K)	120.0	120.0	120.0
Crystal system	orthorhombic	triclinic	orthorhombic
Space group	Pnma	P-1	$Pna2_1$
a/Å	7.1655(2)	8.0108(3)	24.342(2)
b/Å	11.8629(3)	11.6119(4)	9.8877(6)
c/Å	14.2796(4)	13.3724(6)	6.9709(5)
α/°	90.00	87.906(3)	90.00
β/°	90.00	76.043(4)	90.00
γ/°	90.00	85.999(3)	90.00
Volume/$Å^3$	1213.82(6)	1203.99(8)	1677.8(2)
Z	4	2	4
$\rho_{calc}g/cm^3$	1.156	1.080	1.138
μ/mm^{-1}	0.067	0.108	0.065
F(000)	456.0	428.0	616.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Reflections collected	19096	16164	14061
Independent reflections, R_{int}	1841 [R_{int} = 0.0556, R_{sigma} = 0.0237]	5250 [R_{int} = 0.0450, R_{sigma} = 0.0553]	2184 [R_{int} = 0.0883, R_{sigma} = 0.0650]
Data/restraints/parameters	1841/0/124	5250/16/258	2184/1/239
Goodness-of-fit on F^2	1.050	1.031	1.052
Final R_1 indexes [I>=2σ (I)]	R_1 = 0.0444, wR_2 = 0.1158	R_1 = 0.0768, wR_2 = 0.1838	R_1 = 0.0563, wR_2 = 0.1199
Final wR_2 indexes [all data]	R_1 = 0.0544, wR_2 = 0.1246	R_1 = 0.1114, wR_2 = 0.2072	R_1 = 0.0781, wR_2 = 0.1323

Table S2. Crystal and Refinement Data for **1**, **3**, and **4**.

Name	1	3	4
Identification code	15srv057	15srv192	15srv172
Empirical formula	$C_{47}H_{47}IrN_2O_2$ x 0.14 CH_2Cl_2	$C_{61}H_{71}IrN_2O_2Si_2$ x 1.25 CH_2Cl_2	$C_{63}H_{85}IrN_2O_2Si_2$ x $5C_6H_6$
Formula weight	875.91	1218.74	1531.17
Temperature (K)	120.0	120.0	120.0
Crystal system	orthorhombic	triclinic	triclinic
Space group	Pbcn	P-1	P-1
a/Å	60.850(6)	10.7674(7)	12.9934(9)
b/Å	19.0815(18)	22.3710(14)	13.7265(9)
c/Å	25.642(2)	25.6411(17)	23.7151(16)
α/°	90.00	103.153(2)	82.522(2)
β/°	90.00	99.925(2)	77.924(2)
γ/°	90.00	90.329(2)	78.022(2)
Volume/$Å^3$	29773(5)	5917.8(7)	4029.4(5)
Z	28	4	2
$\rho_{calc}g/cm^3$	1.368	1.368	1.262
μ/mm^{-1}	3.195	2.452	1.735
F(000)	12368.0	2498.0	1596.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Reflections collected	454412	87020	59454
Independent reflections, R_{int}	37404 [R_{int} = 0.0910, R_{sigma} = 0.0681]	28506 [R_{int} = 0.1137, R_{sigma} = 0.1692]	18502 [R_{int} = 0.0400, R_{sigma} = 0.0410]
Data/restraints/parameters	37404/0/1657	28506/1341/1261	18502/308/898
Goodness-of-fit on F^2	1.047	1.011	1.045
Final R_1 indexes [I>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.0985	R_1 = 0.0668, wR_2 = 0.1135	R_1 = 0.0366, wR_2 = 0.0893
Final wR_2 indexes [all data]	R_1 = 0.0866, wR_2 = 0.1051	R_1 = 0.1576, wR_2 = 0.1397	R_1 = 0.0490, wR_2 = 0.0975

Table S3. Crystal and Refinement Data for **7**, **12**, and **13**.

Name	7	12	13
Identification code	15srv241	15srv248	15srv240
Empirical formula	$C_{67}H_{55}IrN_2O_2(Cl_{0.1})$ x CH_2Cl_2	$C_{71}H_{71}IrN_2O_2$ x 2 CH_2Cl_2	$C_{87}H_{79}Cl_5IrN_2O_2$ x 2.5 CH_2Cl_2
Formula weight	1200.80	1346.35	1589.04
Temperature (K)	120.0	120.0	120.0
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	P-1	P-1
a/Å	35.154(2)	14.3253(6)	13.0485(7)
b/Å	10.1868(6)	14.4743(7)	14.3392(7)
c/Å	15.3918(9)	17.5054(8)	23.9839(12)
α/°	90.00	99.7869(15)	100.9910(10)
β/°	90.3714(17)	93.9042(15)	95.1830(10)
γ/°	90.00	109.7098(15)	106.0900(10)
Volume/$Å^3$	5515.7(3)	3336.4(3)	4183.6(4)
Z	4	2	2
$\rho_{calc}g/cm^3$	1.446	1.340	1.261
μ/mm^{-1}	2.571	2.206	1.801
F(000)	2431.0	1376.0	1626.0
Radiation	MoKα ($\lambda = 0.71073$)	MoKα ($\lambda = 0.71073$)	MoKα ($\lambda = 0.71073$)
Reflections collected	68154	71327	72657
Independent reflections, R_{int}	12035 [$R_{int} = 0.1404$, $R_{sigma} = 0.1437$]	18528 [$R_{int} = 0.0645$, $R_{sigma} = 0.0802$]	20167 [$R_{int} = 0.0789$, $R_{sigma} = 0.1094$]
Data/restraints/parameters	12035/6/688	18528/55/789	20167/3/925
Goodness-of-fit on F^2	0.997	1.071	1.034
Final R_1 indexes [I>=2σ (I)]	$R_1 = 0.0663$, $wR_2 = 0.1133$	$R_1 = 0.0564$, $wR_2 = 0.1300$	$R_1 = 0.0562$, $wR_2 = 0.1441$
Final wR_2 indexes [all data]	$R_1 = 0.1481$, $wR_2 = 0.1448$	$R_1 = 0.0912$, $wR_2 = 0.1450$	$R_1 = 0.0859$, $wR_2 = 0.1578$

Table S4. Selected bond lengths for **4-(2,3,5,6-tetramethylphenyl)pyridine**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N1	C1	1.341(2)		C6	C7	1.4041(12)
N1	C5	1.340(2)		C6	C7[1]	1.4042(12)
C1	C2	1.385(2)		C7	C8	1.4069(14)
C2	C3	1.394(2)		C7	C10	1.5047(15)
C3	C4	1.3942(18)		C8	C9	1.3923(13)
C3	C6	1.4965(18)		C8	C11	1.5083(16)
C4	C5	1.389(2)		C9	C8[1]	1.3924(13)

Table S5. Selected bond angles for **4-(2,3,5,6-tetramethylphenyl)pyridine**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C5	N1	C1	116.13(13)		C7	C6	C3	119.14(6)
N1	C1	C2	124.04(14)		C7	C6	C7[1]	121.69(12)
C1	C2	C3	119.49(14)		C6	C7	C8	118.90(10)
C2	C3	C4	116.97(13)		C6	C7	C10	121.36(9)
C2	C3	C6	122.29(12)		C8	C7	C10	119.73(9)
C4	C3	C6	120.74(12)		C7	C8	C11	121.06(10)
C5	C4	C3	119.34(14)		C9	C8	C7	119.03(10)
N1	C5	C4	124.04(14)		C9	C8	C11	119.91(10)
C7[1]	C6	C3	119.15(6)		C8	C9	C8[1]	122.42(13)

Table S6. Selected bond lengths for **4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Si1	C17	1.838(3)		C8	C13	1.515(4)
Si1	C18	1.896(2)		C9	C10	1.404(4)
Si1	C18A	1.888(3)		C9	C16	1.441(4)
Si1	C21	1.887(2)		C10	C11	1.400(4)
Si1	C24A	1.893(3)		C10	C14	1.514(3)
Si1	C24B	1.884(2)		C11	C15	1.511(4)
N1	C1	1.335(4)		C16	C17	1.205(4)
N1	C5	1.332(5)		C18	C19	1.551(5)
C1	C2	1.387(4)		C18	C20	1.489(5)
C2	C3	1.390(4)		C18A	C19	1.624(16)
C3	C4	1.391(4)		C18A	C20	1.546(15)
C3	C6	1.497(4)		C21	C22	1.518(4)
C4	C5	1.390(4)		C21	C23	1.518(4)
C6	C7	1.406(4)		C24A	C25	1.557(4)
C6	C11	1.403(3)		C24A	C26B	1.557(4)
C7	C8	1.393(4)		C24B	C25	1.555(3)
C7	C12	1.519(4)		C24B	C26A	1.555(3)
C8	C9	1.406(4)				

Table S7. Selected bond angles for **4-(2,3,5,6-tetramethyl-4-((triisopropylsilyl)ethynyl)phenyl)pyridine**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C17	Si1	C18	105.56(16)		C9	C8	C13	120.1(3)
C17	Si1	C18A	116.2(5)		C8	C9	C16	119.6(2)
C17	Si1	C21	106.91(13)		C10	C9	C8	121.6(2)
C17	Si1	C24A	104.64(16)		C10	C9	C16	118.8(2)
C17	Si1	C24B	111.01(14)		C9	C10	C14	119.7(2)
C18A	Si1	C18	33.0(5)		C11	C10	C9	119.3(2)
C18A	Si1	C24A	98.6(6)		C11	C10	C14	120.9(2)
C21	Si1	C18	107.49(15)		C6	C11	C15	120.8(2)
C21	Si1	C18A	126.7(5)		C10	C11	C6	119.1(2)
C21	Si1	C24A	99.3(3)		C10	C11	C15	120.2(2)
C24A	Si1	C18	131.1(3)		C17	C16	C9	179.5(3)
C24B	Si1	C18	107.70(18)		C16	C17	Si1	177.5(3)
C24B	Si1	C18A	74.8(5)		C19	C18	Si1	110.6(2)
C24B	Si1	C21	117.50(15)		C20	C18	Si1	113.7(3)
C24B	Si1	C24A	24.2(3)		C20	C18	C19	111.2(3)
C5	N1	C1	116.0(3)		C19	C18A	Si1	107.7(7)
N1	C1	C2	124.0(3)		C20	C18A	Si1	111.5(7)
C1	C2	C3	119.5(3)		C20	C18A	C19	104.7(8)
C2	C3	C4	117.1(3)		C18	C19	C18A	39.5(5)
C2	C3	C6	121.0(2)		C18	C20	C18A	41.4(6)
C4	C3	C6	122.0(3)		C22	C21	Si1	111.1(2)
C5	C4	C3	118.8(3)		C22	C21	C23	109.4(3)
N1	C5	C4	124.6(3)		C23	C21	Si1	112.6(2)
C7	C6	C3	119.1(2)		C25	C24A	Si1	111.3(2)
C11	C6	C3	119.4(2)		C26B	C24A	Si1	117.7(6)
C11	C6	C7	121.4(2)		C26B	C24A	C25	108.4(7)
C6	C7	C12	120.5(2)		C25	C24B	Si1	111.9(2)
C8	C7	C6	119.7(2)		C26A	C24B	Si1	110.8(3)
C8	C7	C12	119.8(2)		C26A	C24B	C25	105.0(3)
C7	C8	C9	119.0(2)		C24B	C25	C24A	29.5(4)
C7	C8	C13	121.0(2)					

Table S8. Selected bond lengths for **L^{1}H**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
N1	C3	1.351(4)		C8	C9	1.399(4)
N1	C4	1.343(4)		C8	C13	1.514(4)
C1	C2	1.394(4)		C9	C10	1.394(5)
C1	C5	1.383(5)		C10	C11	1.394(4)
C1	C6	1.494(4)		C10	C14	1.519(4)
C2	C3	1.390(4)		C11	C15	1.501(4)
C3	C16	1.493(4)		C16	C17	1.390(5)
C4	C5	1.376(5)		C16	C21	1.394(5)
C6	C7	1.398(4)		C17	C18	1.393(5)
C6	C11	1.414(4)		C18	C19	1.399(5)
C7	C8	1.398(4)		C19	C20	1.369(5)
C7	C12	1.516(4)		C20	C21	1.399(4)

Table S9. Selected bond angles for **L^{1}H**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C4	N1	C3	116.9(3)		C7	C8	C13	122.2(3)
C2	C1	C6	122.0(3)		C9	C8	C13	118.8(3)
C5	C1	C2	117.6(3)		C10	C9	C8	121.6(3)
C5	C1	C6	120.4(3)		C9	C10	C11	120.0(3)
C3	C2	C1	120.3(3)		C9	C10	C14	118.9(3)
N1	C3	C2	121.8(3)		C11	C10	C14	121.0(3)
N1	C3	C16	115.7(3)		C6	C11	C15	121.3(3)
C2	C3	C16	122.5(3)		C10	C11	C6	118.4(3)
N1	C4	C5	124.6(3)		C10	C11	C15	120.2(3)
C4	C5	C1	118.8(3)		C17	C16	C3	121.7(3)
C7	C6	C1	119.6(3)		C17	C16	C21	118.8(3)
C7	C6	C11	121.4(3)		C21	C16	C3	119.5(3)
C11	C6	C1	119.0(3)		C16	C17	C18	120.9(3)
C6	C7	C8	119.6(3)		C17	C18	C19	119.4(4)
C6	C7	C12	121.3(3)		C20	C19	C18	120.3(3)
C8	C7	C12	119.2(3)		C19	C20	C21	120.1(3)
C7	C8	C9	119.0(3)		C16	C21	C20	120.5(3)

Table S10. Selected bond lengths for **1**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.155(4)		C35A	C36A	1.470(8)
Ir1	O2	2.147(3)		C36A	C37A	1.422(8)
Ir1	N1	2.026(4)		C36A	C41A	1.392(8)
Ir1	N2	2.032(4)		C37A	C38A	1.393(8)
Ir1	C7	1.991(5)		C38A	C39A	1.392(9)
Ir1	C37	1.998(5)		C39A	C40A	1.384(10)
O1	C22	1.265(6)		C40A	C41A	1.383(9)
O2	C24	1.271(7)		C42A	C43A	1.425(8)
N1	C1	1.340(6)		C42A	C47A	1.400(8)
N1	C5	1.360(6)		C43A	C44A	1.405(9)
N2	C31	1.340(7)		C43A	C48A	1.471(9)
N2	C35	1.359(6)		C44A	C45A	1.397(9)
C1	C2	1.378(7)		C44A	C49A	1.513(9)
C2	C3	1.388(7)		C45A	C46A	1.360(9)
C3	C4	1.390(7)		C46A	C47A	1.411(9)
C3	C12	1.481(7)		C46A	C50A	1.516(9)
C4	C5	1.391(7)		C47A	C51A	1.502(9)
C5	C6	1.463(7)		Ir1B	O1B	2.151(3)
C6	C7	1.404(7)		Ir1B	O2B	2.154(4)
C6	C11	1.391(8)		Ir1B	N1B	2.038(4)
C7	C8	1.410(7)		Ir1B	N2B	2.026(4)
C8	C9	1.394(8)		Ir1B	C7B	1.987(5)
C9	C10	1.383(8)		Ir1B	C37B	1.993(5)
C10	C11	1.383(8)		O1B	C22B	1.269(6)
C12	C13	1.409(8)		O2B	C24B	1.267(6)
C12	C17	1.387(8)		N1B	C1B	1.336(6)
C13	C14	1.399(8)		N1B	C5B	1.356(6)
C13	C18	1.520(8)		N2B	C31B	1.330(6)
C14	C15	1.388(9)		N2B	C35B	1.363(6)
C14	C19	1.507(9)		C1B	C2B	1.383(7)
C15	C16	1.377(9)		C2B	C3B	1.387(7)
C16	C17	1.408(8)		C3B	C4B	1.384(7)
C16	C20	1.501(8)		C3B	C12B	1.496(7)
C17	C21	1.501(9)		C4B	C5B	1.395(7)
C22	C23	1.399(8)		C5B	C6B	1.463(7)
C22	C26	1.506(8)		C6B	C7B	1.413(7)
C23	C24	1.410(8)		C6B	C11B	1.400(7)
C24	C25	1.499(8)		C7B	C8B	1.410(7)
C31	C32	1.384(7)		C8B	C9B	1.401(8)
C32	C33	1.377(7)		C9B	C10B	1.373(8)
C33	C34	1.396(7)		C10B	C11B	1.379(8)
C33	C42	1.488(7)		C12B	C13B	1.407(7)
C34	C35	1.384(7)		C12B	C17B	1.392(7)
C35	C36	1.465(7)		C13B	C14B	1.403(7)
C36	C37	1.408(7)		C13B	C18B	1.500(8)
C36	C41	1.399(8)		C14B	C15B	1.387(8)
C37	C38	1.395(7)		C14B	C19B	1.509(8)
C38	C39	1.381(8)		C15B	C16B	1.378(7)
C39	C40	1.386(8)		C16B	C17B	1.401(7)
C40	C41	1.372(8)		C16B	C20B	1.522(7)
C42	C43	1.405(8)		C17B	C21B	1.510(7)
C42	C47	1.398(8)		C22B	C23B	1.401(8)
C43	C44	1.393(7)		C22B	C26B	1.499(8)
C43	C48	1.512(8)		C23B	C24B	1.393(8)

Table S10 continued. Selected bond lengths for **1**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
C44	C45	1.370(9)		C24B	C25B	1.525(8)
C44	C49	1.500(9)		C31B	C32B	1.380(7)
C45	C46	1.375(9)		C32B	C33B	1.396(7)
C46	C47	1.410(8)		C33B	C34B	1.384(7)
C46	C50	1.495(9)		C33B	C42B	1.507(7)
C47	C51	1.518(9)		C34B	C35B	1.399(7)
Ir1A	O1A	2.149(4)		C35B	C36B	1.459(7)
Ir1A	O2A	2.140(4)		C36B	C37B	1.415(7)
Ir1A	N1A	2.035(5)		C36B	C41B	1.386(7)
Ir1A	N2A	2.020(5)		C37B	C38B	1.403(7)
Ir1A	C7A	1.984(5)		C38B	C39B	1.383(7)
Ir1A	C37A	1.984(6)		C39B	C40B	1.386(8)
O1A	C22A	1.272(7)		C40B	C41B	1.378(7)
O2A	C24A	1.275(7)		C42B	C43B	1.390(8)
N1A	C1A	1.314(8)		C42B	C47B	1.397(8)
N1A	C5A	1.374(7)		C43B	C44B	1.402(7)
N2A	C31A	1.354(7)		C43B	C48B	1.495(8)
N2A	C35A	1.371(7)		C44B	C45B	1.379(8)
C1A	C2A	1.385(8)		C44B	C49B	1.514(8)
C2A	C3A	1.375(8)		C45B	C46B	1.397(9)
C3A	C4A	1.400(8)		C46B	C47B	1.402(8)
C3A	C12A	1.483(8)		C46B	C50B	1.500(9)
C3A	C12K	1.516(9)		C47B	C51B	1.499(8)
C4A	C5A	1.392(8)		Ir1C	O1C^{1}	2.157(4)
C5A	C6A	1.463(8)		Ir1C	O1C	2.157(4)
C6A	C7A	1.412(8)		Ir1C	N1C	2.035(4)
C6A	C11A	1.400(8)		Ir1C	N1C^{1}	2.035(4)
C7A	C8A	1.408(8)		Ir1C	C7C^{1}	2.000(5)
C8A	C9A	1.392(9)		Ir1C	C7C	2.000(5)
C9A	C10A	1.379(9)		O1C	C22C	1.264(7)
C10A	C11A	1.368(9)		N1C	C1M	1.334(6)
C12A	C17A	1.3900		N1C	C5C	1.357(6)
C12A	C13A	1.3900		C1M	C2C	1.382(7)
C17A	C16A	1.3900		C2C	C3C	1.380(7)
C17A	C21K	1.86(2)		C3C	C4C	1.390(7)
C16A	C15A	1.3900		C3C	C12C	1.490(7)
C16A	C20A	1.55(2)		C4C	C5C	1.385(7)
C15A	C14A	1.3900		C5C	C6C	1.466(7)
C14A	C13A	1.3900		C6C	C7C	1.407(7)
C14A	C19A	1.488(17)		C6C	C11C	1.403(7)
C13A	C18K	1.125(19)		C7C	C8C	1.400(7)
C12K	C13K	1.3900		C8C	C9C	1.382(8)
C12K	C17K	1.3900		C9C	C10C	1.377(8)
C13K	C14K	1.3900		C10C	C11C	1.382(7)
C13K	C18A	1.909(19)		C12C	C13C	1.399(8)
C14K	C15K	1.3900		C12C	C17C	1.399(7)
C14K	C19K	1.544(19)		C13C	C14C	1.406(8)
C15K	C16K	1.3900		C13C	C18C	1.517(8)
C16K	C17K	1.3900		C14C	C15C	1.377(9)
C16K	C20K	1.49(2)		C14C	C19C	1.520(9)
C17K	C21A	1.21(2)		C15C	C16C	1.384(9)
C22A	C23A	1.394(9)		C16C	C17C	1.404(8)

Table S10 continued. Selected bond lengths for **1**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
C22A	C26A	1.500(8)		C16C	C20C	1.496(8)
C23A	C24A	1.400(9)		C17C	C21C	1.498(8)
C24A	C25A	1.516(9)		C22C	C23C	1.399(7)
C31A	C32A	1.385(9)		C22C	C24C	1.513(8)
C32A	C33A	1.396(8)		C23C	$C22C^{1}$	1.399(7)
C33A	C34A	1.392(8)		Cl2	C1S	1.744(6)
C33A	C42A	1.492(8)		C1S	$Cl2^{2}$	1.744(6)
C34A	C35A	1.383(8)				

Table S11. Selected bond angles for **1**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O2	Ir1	O1	88.18(14)		C35A	C34A	C33A	121.1(6)
N1	Ir1	O1	97.35(15)		N2A	C35A	C34A	120.9(6)
N1	Ir1	O2	88.97(15)		N2A	C35A	C36A	112.4(5)
N1	Ir1	N2	174.46(16)		C34A	C35A	C36A	126.6(6)
N2	Ir1	O1	85.11(16)		C37A	C36A	C35A	114.9(5)
N2	Ir1	O2	96.08(15)		C41A	C36A	C35A	123.0(5)
C7	Ir1	O1	177.40(18)		C41A	C36A	C37A	122.1(5)
C7	Ir1	O2	91.02(17)		C36A	C37A	Ir1A	114.5(4)
C7	Ir1	N1	80.16(19)		C38A	C37A	Ir1A	129.0(5)
C7	Ir1	N2	97.43(19)		C38A	C37A	C36A	116.5(5)
C7	Ir1	C37	92.0(2)		C39A	C38A	C37A	121.7(6)
C37	Ir1	O1	88.91(18)		C40A	C39A	C38A	120.3(6)
C37	Ir1	O2	175.95(18)		C41A	C40A	C39A	120.3(6)
C37	Ir1	N1	94.20(19)		C40A	C41A	C36A	119.1(6)
C37	Ir1	N2	80.86(19)		C43A	C42A	C33A	119.5(5)
C22	O1	Ir1	124.3(4)		C47A	C42A	C33A	119.0(5)
C24	O2	Ir1	124.8(3)		C47A	C42A	C43A	121.5(6)
C1	N1	Ir1	124.0(3)		C42A	C43A	C48A	120.7(6)
C1	N1	C5	119.0(4)		C44A	C43A	C42A	117.6(6)
C5	N1	Ir1	116.6(3)		C44A	C43A	C48A	121.6(6)
C31	N2	Ir1	124.4(3)		C43A	C44A	C49A	121.0(6)
C31	N2	C35	119.5(4)		C45A	C44A	C43A	119.1(6)
C35	N2	Ir1	116.0(3)		C45A	C44A	C49A	119.6(6)
N1	C1	C2	122.7(5)		C46A	C45A	C44A	123.8(6)
C1	C2	C3	119.7(5)		C45A	C46A	C47A	118.3(6)
C2	C3	C4	117.3(5)		C45A	C46A	C50A	119.9(6)
C2	C3	C12	121.7(5)		C47A	C46A	C50A	121.8(6)
C4	C3	C12	121.0(5)		C42A	C47A	C46A	119.5(6)
C3	C4	C5	121.0(5)		C42A	C47A	C51A	122.0(6)
N1	C5	C4	120.1(4)		C46A	C47A	C51A	118.5(6)
N1	C5	C6	113.1(4)		O1B	Ir1B	O2B	88.44(14)
C4	C5	C6	126.7(5)		N1B	Ir1B	O1B	96.43(15)
C7	C6	C5	114.7(5)		N1B	Ir1B	O2B	87.86(15)
C11	C6	C5	123.2(5)		N2B	Ir1B	O1B	87.82(15)
C11	C6	C7	122.1(5)		N2B	Ir1B	O2B	96.30(15)
C6	C7	Ir1	115.2(4)		N2B	Ir1B	N1B	174.15(17)
C6	C7	C8	116.0(5)		C7B	Ir1B	O1B	177.04(17)
C8	C7	Ir1	128.8(4)		C7B	Ir1B	O2B	90.53(17)
C9	C8	C7	121.9(5)		C7B	Ir1B	N1B	80.76(18)
C10	C9	C8	120.2(5)		C7B	Ir1B	N2B	95.05(19)
C11	C10	C9	119.4(5)		C7B	Ir1B	C37B	91.0(2)
C10	C11	C6	120.2(5)		C37B	Ir1B	O1B	90.16(17)
C13	C12	C3	118.4(5)		C37B	Ir1B	O2B	176.74(17)
C17	C12	C3	119.9(5)		C37B	Ir1B	N1B	95.22(18)
C17	C12	C13	121.7(5)		C37B	Ir1B	N2B	80.70(19)
C12	C13	C18	120.9(5)		C22B	O1B	Ir1B	125.0(3)
C14	C13	C12	118.7(5)		C24B	O2B	Ir1B	123.8(4)
C14	C13	C18	120.4(6)		C1B	N1B	Ir1B	124.8(3)
C13	C14	C19	120.6(6)		C1B	N1B	C5B	119.8(4)
C15	C14	C13	118.7(6)		C5B	N1B	Ir1B	115.4(3)
C15	C14	C19	120.7(6)		C31B	N2B	Ir1B	124.2(4)
C16	C15	C14	123.0(5)		C31B	N2B	C35B	119.6(4)
C15	C16	C17	118.7(5)		C35B	N2B	Ir1B	116.2(3)
C15	C16	C20	119.8(6)		N1B	C1B	C2B	122.0(5)

Table S11 continued. Selected bond angles for **1**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C17	C16	C20	121.5(6)		C1B	C2B	C3B	119.9(5)
C12	C17	C16	119.1(6)		C2B	C3B	C12B	122.4(5)
C12	C17	C21	121.7(5)		C4B	C3B	C2B	117.3(5)
C16	C17	C21	119.1(5)		C4B	C3B	C12B	120.3(4)
O1	C22	C23	127.6(5)		C3B	C4B	C5B	121.2(5)
O1	C22	C26	114.6(5)		N1B	C5B	C4B	119.6(4)
C23	C22	C26	117.8(5)		N1B	C5B	C6B	114.4(4)
C22	C23	C24	126.6(5)		C4B	C5B	C6B	126.0(5)
O2	C24	C23	127.0(5)		C7B	C6B	C5B	114.4(4)
O2	C24	C25	114.8(5)		C11B	C6B	C5B	124.3(5)
C23	C24	C25	118.1(5)		C11B	C6B	C7B	121.3(5)
N2	C31	C32	122.5(5)		C6B	C7B	Ir1B	114.9(4)
C33	C32	C31	119.1(5)		C8B	C7B	Ir1B	127.9(4)
C32	C33	C34	118.3(5)		C8B	C7B	C6B	117.1(5)
C32	C33	C42	121.6(5)		C9B	C8B	C7B	120.6(5)
C34	C33	C42	120.1(5)		C10B	C9B	C8B	120.8(5)
C35	C34	C33	120.6(5)		C9B	C10B	C11B	120.2(5)
N2	C35	C34	120.1(5)		C10B	C11B	C6B	120.0(5)
N2	C35	C36	113.6(4)		C13B	C12B	C3B	117.0(5)
C34	C35	C36	126.2(5)		C17B	C12B	C3B	120.8(5)
C37	C36	C35	115.4(5)		C17B	C12B	C13B	122.2(5)
C41	C36	C35	123.4(5)		C12B	C13B	C18B	121.2(5)
C41	C36	C37	121.0(5)		C14B	C13B	C12B	118.2(5)
C36	C37	Ir1	114.1(4)		C14B	C13B	C18B	120.5(5)
C38	C37	Ir1	128.2(4)		C13B	C14B	C19B	121.1(5)
C38	C37	C36	117.4(5)		C15B	C14B	C13B	118.9(5)
C39	C38	C37	121.2(5)		C15B	C14B	C19B	120.0(5)
C38	C39	C40	120.5(5)		C16B	C15B	C14B	122.8(5)
C41	C40	C39	120.0(5)		C15B	C16B	C17B	119.3(5)
C40	C41	C36	119.9(5)		C15B	C16B	C20B	120.2(5)
C43	C42	C33	119.2(5)		C17B	C16B	C20B	120.5(5)
C47	C42	C33	119.7(5)		C12B	C17B	C16B	118.5(5)
C47	C42	C43	121.1(5)		C12B	C17B	C21B	121.6(5)
C42	C43	C48	121.5(5)		C16B	C17B	C21B	119.9(5)
C44	C43	C42	118.8(5)		O1B	C22B	C23B	126.5(5)
C44	C43	C48	119.7(5)		O1B	C22B	C26B	115.9(5)
C43	C44	C49	120.0(6)		C23B	C22B	C26B	117.5(5)
C45	C44	C43	119.4(6)		C24B	C23B	C22B	127.9(5)
C45	C44	C49	120.6(6)		O2B	C24B	C23B	127.8(5)
C44	C45	C46	123.4(5)		O2B	C24B	C25B	113.9(5)
C45	C46	C47	118.3(6)		C23B	C24B	C25B	118.3(5)
C45	C46	C50	121.3(6)		N2B	C31B	C32B	122.6(5)
C47	C46	C50	120.4(6)		C31B	C32B	C33B	119.5(5)
C42	C47	C46	119.1(5)		C32B	C33B	C42B	119.4(5)
C42	C47	C51	120.8(5)		C34B	C33B	C32B	117.8(5)
C46	C47	C51	120.1(5)		C34B	C33B	C42B	122.7(5)
O2A	Ir1A	O1A	88.11(16)		C33B	C34B	C35B	120.5(5)
N1A	Ir1A	O1A	96.30(18)		N2B	C35B	C34B	120.0(5)
N1A	Ir1A	O2A	88.63(18)		N2B	C35B	C36B	113.6(4)
N2A	Ir1A	O1A	89.17(17)		C34B	C35B	C36B	126.3(5)
N2A	Ir1A	O2A	97.37(18)		C37B	C36B	C35B	114.9(4)
N2A	Ir1A	N1A	172.03(19)		C41B	C36B	C35B	123.8(5)
C7A	Ir1A	O1A	176.8(2)		C41B	C36B	C37B	121.3(5)
C7A	Ir1A	O2A	90.2(2)		C36B	C37B	Ir1B	114.5(4)

Table S11 continued. Selected bond angles for **1**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C7A	Ir1A	N1A	80.9(2)		C38B	C37B	Ir1B	128.4(4)
C7A	Ir1A	N2A	93.8(2)		C38B	C37B	C36B	117.1(5)
C37A	Ir1A	O1A	92.5(2)		C39B	C38B	C37B	121.3(5)
C37A	Ir1A	O2A	178.1(2)		C38B	C39B	C40B	120.3(5)
C37A	Ir1A	N1A	93.2(2)		C41B	C40B	C39B	120.1(5)
C37A	Ir1A	N2A	80.8(2)		C40B	C41B	C36B	120.0(5)
C37A	Ir1A	C7A	89.3(2)		C43B	C42B	C33B	117.8(5)
C22A	O1A	Ir1A	125.2(4)		C43B	C42B	C47B	121.9(5)
C24A	O2A	Ir1A	124.7(4)		C47B	C42B	C33B	120.2(5)
C1A	N1A	Ir1A	125.7(4)		C42B	C43B	C44B	119.0(5)
C1A	N1A	C5A	118.8(5)		C42B	C43B	C48B	122.2(5)
C5A	N1A	Ir1A	115.3(4)		C44B	C43B	C48B	118.8(5)
C31A	N2A	Ir1A	125.3(4)		C43B	C44B	C49B	120.1(5)
C31A	N2A	C35A	117.8(5)		C45B	C44B	C43B	118.6(5)
C35A	N2A	Ir1A	116.4(4)		C45B	C44B	C49B	121.3(5)
N1A	C1A	C2A	123.2(6)		C44B	C45B	C46B	123.4(5)
C3A	C2A	C1A	120.1(6)		C45B	C46B	C47B	117.8(5)
C2A	C3A	C4A	116.8(6)		C45B	C46B	C50B	120.2(6)
C2A	C3A	C12A	121.8(7)		C47B	C46B	C50B	122.0(6)
C2A	C3A	C12K	123.7(7)		C42B	C47B	C46B	119.3(5)
C4A	C3A	C12A	120.8(6)		C42B	C47B	C51B	121.3(5)
C4A	C3A	C12K	119.2(7)		C46B	C47B	C51B	119.4(6)
C12A	C3A	C12K	12.4(6)		O1C^{1}	Ir1C	O1C	88.0(2)
C5A	C4A	C3A	120.9(6)		N1C	Ir1C	O1C	89.69(15)
N1A	C5A	C4A	119.8(5)		N1C^{1}	Ir1C	O1C^{1}	89.68(15)
N1A	C5A	C6A	113.8(5)		N1C^{1}	Ir1C	O1C	96.72(15)
C4A	C5A	C6A	126.2(5)		N1C	Ir1C	O1C^{1}	96.72(15)
C7A	C6A	C5A	114.6(5)		N1C	Ir1C	N1C^{1}	171.1(2)
C11A	C6A	C5A	123.6(6)		C7C^{1}	Ir1C	O1C	177.40(17)
C11A	C6A	C7A	121.9(5)		C7C^{1}	Ir1C	O1C^{1}	92.02(17)
C6A	C7A	Ir1A	115.1(4)		C7C	Ir1C	O1C	92.03(17)
C8A	C7A	Ir1A	128.3(5)		C7C	Ir1C	O1C^{1}	177.40(17)
C8A	C7A	C6A	116.5(5)		C7C^{1}	Ir1C	N1C	92.89(19)
C9A	C8A	C7A	121.5(6)		C7C	Ir1C	N1C	80.68(18)
C10A	C9A	C8A	119.8(6)		C7C^{1}	Ir1C	N1C^{1}	80.68(18)
C11A	C10A	C9A	121.2(6)		C7C	Ir1C	N1C^{1}	92.89(19)
C10A	C11A	C6A	119.2(6)		C7C	Ir1C	C7C^{1}	88.0(3)
C17A	C12A	C3A	117.5(6)		C22C	O1C	Ir1C	124.6(3)
C17A	C12A	C13A	120.0		C1M	N1C	Ir1C	123.9(4)
C13A	C12A	C3A	122.4(6)		C1M	N1C	C5C	119.9(4)
C12A	C17A	C21K	117.9(9)		C5C	N1C	Ir1C	115.6(3)
C16A	C17A	C12A	120.0		N1C	C1M	C2C	122.0(5)
C16A	C17A	C21K	121.2(9)		C3C	C2C	C1M	119.6(5)
C17A	C16A	C20A	121.4(9)		C2C	C3C	C4C	117.5(5)
C15A	C16A	C17A	120.0		C2C	C3C	C12C	120.7(5)
C15A	C16A	C20A	118.6(9)		C4C	C3C	C12C	121.7(5)
C16A	C15A	C14A	120.0		C5C	C4C	C3C	121.2(5)
C15A	C14A	C13A	120.0		N1C	C5C	C4C	119.5(4)
C15A	C14A	C19A	117.6(8)		N1C	C5C	C6C	113.9(4)
C13A	C14A	C19A	122.4(8)		C4C	C5C	C6C	126.4(5)
C14A	C13A	C12A	120.0		C7C	C6C	C5C	114.9(4)
C18K	C13A	C12A	129.1(12)		C11C	C6C	C5C	123.8(5)
C18K	C13A	C14A	110.5(12)		C11C	C6C	C7C	121.3(5)

Table S11 continued. Selected bond angles for **1**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C13K	C12K	C3A	116.2(7)		C6C	C7C	Ir1C	114.4(4)
C13K	C12K	C17K	120.0		C8C	C7C	Ir1C	128.5(4)
C17K	C12K	C3A	123.4(7)		C8C	C7C	C6C	117.1(5)
C12K	C13K	C14K	120.0		C9C	C8C	C7C	121.1(5)
C12K	C13K	C18A	115.1(8)		C10C	C9C	C8C	121.2(5)
C14K	C13K	C18A	124.9(8)		C9C	C10C	C11C	119.5(5)
C13K	C14K	C15K	120.0		C10C	C11C	C6C	119.7(5)
C13K	C14K	C19K	124.6(9)		C13C	C12C	C3C	118.1(5)
C15K	C14K	C19K	115.4(9)		C13C	C12C	C17C	122.2(5)
C16K	C15K	C14K	120.0		C17C	C12C	C3C	119.7(5)
C15K	C16K	C17K	120.0		C12C	C13C	C14C	118.3(5)
C15K	C16K	C20K	119.4(11)		C12C	C13C	C18C	121.2(5)
C17K	C16K	C20K	120.6(11)		C14C	C13C	C18C	120.5(5)
C16K	C17K	C12K	120.0		C13C	C14C	C19C	121.1(6)
C21A	C17K	C12K	122.0(14)		C15C	C14C	C13C	119.2(6)
C21A	C17K	C16K	117.5(14)		C15C	C14C	C19C	119.7(6)
O1A	C22A	C23A	126.3(6)		C14C	C15C	C16C	122.9(5)
O1A	C22A	C26A	116.1(6)		C15C	C16C	C17C	118.9(5)
C23A	C22A	C26A	117.5(6)		C15C	C16C	C20C	120.2(5)
C22A	C23A	C24A	127.8(6)		C17C	C16C	C20C	120.9(6)
O2A	C24A	C23A	126.8(6)		C12C	C17C	C16C	118.5(5)
O2A	C24A	C25A	114.3(6)		C12C	C17C	C21C	121.8(5)
C23A	C24A	C25A	119.0(6)		C16C	C17C	C21C	119.6(5)
N2A	C31A	C32A	123.4(6)		O1C	C22C	C23C	127.6(6)
C31A	C32A	C33A	118.9(6)		O1C	C22C	C24C	115.6(5)
C32A	C33A	C42A	119.7(5)		C23C	C22C	C24C	116.8(6)
C34A	C33A	C32A	117.7(6)		C22C	C23C	C22C[1]	127.0(8)
C34A	C33A	C42A	122.6(5)		Cl2	C1S	Cl2[2]	114.1(6)

Table S12. Selected bond lengths for **3**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.151(4)		Si21	C26C	1.875(5)
Ir1	O2	2.160(5)		Si21	C219	1.834(9)
Ir1	N1	2.029(6)		Si21	C220	1.869(4)
Ir1	N2	2.038(5)		Si21	C223	1.873(4)
Ir1	C7	1.987(7)		Si21	C226	1.877(5)
Ir1	C37	1.979(7)		Si22	C49C	1.846(7)
Si1A	C19A	1.849(6)		Si22	C50C	1.874(5)
Si1A	C20A	1.772(10)		Si22	C53C	1.873(3)
Si1A	C23A	1.875(4)		Si22	C56C	1.873(5)
Si1A	C26A	1.874(5)		Si23	C249	1.847(7)
Si1B	C19B	1.850(6)		Si23	C250	1.874(5)
Si1B	C20A	2.058(10)		Si23	C253	1.873(5)
Si1B	C23B	1.875(5)		Si23	C256	1.872(5)
Si1B	C26B	1.876(5)		O21	C263	1.257(8)
Si2A	C49A	1.848(6)		O22	C261	1.268(8)
Si2A	C50A	1.876(4)		N21	C201	1.341(9)
Si2A	C53A	1.879(5)		N21	C205	1.364(8)
Si2A	C56A	1.878(5)		N22	C231	1.353(9)
Si2B	C49B	1.847(7)		N22	C235	1.363(9)
Si2B	C50B	1.875(5)		C20C	C21C	1.526(4)
Si2B	C53B	1.868(5)		C20C	C22C	1.526(4)
Si2B	C56B	1.873(5)		C23C	C24C	1.526(4)
O1	C61	1.262(8)		C23C	C25C	1.525(4)
O2	C63	1.284(8)		C26C	C27C	1.526(4)
N1	C1	1.335(8)		C26C	C227	1.530(4)
N1	C5	1.357(8)		C42C	C47C	1.3900
N2	C31	1.336(8)		C42C	C43C	1.3900
N2	C35	1.357(8)		C42C	C233	1.361(10)
C1	C2	1.360(9)		C47C	C46C	1.3900
C2	C3	1.394(9)		C46C	C45C	1.3900
C3	C4	1.397(9)		C45C	C44C	1.3900
C3	C12	1.475(9)		C45C	C48C	1.434(10)
C4	C5	1.403(9)		C44C	C43C	1.3900
C5	C6	1.453(9)		C48C	C49C	1.192(8)
C6	C7	1.421(9)		C50C	C51C	1.524(4)
C6	C11	1.388(9)		C50C	C52C	1.525(4)
C7	C8	1.396(9)		C53C	C54C	1.522(4)
C8	C9	1.390(9)		C53C	C55C	1.523(4)
C9	C10	1.383(9)		C56C	C57C	1.526(4)
C10	C11	1.377(10)		C56C	C58C	1.524(4)
C12	C13	1.394(10)		C201	C202	1.367(9)
C12	C17	1.389(10)		C202	C203	1.393(9)
C13	C14	1.382(10)		C203	C204	1.394(10)
C14	C15	1.393(11)		C203	C212	1.464(10)
C15	C16	1.397(10)		C204	C205	1.385(9)
C15	C18A	1.381(10)		C205	C206	1.457(10)
C15	C18B	1.538(11)		C206	C207	1.422(10)
C16	C17	1.379(9)		C206	C211	1.400(9)
C18A	C19A	1.194(8)		C207	C208	1.406(10)
C18B	C19B	1.194(8)		C208	C209	1.374(10)
C20A	C21A	1.526(4)		C209	C210	1.384(10)
C20A	C22A	1.528(4)		C210	C211	1.369(10)
C23A	C24A	1.526(4)		C212	C213	1.386(9)
C23A	C25A	1.525(4)		C212	C217	1.403(10)

Table S12 continued. Selected bond lengths for **3**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
C23B	C24B	1.526(4)		C213	C214	1.354(10)
C23B	C25B	1.525(4)		C214	C215	1.369(10)
C26A	C27A	1.525(4)		C215	C216	1.391(10)
C26A	C28A	1.525(5)		C215	C218	1.427(11)
C26B	C27B	1.526(4)		C216	C217	1.390(10)
C26B	C28B	1.525(4)		C218	C219	1.203(11)
C31	C32	1.364(9)		C220	C221	1.525(4)
C32	C33	1.391(9)		C220	C222	1.525(4)
C33	C34	1.386(9)		C223	C224	1.523(4)
C33	C42	1.478(9)		C223	C225	1.525(4)
C34	C35	1.386(9)		C226	C227	1.530(4)
C35	C36	1.467(9)		C226	C228	1.526(4)
C36	C37	1.399(9)		C231	C232	1.370(11)
C36	C41	1.400(9)		C232	C233	1.384(11)
C37	C38	1.399(9)		C233	C234	1.393(9)
C38	C39	1.388(9)		C233	C242	1.618(10)
C39	C40	1.381(10)		C234	C235	1.370(9)
C40	C41	1.381(10)		C235	C236	1.464(9)
C42	C43	1.403(10)		C236	C237	1.402(9)
C42	C47	1.391(9)		C236	C241	1.391(9)
C43	C44	1.390(10)		C237	C238	1.409(9)
C44	C45	1.386(10)		C238	C239	1.385(9)
C45	C46	1.386(10)		C239	C240	1.373(10)
C45	C48A	1.553(10)		C240	C241	1.383(10)
C45	C48B	1.351(10)		C242	C247	1.3900
C46	C47	1.377(10)		C242	C243	1.3900
C48A	C49A	1.194(8)		C247	C246	1.3900
C48B	C49B	1.193(8)		C246	C245	1.3900
C50A	C51A	1.525(4)		C245	C244	1.3900
C50A	C52A	1.525(4)		C245	C248	1.446(10)
C50B	C51B	1.524(4)		C244	C243	1.3900
C50B	C52B	1.526(4)		C248	C249	1.193(8)
C53A	C54A	1.525(4)		C250	C251	1.524(4)
C53A	C55A	1.528(4)		C250	C252	1.525(4)
C53B	C54B	1.523(4)		C253	C254	1.524(4)
C53B	C55B	1.522(4)		C253	C255	1.526(4)
C56A	C57A	1.526(4)		C256	C257	1.527(4)
C56A	C58A	1.526(4)		C256	C258	1.525(4)
C56B	C57B	1.525(4)		C261	C262	1.379(10)
C56B	C58B	1.525(4)		C261	C265	1.506(10)
C61	C62	1.397(9)		C262	C263	1.398(10)
C61	C65	1.505(9)		C263	C264	1.506(10)
C62	C63	1.378(10)		Cl1	C1S	1.777(7)
C63	C64	1.509(10)		Cl1	C1SA	1.772(7)
Ir2	O21	2.152(5)		Cl2A	C1S	1.778(7)
Ir2	O22	2.141(5)		Cl2B	C1SA	1.775(7)
Ir2	N21	2.026(6)		Cl3A	C3S	1.776(7)
Ir2	N22	2.029(6)		Cl3B	C2S	1.775(6)
Ir2	C207	1.990(7)		Cl4A	C3S	1.778(7)
Ir2	C237	1.980(7)		Cl4B	C2S	1.776(6)
Si21	C20C	1.877(5)		Cl5	C4S	1.775(7)
Si21	C23C	1.879(5)		Cl6	C4S	1.773(7)

Table S12. Selected bond angles for **3**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Ir1	O2	87.36(17)		C237	Ir2	O22	174.1(2)
N1	Ir1	O1	94.91(19)		C237	Ir2	N21	93.9(2)
N1	Ir1	O2	90.26(19)		C237	Ir2	N22	80.4(3)
N1	Ir1	N2	175.7(2)		C237	Ir2	C207	92.2(3)
N2	Ir1	O1	86.22(19)		C20C	Si21	C23C	103.9(6)
N2	Ir1	O2	94.0(2)		C20C	Si21	C226	68.4(5)
C7	Ir1	O1	174.8(2)		C26C	Si21	C20C	116.0(6)
C7	Ir1	O2	93.2(2)		C26C	Si21	C23C	104.8(6)
C7	Ir1	N1	79.9(3)		C26C	Si21	C226	53.1(5)
C7	Ir1	N2	98.9(3)		C219	Si21	C20C	107.2(5)
C37	Ir1	O1	90.9(2)		C219	Si21	C23C	115.9(7)
C37	Ir1	O2	174.3(2)		C219	Si21	C26C	109.3(5)
C37	Ir1	N1	95.3(2)		C219	Si21	C220	103.5(4)
C37	Ir1	N2	80.5(2)		C219	Si21	C223	101.9(4)
C37	Ir1	C7	89.0(3)		C219	Si21	C226	103.2(5)
C19A	Si1A	C23A	108.2(6)		C220	Si21	C20C	48.1(6)
C19A	Si1A	C26A	104.7(8)		C220	Si21	C23C	62.4(6)
C20A	Si1A	C19A	108.8(6)		C220	Si21	C26C	147.0(6)
C20A	Si1A	C23A	107.0(5)		C220	Si21	C223	119.3(6)
C20A	Si1A	C26A	116.9(6)		C220	Si21	C226	115.8(5)
C26A	Si1A	C23A	110.9(7)		C223	Si21	C20C	150.4(5)
C19B	Si1B	C20A	102.8(6)		C223	Si21	C23C	56.9(6)
C19B	Si1B	C23B	110.0(7)		C223	Si21	C26C	57.4(5)
C19B	Si1B	C26B	106.5(7)		C223	Si21	C226	110.4(5)
C23B	Si1B	C20A	115.9(6)		C226	Si21	C23C	140.3(7)
C23B	Si1B	C26B	114.6(7)		C49C	Si22	C50C	105.7(7)
C26B	Si1B	C20A	106.0(5)		C49C	Si22	C53C	108.0(5)
C49A	Si2A	C50A	108.6(6)		C49C	Si22	C56C	109.2(8)
C49A	Si2A	C53A	106.2(6)		C53C	Si22	C50C	111.4(6)
C49A	Si2A	C56A	107.7(6)		C53C	Si22	C56C	112.3(5)
C50A	Si2A	C53A	110.4(5)		C56C	Si22	C50C	110.0(7)
C50A	Si2A	C56A	111.2(6)		C249	Si23	C250	106.9(6)
C56A	Si2A	C53A	112.5(5)		C249	Si23	C253	108.2(6)
C49B	Si2B	C50B	106.0(6)		C249	Si23	C256	107.9(7)
C49B	Si2B	C53B	108.2(7)		C253	Si23	C250	108.9(7)
C49B	Si2B	C56B	110.2(7)		C256	Si23	C250	110.9(6)
C53B	Si2B	C50B	123.1(8)		C256	Si23	C253	113.8(6)
C53B	Si2B	C56B	98.3(7)		C263	O21	Ir2	125.7(4)
C56B	Si2B	C50B	110.7(6)		C261	O22	Ir2	126.2(5)
C61	O1	Ir1	125.9(4)		C201	N21	Ir2	124.7(5)
C63	O2	Ir1	124.8(4)		C201	N21	C205	119.1(6)
C1	N1	Ir1	124.1(5)		C205	N21	Ir2	115.9(5)
C1	N1	C5	119.0(6)		C231	N22	Ir2	125.4(5)
C5	N1	Ir1	116.9(5)		C231	N22	C235	118.4(6)
C31	N2	Ir1	125.1(4)		C235	N22	Ir2	116.2(5)
C31	N2	C35	118.6(6)		C21C	C20C	Si21	118.0(10)
C35	N2	Ir1	116.1(5)		C21C	C20C	C22C	106.5(11)
N1	C1	C2	123.7(6)		C22C	C20C	Si21	110.6(8)
C1	C2	C3	119.1(7)		C24C	C23C	Si21	115.9(10)
C2	C3	C4	118.1(6)		C25C	C23C	Si21	114.5(11)
C2	C3	C12	119.9(7)		C25C	C23C	C24C	105.6(14)
C4	C3	C12	122.0(6)		C27C	C26C	Si21	117.6(11)
C3	C4	C5	119.7(6)		C27C	C26C	C227	110.0(11)
N1	C5	C4	120.4(6)		C227	C26C	Si21	108.7(5)

Table S12 continued. Selected bond angles for **3**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
N1	C5	C6	113.6(6)		C47C	C42C	C43C	120.0
C4	C5	C6	126.0(6)		C233	C42C	C47C	116.3(7)
C7	C6	C5	114.2(6)		C233	C42C	C43C	123.7(8)
C11	C6	C5	124.8(6)		C42C	C47C	C46C	120.0
C11	C6	C7	121.0(6)		C45C	C46C	C47C	120.0
C6	C7	Ir1	115.4(5)		C46C	C45C	C44C	120.0
C8	C7	Ir1	128.1(5)		C46C	C45C	C48C	117.7(9)
C8	C7	C6	116.5(6)		C44C	C45C	C48C	122.3(9)
C9	C8	C7	122.3(7)		C43C	C44C	C45C	120.0
C10	C9	C8	119.6(7)		C44C	C43C	C42C	120.0
C11	C10	C9	120.1(7)		C49C	C48C	C45C	175.7(16)
C10	C11	C6	120.5(7)		C48C	C49C	Si22	174.5(15)
C13	C12	C3	121.1(7)		C51C	C50C	Si22	114.0(11)
C17	C12	C3	120.9(6)		C51C	C50C	C52C	112.4(14)
C17	C12	C13	117.9(7)		C52C	C50C	Si22	112.1(11)
C14	C13	C12	120.5(7)		C54C	C53C	Si22	123.6(14)
C13	C14	C15	121.7(7)		C54C	C53C	C55C	119.9(15)
C14	C15	C16	117.6(7)		C55C	C53C	Si22	116.4(7)
C14	C15	C18B	122.8(8)		C57C	C56C	Si22	112.8(11)
C16	C15	C18B	118.3(8)		C58C	C56C	Si22	110.4(11)
C18A	C15	C14	119.4(9)		C58C	C56C	C57C	106.9(14)
C18A	C15	C16	121.7(9)		N21	C201	C202	122.7(7)
C18A	C15	C18B	23.0(7)		C201	C202	C203	120.7(7)
C17	C16	C15	120.7(7)		C202	C203	C204	115.5(7)
C16	C17	C12	121.6(7)		C202	C203	C212	122.8(7)
C19A	C18A	C15	172.3(17)		C204	C203	C212	121.7(6)
C19B	C18B	C15	167.9(16)		C205	C204	C203	122.7(7)
C18A	C19A	Si1A	178.1(16)		N21	C205	C204	119.2(7)
C18B	C19B	Si1B	174.6(15)		N21	C205	C206	113.6(6)
Si1A	C20A	Si1B	22.14(19)		C204	C205	C206	127.1(7)
C21A	C20A	Si1A	121.2(6)		C207	C206	C205	115.2(6)
C21A	C20A	Si1B	103.8(6)		C211	C206	C205	123.7(7)
C21A	C20A	C22A	110.2(8)		C211	C206	C207	121.2(7)
C22A	C20A	Si1A	114.0(7)		C206	C207	Ir2	113.9(5)
C22A	C20A	Si1B	113.4(7)		C208	C207	Ir2	129.6(6)
C24A	C23A	Si1A	114.1(9)		C208	C207	C206	116.4(7)
C25A	C23A	Si1A	115.7(9)		C209	C208	C207	121.5(8)
C25A	C23A	C24A	107.3(11)		C208	C209	C210	120.9(7)
C24B	C23B	Si1B	112.2(12)		C211	C210	C209	120.0(7)
C25B	C23B	Si1B	113.7(11)		C210	C211	C206	119.9(7)
C25B	C23B	C24B	107.9(14)		C213	C212	C203	123.8(7)
C27A	C26A	Si1A	110.3(10)		C213	C212	C217	116.9(7)
C28A	C26A	Si1A	116.1(11)		C217	C212	C203	119.2(6)
C28A	C26A	C27A	111.0(14)		C214	C213	C212	122.0(7)
C27B	C26B	Si1B	112.5(10)		C213	C214	C215	121.4(7)
C28B	C26B	Si1B	111.3(10)		C214	C215	C216	119.0(7)
C28B	C26B	C27B	110.6(12)		C214	C215	C218	119.5(7)
N2	C31	C32	122.5(6)		C216	C215	C218	121.3(7)
C31	C32	C33	120.7(7)		C217	C216	C215	119.6(7)
C32	C33	C42	120.4(6)		C216	C217	C212	121.1(7)
C34	C33	C32	116.4(6)		C219	C218	C215	178.8(9)
C34	C33	C42	123.2(6)		C218	C219	Si21	174.5(8)
C33	C34	C35	120.9(6)		C221	C220	Si21	107.6(8)
N2	C35	C34	120.8(6)		C222	C220	Si21	113.9(8)

Table S12 continued. Selected bond angles for **3**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
N2	C35	C36	112.7(6)		C222	C220	C221	113.7(11)
C34	C35	C36	126.4(6)		C224	C223	Si21	108.0(8)
C37	C36	C35	115.6(6)		C224	C223	C225	113.0(12)
C37	C36	C41	121.5(6)		C225	C223	Si21	110.4(9)
C41	C36	C35	122.9(6)		C227	C226	Si21	108.5(5)
C36	C37	Ir1	114.8(5)		C228	C226	Si21	113.6(8)
C36	C37	C38	117.1(6)		C228	C226	C227	114.5(10)
C38	C37	Ir1	128.0(5)		C26C	C227	C226	66.5(7)
C39	C38	C37	120.9(7)		N22	C231	C232	122.4(8)
C40	C39	C38	121.5(7)		C231	C232	C233	120.3(7)
C39	C40	C41	118.7(7)		C42C	C233	C232	115.3(8)
C40	C41	C36	120.2(7)		C42C	C233	C234	128.0(9)
C43	C42	C33	119.6(7)		C42C	C233	C242	14.5(6)
C47	C42	C33	122.5(7)		C232	C233	C234	116.6(7)
C47	C42	C43	117.9(7)		C232	C233	C242	127.1(7)
C44	C43	C42	120.3(7)		C234	C233	C242	116.1(8)
C45	C44	C43	120.8(7)		C235	C234	C233	121.8(7)
C44	C45	C46	118.9(7)		N22	C235	C234	120.3(6)
C44	C45	C48A	116.1(8)		N22	C235	C236	112.7(6)
C46	C45	C48A	124.4(8)		C234	C235	C236	127.0(7)
C48B	C45	C44	119.3(9)		C237	C236	C235	115.2(6)
C48B	C45	C46	120.1(10)		C241	C236	C235	122.8(7)
C48B	C45	C48A	21.0(8)		C241	C236	C237	122.0(6)
C47	C46	C45	120.6(7)		C236	C237	Ir2	114.6(5)
C46	C47	C42	121.3(7)		C236	C237	C238	116.6(6)
C49A	C48A	C45	173.8(16)		C238	C237	Ir2	128.7(5)
C49B	C48B	C45	171.1(17)		C239	C238	C237	121.5(7)
C48A	C49A	Si2A	175.4(14)		C240	C239	C238	120.1(7)
C48B	C49B	Si2B	170.4(14)		C239	C240	C241	120.6(7)
C51A	C50A	Si2A	113.7(8)		C240	C241	C236	119.2(7)
C51A	C50A	C52A	108.6(10)		C247	C242	C233	124.7(7)
C52A	C50A	Si2A	113.3(8)		C247	C242	C243	120.0
C51B	C50B	Si2B	113.2(10)		C243	C242	C233	115.3(7)
C51B	C50B	C52B	110.2(12)		C246	C247	C242	120.0
C52B	C50B	Si2B	113.4(9)		C247	C246	C245	120.0
C54A	C53A	Si2A	110.7(9)		C246	C245	C248	116.6(9)
C54A	C53A	C55A	95.7(11)		C244	C245	C246	120.0
C55A	C53A	Si2A	121.0(9)		C244	C245	C248	123.4(9)
C54B	C53B	Si2B	117.8(11)		C245	C244	C243	120.0
C55B	C53B	Si2B	119.5(11)		C244	C243	C242	120.0
C55B	C53B	C54B	117.6(13)		C249	C248	C245	175.6(17)
C57A	C56A	Si2A	113.1(8)		C248	C249	Si23	176.1(15)
C57A	C56A	C58A	110.0(11)		C251	C250	Si23	113.7(9)
C58A	C56A	Si2A	111.2(8)		C251	C250	C252	111.3(12)
C57B	C56B	Si2B	112.1(10)		C252	C250	Si23	112.1(9)
C58B	C56B	Si2B	109.5(9)		C254	C253	Si23	116.1(12)
C58B	C56B	C57B	112.2(14)		C254	C253	C255	110.4(13)
O1	C61	C62	126.8(7)		C255	C253	Si23	114.7(9)
O1	C61	C65	115.0(6)		C257	C256	Si23	109.9(10)
C62	C61	C65	118.2(6)		C258	C256	Si23	109.9(10)
C63	C62	C61	127.9(7)		C258	C256	C257	113.3(13)
O2	C63	C62	127.3(7)		O22	C261	C262	126.0(7)
O2	C63	C64	114.5(6)		O22	C261	C265	113.7(7)
C62	C63	C64	118.2(7)		C262	C261	C265	120.2(7)

Table S12 continued. Selected bond angles for **3**.

O22	Ir2	O21	86.80(18)		C261	C262	C263	127.8(7)
N21	Ir2	O21	93.0(2)		O21	C263	C262	126.6(7)
N21	Ir2	O22	91.8(2)		O21	C263	C264	114.8(6)
N21	Ir2	N22	174.1(2)		C262	C263	C264	118.6(7)
N22	Ir2	O21	88.6(2)		C1SA	Cl1	C1S	24.2(3)
N22	Ir2	O22	93.9(2)		Cl1	C1S	Cl2A	117.6(7)
C207	Ir2	O21	173.4(3)		Cl1	C1SA	Cl2B	100.7(6)
C207	Ir2	O22	90.3(2)		Cl3B	C2S	Cl4B	111.0(6)
C207	Ir2	N21	81.1(3)		Cl3A	C3S	Cl4A	108.0(7)
C207	Ir2	N22	97.5(3)		Cl6	C4S	Cl5	107.8(7)
C237	Ir2	O21	91.2(2)					

Table S13. Selected bond lengths for **4**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.143(2)		C34	C35	1.389(6)
Ir1	O2	2.141(2)		C35	C36	1.395(5)
Ir1	N1	2.034(3)		C35	C39	1.435(5)
Ir1	N2	2.039(3)		C36	C37	1.383(5)
Ir1	C7	1.994(3)		C39	C40	1.209(6)
Ir1	C27	1.998(3)		C41	C42	1.399(5)
Si1	C20	1.834(4)		C41	C45	1.519(5)
Si1	C51	1.902(4)		C42	C43	1.411(5)
Si1	C51A	1.885(4)		C43	C44	1.514(5)
Si1	C54	1.900(4)		C51	C52	1.529(5)
Si1	C54A	1.893(5)		C51	C53	1.530(4)
Si1	C57	1.885(4)		C51A	C52A	1.527(5)
Si1	C57A	1.900(5)		C51A	C53A	1.526(5)
Si2	C40	1.829(4)		C54	C55	1.528(4)
Si2	C61	1.886(5)		C54	C56	1.530(5)
Si2	C61A	1.897(5)		C54A	C55A	1.528(5)
Si2	C64	1.897(4)		C54A	C56A	1.526(5)
Si2	C67	1.916(4)		C57	C58	1.527(5)
Si2	C67A	1.890(5)		C57	C59	1.534(4)
O1	C41	1.269(4)		C57A	C58A	1.532(5)
O2	C43	1.258(4)		C57A	C59A	1.528(5)
N1	C1	1.343(4)		C61	C62	1.522(5)
N1	C5	1.373(4)		C61	C63	1.530(5)
N2	C21	1.347(4)		C61A	C62A	1.529(5)
N2	C25	1.368(4)		C61A	C63A	1.534(5)
C1	C2	1.386(5)		C64	C65	1.536(4)
C2	C3	1.390(5)		C64	C66	1.522(4)
C3	C4	1.392(5)		C64	C66A	1.525(5)
C3	C12	1.496(5)		C67	C68	1.537(5)
C4	C5	1.387(5)		C67	C69	1.530(4)
C5	C6	1.469(5)		C67A	C68A	1.526(5)
C6	C7	1.415(5)		C67A	C69A	1.527(5)
C6	C11	1.402(5)		C1S	C2S	1.387(8)
C7	C8	1.388(5)		C1S	C6S	1.375(8)
C8	C9	1.388(5)		C2S	C3S	1.380(8)
C9	C10	1.386(6)		C3S	C4S	1.359(7)
C10	C11	1.390(5)		C4S	C5S	1.362(6)
C12	C13	1.402(5)		C5S	C6S	1.359(7)
C12	C17	1.403(5)		C11S	C12S	1.360(12)
C13	C14	1.394(5)		C11S	C16S	1.357(10)
C13	C18	1.511(6)		C12S	C13S	1.375(12)
C14	C15	1.388(6)		C13S	C14S	1.383(11)
C15	C16	1.384(6)		C14S	C15S	1.342(11)
C15	C19	1.445(5)		C15S	C16S	1.390(9)
C16	C17	1.386(5)		C21S	C22S	1.375(7)
C19	C20	1.210(6)		C21S	C26S	1.375(7)
C21	C22	1.377(4)		C22S	C23S	1.379(7)
C22	C23	1.397(4)		C23S	C24S	1.374(8)
C23	C24	1.394(5)		C24S	C25S	1.384(8)
C23	C32	1.480(4)		C25S	C26S	1.372(7)
C24	C25	1.384(5)		C31S	C32S	1.385(8)
C25	C26	1.469(5)		C31S	C36S	1.358(7)
C26	C27	1.414(5)		C32S	C33S	1.364(8)
C26	C31	1.405(5)		C33S	C34S	1.382(7)

Table S13 continued. Selected bond lengths for **4**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
C27	C28	1.399(5)		C34S	C35S	1.368(7)
C28	C29	1.390(5)		C35S	C36S	1.388(7)
C29	C30	1.391(5)		C41S	C42S	1.360(10)
C30	C31	1.383(5)		C41S	C46S	1.361(9)
C32	C33	1.411(5)		C42S	C43S	1.369(9)
C32	C37	1.401(5)		C43S	C44S	1.371(10)
C33	C34	1.393(5)		C44S	C45S	1.367(10)
C33	C38	1.510(5)		C45S	C46S	1.353(9)

Table S14. Selected bond angles for **4**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O2	Ir1	O1	88.09(9)		N2	C25	C26	113.1(3)
N1	Ir1	O1	87.12(9)		C24	C25	C26	126.5(3)
N1	Ir1	O2	94.97(10)		C27	C26	C25	115.5(3)
N1	Ir1	N2	177.67(10)		C31	C26	C25	123.2(3)
N2	Ir1	O1	94.61(9)		C31	C26	C27	121.3(3)
N2	Ir1	O2	86.66(10)		C26	C27	Ir1	114.4(2)
C7	Ir1	O1	89.55(10)		C28	C27	Ir1	128.6(3)
C7	Ir1	O2	175.38(11)		C28	C27	C26	117.0(3)
C7	Ir1	N1	80.95(12)		C29	C28	C27	121.4(3)
C7	Ir1	N2	97.49(12)		C28	C29	C30	121.0(3)
C7	Ir1	C27	91.97(12)		C31	C30	C29	119.2(3)
C27	Ir1	O1	175.23(11)		C30	C31	C26	120.1(3)
C27	Ir1	O2	90.69(11)		C33	C32	C23	122.8(3)
C27	Ir1	N1	97.58(12)		C37	C32	C23	117.9(3)
C27	Ir1	N2	80.72(12)		C37	C32	C33	119.3(3)
C20	Si1	C51	107.0(3)		C32	C33	C38	124.0(3)
C20	Si1	C51A	107.6(3)		C34	C33	C32	118.2(3)
C20	Si1	C54	107.1(3)		C34	C33	C38	117.8(3)
C20	Si1	C54A	106.1(4)		C35	C34	C33	122.4(3)
C20	Si1	C57	115.3(3)		C34	C35	C36	118.9(3)
C20	Si1	C57A	102.3(4)		C34	C35	C39	119.6(4)
C51A	Si1	C51	17.7(4)		C36	C35	C39	121.5(4)
C51A	Si1	C54	87.4(4)		C37	C36	C35	119.8(4)
C51A	Si1	C54A	116.4(5)		C36	C37	C32	121.4(3)
C51A	Si1	C57	122.8(4)		C40	C39	C35	177.7(6)
C51A	Si1	C57A	112.0(6)		C39	C40	Si2	176.2(5)
C54	Si1	C51	104.2(3)		O1	C41	C42	126.6(3)
C54	Si1	C57A	137.6(5)		O1	C41	C45	114.8(3)
C54A	Si1	C51	131.3(4)		C42	C41	C45	118.6(3)
C54A	Si1	C54	31.2(4)		C41	C42	C43	127.0(3)
C54A	Si1	C57A	111.1(5)		O2	C43	C42	127.4(3)
C57	Si1	C51	109.9(3)		O2	C43	C44	115.2(3)
C57	Si1	C54	112.5(4)		C42	C43	C44	117.4(3)
C57	Si1	C54A	86.3(4)		C52	C51	Si1	118.1(6)
C57	Si1	C57A	25.3(4)		C52	C51	C53	105.0(7)
C57A	Si1	C51	95.4(5)		C53	C51	Si1	113.2(5)
C40	Si2	C61	108.4(3)		C52A	C51A	Si1	105.1(7)
C40	Si2	C61A	104.3(6)		C53A	C51A	Si1	107.7(8)
C40	Si2	C64	108.1(3)		C53A	C51A	C52A	112.1(11)
C40	Si2	C67	104.8(3)		C55	C54	Si1	118.3(6)
C40	Si2	C67A	110.8(4)		C55	C54	C56	109.9(8)
C61	Si2	C61A	22.5(5)		C56	C54	Si1	110.5(6)
C61	Si2	C64	123.4(4)		C55A	C54A	Si1	108.2(7)
C61	Si2	C67	109.2(4)		C56A	C54A	Si1	116.2(10)
C61	Si2	C67A	79.9(7)		C56A	C54A	C55A	108.7(11)
C61A	Si2	C64	106.3(5)		C58	C57	Si1	111.2(7)
C61A	Si2	C67	130.5(6)		C58	C57	C59	108.8(8)
C64	Si2	C67	101.4(3)		C59	C57	Si1	111.7(5)
C67A	Si2	C61A	101.9(8)		C58A	C57A	Si1	115.2(9)
C67A	Si2	C64	123.4(7)		C59A	C57A	Si1	115.0(10)
C67A	Si2	C67	29.7(6)		C59A	C57A	C58A	103.9(13)
C41	O1	Ir1	124.6(2)		C62	C61	Si2	118.3(8)
C43	O2	Ir1	124.2(2)		C62	C61	C63	115.2(9)
C1	N1	Ir1	124.5(2)		C63	C61	Si2	107.7(6)

Table S14 continued. Selected bond angles for **4**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C1	N1	C5	119.5(3)		C62A	C61A	Si2	106.2(17)
C5	N1	Ir1	116.0(2)		C62A	C61A	C63A	129(2)
C21	N2	Ir1	125.0(2)		C63A	C61A	Si2	102.1(9)
C21	N2	C25	118.7(3)		C65	C64	Si2	105.6(6)
C25	N2	Ir1	116.2(2)		C66	C64	Si2	120.8(5)
N1	C1	C2	122.4(3)		C66	C64	C65	113.3(7)
C1	C2	C3	119.5(3)		C66	C64	C66A	106.6(13)
C2	C3	C4	117.7(3)		C66A	C64	Si2	112.9(13)
C2	C3	C12	120.5(3)		C66A	C64	C65	94.7(13)
C4	C3	C12	121.8(3)		C68	C67	Si2	106.8(6)
C5	C4	C3	121.4(3)		C69	C67	Si2	119.5(5)
N1	C5	C4	119.5(3)		C69	C67	C68	107.3(8)
N1	C5	C6	112.6(3)		C68A	C67A	Si2	115.4(7)
C4	C5	C6	127.8(3)		C68A	C67A	C69A	121.6(12)
C7	C6	C5	115.9(3)		C69A	C67A	Si2	111.6(9)
C11	C6	C5	122.8(3)		C6S	C1S	C2S	119.5(4)
C11	C6	C7	121.2(3)		C3S	C2S	C1S	119.4(5)
C6	C7	Ir1	113.6(2)		C4S	C3S	C2S	120.3(5)
C8	C7	Ir1	128.5(3)		C3S	C4S	C5S	120.0(4)
C8	C7	C6	117.8(3)		C6S	C5S	C4S	121.0(5)
C9	C8	C7	121.2(3)		C5S	C6S	C1S	119.9(5)
C10	C9	C8	120.5(3)		C16S	C11S	C12S	121.2(7)
C9	C10	C11	120.2(3)		C11S	C12S	C13S	121.5(8)
C10	C11	C6	119.0(3)		C12S	C13S	C14S	116.7(8)
C13	C12	C3	123.2(3)		C15S	C14S	C13S	122.0(8)
C13	C12	C17	118.8(3)		C14S	C15S	C16S	120.5(7)
C17	C12	C3	118.0(3)		C11S	C16S	C15S	118.0(8)
C12	C13	C18	123.2(3)		C26S	C21S	C22S	120.7(5)
C14	C13	C12	118.6(4)		C21S	C22S	C23S	119.1(5)
C14	C13	C18	118.2(4)		C24S	C23S	C22S	120.6(5)
C15	C14	C13	122.3(4)		C23S	C24S	C25S	119.8(5)
C14	C15	C19	120.1(4)		C26S	C25S	C24S	119.7(5)
C16	C15	C14	118.8(4)		C25S	C26S	C21S	120.1(5)
C16	C15	C19	121.0(4)		C36S	C31S	C32S	120.4(5)
C15	C16	C17	119.9(4)		C33S	C32S	C31S	119.4(5)
C16	C17	C12	121.4(4)		C32S	C33S	C34S	120.6(5)
C20	C19	C15	179.0(5)		C35S	C34S	C33S	119.6(5)
C19	C20	Si1	179.5(5)		C34S	C35S	C36S	119.9(5)
N2	C21	C22	122.8(3)		C31S	C36S	C35S	120.0(5)
C21	C22	C23	119.6(3)		C42S	C41S	C46S	120.1(7)
C22	C23	C32	120.0(3)		C41S	C42S	C43S	120.1(6)
C24	C23	C22	117.2(3)		C42S	C43S	C44S	119.5(7)
C24	C23	C32	122.8(3)		C45S	C44S	C43S	119.6(7)
C25	C24	C23	121.3(3)		C46S	C45S	C44S	120.5(6)
N2	C25	C24	120.3(3)		C45S	C46S	C41S	120.0(7)

Table S15. Selected bond lengths for **7**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.144(5)		C24	C25	1.379(11)
Ir1	O2	2.145(6)		C25	C26	1.376(11)
Ir1	N1	2.026(6)		C25	C28	1.554(10)
Ir1	N2	2.018(6)		C26	C27	1.398(10)
Ir1	C7	1.976(8)		C28	C29	1.546(12)
Ir1	C47	1.985(8)		C28	C30	1.543(11)
O1	C1A	1.270(10)		C28	C31	1.507(11)
O2	C3A	1.269(10)		C41	C42	1.371(9)
N1	C1	1.359(9)		C42	C43	1.392(10)
N1	C5	1.388(9)		C43	C44	1.384(11)
N2	C41	1.333(9)		C43	C52	1.448(10)
N2	C45	1.402(9)		C44	C45	1.388(9)
C1	C2	1.364(9)		C45	C46	1.445(10)
C1A	C2A	1.382(12)		C46	C47	1.417(9)
C1A	C5A	1.490(11)		C46	C51	1.387(10)
C2	C3	1.432(10)		C47	C48	1.398(10)
C2A	C3A	1.393(12)		C48	C49	1.374(10)
C3	C4	1.455(11)		C49	C50	1.391(10)
C3	C12	1.458(10)		C50	C51	1.400(11)
C3A	C4A	1.499(11)		C52	C53	1.168(10)
C4	C5	1.373(9)		C53	C54	1.453(11)
C5	C6	1.425(10)		C54	C55	1.380(12)
C6	C7	1.432(9)		C54	C59	1.391(12)
C6	C11	1.408(10)		C55	C56	1.403(11)
C7	C8	1.414(11)		C56	C57	1.384(13)
C8	C9	1.371(10)		C57	C58	1.358(13)
C9	C10	1.384(10)		C57	C60	1.451(11)
C10	C11	1.378(10)		C58	C59	1.393(11)
C12	C13	1.173(9)		C60	C61	1.193(10)
C13	C14	1.456(10)		C61	C62	1.449(11)
C14	C15	1.393(10)		C62	C63	1.371(12)
C14	C19	1.371(11)		C62	C67	1.377(12)
C15	C16	1.387(10)		C63	C64	1.385(10)
C16	C17	1.367(11)		C64	C65	1.344(10)
C17	C18	1.375(11)		C65	C66	1.388(11)
C17	C20	1.428(10)		C65	C68	1.528(9)
C18	C19	1.391(9)		C66	C67	1.377(10)
C20	C21	1.208(9)		C68	C69	1.537(10)
C21	C22	1.440(10)		C68	C70	1.531(11)
C22	C23	1.383(12)		C68	C71	1.518(11)
C22	C27	1.353(11)		Cl1	C1S	1.733(10)
C23	C24	1.404(10)		Cl2	C1S	1.718(9)

Table S16. Selected bond angles for **7**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Ir1	O2	87.8(2)		C27	C22	C23	118.7(8)
N1	Ir1	O1	91.3(2)		C22	C23	C24	120.4(9)
N1	Ir1	O2	93.1(2)		C25	C24	C23	120.6(9)
N2	Ir1	O1	93.8(2)		C24	C25	C28	122.0(8)
N2	Ir1	O2	88.3(2)		C26	C25	C24	118.1(7)
N2	Ir1	N1	174.7(2)		C26	C25	C28	119.8(8)
C7	Ir1	O1	88.0(3)		C25	C26	C27	120.9(9)
C7	Ir1	O2	172.9(2)		C22	C27	C26	121.2(9)
C7	Ir1	N1	81.3(3)		C29	C28	C25	111.0(7)
C7	Ir1	N2	97.7(3)		C30	C28	C25	108.5(6)
C7	Ir1	C47	90.9(3)		C30	C28	C29	109.9(7)
C47	Ir1	O1	174.6(2)		C31	C28	C25	110.7(7)
C47	Ir1	O2	93.7(3)		C31	C28	C29	108.6(7)
C47	Ir1	N1	93.8(3)		C31	C28	C30	108.1(7)
C47	Ir1	N2	81.1(3)		N2	C41	C42	123.7(8)
C1A	O1	Ir1	126.4(6)		C41	C42	C43	119.8(8)
C3A	O2	Ir1	124.2(6)		C42	C43	C52	121.3(8)
C1	N1	Ir1	125.1(5)		C44	C43	C42	117.6(7)
C1	N1	C5	119.0(6)		C44	C43	C52	121.1(8)
C5	N1	Ir1	115.8(5)		C43	C44	C45	121.2(7)
C41	N2	Ir1	127.0(5)		N2	C45	C46	113.6(6)
C41	N2	C45	117.7(6)		C44	C45	N2	119.9(7)
C45	N2	Ir1	115.3(5)		C44	C45	C46	126.4(7)
N1	C1	C2	124.6(8)		C47	C46	C45	114.9(7)
O1	C1A	C2A	125.3(9)		C51	C46	C45	123.7(7)
O1	C1A	C5A	113.9(9)		C51	C46	C47	121.4(8)
C2A	C1A	C5A	120.8(9)		C46	C47	Ir1	115.1(6)
C1	C2	C3	116.0(8)		C48	C47	Ir1	128.7(5)
C1A	C2A	C3A	128.5(9)		C48	C47	C46	116.1(7)
C2	C3	C4	121.4(7)		C49	C48	C47	122.7(8)
C2	C3	C12	118.4(8)		C48	C49	C50	120.9(8)
C4	C3	C12	120.1(7)		C49	C50	C51	118.0(8)
O2	C3A	C2A	127.7(9)		C46	C51	C50	120.9(7)
O2	C3A	C4A	115.4(9)		C53	C52	C43	177.9(11)
C2A	C3A	C4A	116.9(9)		C52	C53	C54	176.8(11)
C5	C4	C3	116.3(7)		C55	C54	C53	119.5(9)
N1	C5	C6	112.5(6)		C55	C54	C59	119.5(8)
C4	C5	N1	122.6(8)		C59	C54	C53	121.0(9)
C4	C5	C6	124.9(7)		C54	C55	C56	119.4(10)
C5	C6	C7	117.0(7)		C57	C56	C55	120.7(10)
C11	C6	C5	123.2(7)		C56	C57	C60	119.5(10)
C11	C6	C7	119.8(8)		C58	C57	C56	119.4(9)
C6	C7	Ir1	113.2(6)		C58	C57	C60	121.1(10)
C8	C7	Ir1	129.9(5)		C57	C58	C59	121.0(10)
C8	C7	C6	116.8(7)		C54	C59	C58	119.9(10)
C9	C8	C7	121.9(7)		C61	C60	C57	179.2(12)
C8	C9	C10	120.9(8)		C60	C61	C62	178.2(11)
C11	C10	C9	119.7(7)		C63	C62	C61	121.9(10)
C10	C11	C6	120.9(7)		C63	C62	C67	118.3(8)
C13	C12	C3	174.5(9)		C67	C62	C61	119.8(10)
C12	C13	C14	174.7(9)		C62	C63	C64	120.1(9)
C15	C14	C13	119.3(8)		C65	C64	C63	123.1(9)
C19	C14	C13	121.7(8)		C64	C65	C66	116.0(7)
C19	C14	C15	119.0(7)		C64	C65	C68	123.0(8)

Table S17 continued. Selected bond angles for **7**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C16	C15	C14	120.1(8)		C66	C65	C68	120.9(8)
C17	C16	C15	121.0(8)		C67	C66	C65	122.5(9)
C16	C17	C18	118.4(7)		C62	C67	C66	119.8(9)
C16	C17	C20	120.5(8)		C65	C68	C69	109.5(7)
C18	C17	C20	121.1(8)		C65	C68	C70	111.0(7)
C17	C18	C19	121.5(8)		C70	C68	C69	107.6(7)
C14	C19	C18	119.8(8)		C71	C68	C65	110.1(7)
C21	C20	C17	178.2(10)		C71	C68	C69	111.5(7)
C20	C21	C22	178.5(9)		C71	C68	C70	107.1(7)
C23	C22	C21	120.8(9)		Cl2	C1S	Cl1	111.3(5)
C27	C22	C21	120.4(8)					

Table S18. Selected bond lengths for **12**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.149(4)		C30	C32	1.503(9)
Ir1	O2	2.145(4)		C30	C33	1.508(9)
Ir1	N1	2.026(4)		C41	C42	1.380(6)
Ir1	N2	2.029(4)		C42	C43	1.381(7)
Ir1	C7	1.988(5)		C43	C44	1.389(7)
Ir1	C47	2.002(5)		C43	C52	1.488(6)
O1	C2A	1.256(7)		C44	C45	1.390(6)
O2	C4A	1.256(7)		C45	C46	1.457(7)
N1	C1	1.341(6)		C46	C47	1.410(6)
N1	C5	1.364(6)		C46	C51	1.400(7)
N2	C41	1.346(6)		C47	C48	1.397(7)
N2	C45	1.352(6)		C48	C49	1.381(8)
C1	C2	1.370(6)		C49	C50	1.382(7)
C1A	C2A	1.495(8)		C50	C51	1.363(7)
C2	C3	1.391(7)		C52	C53	1.394(7)
C2A	C3A	1.417(8)		C52	C57	1.411(7)
C3	C4	1.386(7)		C53	C54	1.391(7)
C3	C12	1.494(6)		C53	C58	1.501(8)
C3A	C4A	1.395(8)		C54	C55	1.408(8)
C4	C5	1.394(6)		C54	C59	1.503(8)
C4A	C5A	1.506(8)		C55	C56	1.410(8)
C5	C6	1.463(7)		C55	C62	1.425(7)
C6	C7	1.419(6)		C56	C57	1.394(7)
C6	C11	1.379(8)		C56	C60	1.507(8)
C7	C8	1.386(7)		C57	C61	1.497(7)
C8	C9	1.376(8)		C62	C63	1.208(7)
C9	C10	1.386(8)		C63	C64	1.427(7)
C10	C11	1.394(8)		C64	C65	1.412(8)
C12	C13	1.401(8)		C64	C69	1.371(8)
C12	C17	1.408(7)		C65	C66	1.371(7)
C13	C14	1.397(6)		C66	C67	1.396(8)
C13	C18	1.520(8)		C67	C68	1.382(8)
C14	C15	1.397(7)		C67	C70	1.525(7)
C14	C19	1.504(8)		C68	C69	1.388(7)
C15	C16	1.400(7)		C70	C71	1.527(11)
C15	C22	1.451(6)		C70	C72	1.532(12)
C16	C17	1.392(6)		C70	C73	1.529(11)
C16	C20	1.510(7)		Cl1	C1S	1.739(5)
C17	C21	1.512(7)		Cl2	C1S	1.734(5)
C22	C23	1.190(7)		Cl2A	C1S	1.742(5)
C23	C24	1.441(6)		Cl3	C2S	1.733(5)
C24	C25	1.389(7)		Cl3	C2SA	1.735(6)
C24	C29	1.393(7)		Cl4	C2S	1.729(5)
C25	C26	1.376(7)		Cl4A	C2SA	1.732(6)
C26	C27	1.395(7)		Cl5	C3SA	1.736(6)
C27	C28	1.397(7)		Cl5	C3SB	1.735(6)
C27	C30	1.528(6)		Cl6	C3SA[1]	1.738(6)
C28	C29	1.378(6)		Cl6	C3SA	1.738(6)
C30	C31	1.549(9)		Cl6A	C3SB	1.732(6)

Table S19. Selected bond angles for **12**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O2	Ir1	O1	87.93(14)		C26	C27	C30	123.0(5)
N1	Ir1	O1	95.73(14)		C28	C27	C30	120.3(4)
N1	Ir1	O2	85.86(15)		C29	C28	C27	122.0(5)
N1	Ir1	N2	177.78(16)		C28	C29	C24	120.8(5)
N2	Ir1	O1	85.43(14)		C27	C30	C31	110.0(5)
N2	Ir1	O2	96.08(15)		C32	C30	C27	113.1(5)
C7	Ir1	O1	176.38(16)		C32	C30	C31	107.1(6)
C7	Ir1	O2	91.90(17)		C32	C30	C33	109.0(6)
C7	Ir1	N1	80.65(17)		C33	C30	C27	110.0(5)
C7	Ir1	N2	98.18(17)		C33	C30	C31	107.5(6)
C7	Ir1	C47	88.01(19)		N2	C41	C42	121.8(5)
C47	Ir1	O1	92.37(16)		C41	C42	C43	120.4(5)
C47	Ir1	O2	176.56(16)		C42	C43	C44	117.1(4)
C47	Ir1	N1	97.52(17)		C42	C43	C52	120.0(4)
C47	Ir1	N2	80.53(17)		C44	C43	C52	123.0(4)
C2A	O1	Ir1	125.4(4)		C43	C44	C45	121.1(4)
C4A	O2	Ir1	125.2(4)		N2	C45	C44	120.3(4)
C1	N1	Ir1	124.2(3)		N2	C45	C46	113.8(4)
C1	N1	C5	119.2(4)		C44	C45	C46	125.9(4)
C5	N1	Ir1	116.6(3)		C47	C46	C45	115.2(4)
C41	N2	Ir1	124.4(3)		C51	C46	C45	123.7(4)
C41	N2	C45	119.3(4)		C51	C46	C47	121.1(4)
C45	N2	Ir1	116.1(3)		C46	C47	Ir1	114.1(3)
N1	C1	C2	122.6(5)		C48	C47	Ir1	129.1(4)
C1	C2	C3	119.9(5)		C48	C47	C46	116.8(4)
O1	C2A	C1A	115.4(5)		C49	C48	C47	121.2(5)
O1	C2A	C3A	126.3(5)		C48	C49	C50	121.1(5)
C3A	C2A	C1A	118.2(6)		C51	C50	C49	119.4(5)
C2	C3	C12	121.4(4)		C50	C51	C46	120.4(5)
C4	C3	C2	117.6(4)		C53	C52	C43	119.2(4)
C4	C3	C12	121.0(4)		C53	C52	C57	121.2(4)
C4A	C3A	C2A	127.3(6)		C57	C52	C43	119.6(4)
C3	C4	C5	120.8(5)		C52	C53	C58	121.2(4)
O2	C4A	C3A	127.1(5)		C54	C53	C52	119.6(5)
O2	C4A	C5A	115.6(5)		C54	C53	C58	119.1(5)
C3A	C4A	C5A	117.3(6)		C53	C54	C55	119.7(5)
N1	C5	C4	120.0(4)		C53	C54	C59	120.5(5)
N1	C5	C6	113.1(4)		C55	C54	C59	119.8(5)
C4	C5	C6	126.9(4)		C54	C55	C56	120.4(4)
C7	C6	C5	115.0(4)		C54	C55	C62	119.8(5)
C11	C6	C5	123.5(4)		C56	C55	C62	119.8(5)
C11	C6	C7	121.5(5)		C55	C56	C60	120.3(5)
C6	C7	Ir1	114.6(4)		C57	C56	C55	119.8(5)
C8	C7	Ir1	128.6(4)		C57	C56	C60	119.9(5)
C8	C7	C6	116.8(5)		C52	C57	C61	122.0(4)
C9	C8	C7	122.3(5)		C56	C57	C52	118.9(5)
C8	C9	C10	120.1(5)		C56	C57	C61	119.1(5)
C9	C10	C11	119.6(6)		C63	C62	C55	179.4(7)
C6	C11	C10	119.8(5)		C62	C63	C64	179.5(7)
C13	C12	C3	119.2(5)		C65	C64	C63	120.3(5)
C13	C12	C17	121.1(4)		C69	C64	C63	121.6(5)
C17	C12	C3	119.7(5)		C69	C64	C65	117.9(5)
C12	C13	C18	121.5(4)		C66	C65	C64	120.5(5)
C14	C13	C12	119.3(5)		C65	C66	C67	121.5(5)

Table S19 continued. Selected bond angles for **12**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C14	C13	C18	119.3(5)		C66	C67	C70	119.6(5)
C13	C14	C19	119.2(5)		C68	C67	C66	117.3(5)
C15	C14	C13	119.4(5)		C68	C67	C70	123.1(5)
C15	C14	C19	121.4(4)		C67	C68	C69	121.6(5)
C14	C15	C16	121.6(4)		C64	C69	C68	121.0(5)
C14	C15	C22	118.4(5)		C67	C70	C71	109.6(6)
C16	C15	C22	120.0(5)		C67	C70	C72	108.6(6)
C15	C16	C20	120.4(4)		C67	C70	C73	111.2(6)
C17	C16	C15	119.1(5)		C71	C70	C72	109.0(6)
C17	C16	C20	120.5(5)		C71	C70	C73	109.3(8)
C12	C17	C21	120.6(4)		C73	C70	C72	109.2(8)
C16	C17	C12	119.5(5)		Cl1	C1S	Cl2A	129.3(7)
C16	C17	C21	119.8(5)		Cl2	C1S	Cl1	107.2(4)
C23	C22	C15	177.6(6)		Cl2	C1S	Cl2A	81.9(5)
C22	C23	C24	178.4(5)		C2S	Cl3	C2SA	45.6(11)
C25	C24	C23	121.8(4)		Cl4	C2S	Cl3	105.1(5)
C25	C24	C29	117.7(4)		Cl4A	C2SA	Cl3	118.7(9)
C29	C24	C23	120.6(5)		C3SB	Cl5	C3SA	17.8(7)
C26	C25	C24	121.4(5)		C3SA[1]	Cl6	C3SA	179.999(7)
C25	C26	C27	121.6(5)		Cl5	C3SA	Cl6	117.2(6)
C26	C27	C28	116.6(4)		Cl6A	C3SB	Cl5	116.4(8)

Table S20. Selected bond lengths for **13**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Ir1	O1	2.162(4)		C36	C37	1.382(8)
Ir1	O2	2.164(4)		C38	C39	1.519(9)
Ir1	N1	2.035(4)		C38	C40	1.581(12)
Ir1	N2	2.042(4)		C38	C41	1.512(11)
Ir1	C7	2.004(6)		C51	C52	1.383(7)
Ir1	C57	1.992(5)		C52	C53	1.404(7)
O1	C1A	1.224(7)		C53	C54	1.389(7)
O2	C3A	1.254(7)		C53	C62	1.499(7)
N1	C1	1.340(6)		C54	C55	1.389(7)
N1	C5	1.369(7)		C55	C56	1.460(7)
N2	C51	1.341(7)		C56	C57	1.412(7)
N2	C55	1.359(6)		C56	C61	1.400(7)
C1	C2	1.386(7)		C57	C58	1.387(7)
C1A	C2A	1.440(10)		C58	C59	1.400(7)
C1A	C5A	1.512(9)		C59	C60	1.375(7)
C2	C3	1.396(8)		C60	C61	1.380(8)
C2A	C3A	1.387(9)		C62	C63	1.394(7)
C3	C4	1.379(7)		C62	C67	1.407(7)
C3	C12	1.496(7)		C63	C64	1.401(7)
C3A	C4A	1.508(9)		C63	C68	1.513(7)
C4	C5	1.378(7)		C64	C65	1.399(8)
C5	C6	1.476(7)		C64	C69	1.505(8)
C6	C7	1.417(7)		C65	C66	1.411(8)
C6	C11	1.379(8)		C65	C72	1.438(7)
C7	C8	1.379(7)		C66	C67	1.407(7)
C8	C9	1.378(9)		C66	C70	1.482(8)
C9	C10	1.359(9)		C67	C71	1.498(7)
C10	C11	1.384(8)		C72	C73	1.195(7)
C12	C13	1.386(7)		C73	C74	1.446(7)
C12	C17	1.406(8)		C74	C75	1.376(9)
C13	C14	1.404(7)		C74	C79	1.380(8)
C13	C18	1.520(8)		C75	C76	1.387(8)
C14	C15	1.398(7)		C76	C77	1.378(9)
C14	C19	1.511(8)		C77	C78	1.385(10)
C15	C16	1.405(8)		C77	C80	1.453(8)
C15	C22	1.439(7)		C78	C79	1.384(8)
C16	C17	1.403(7)		C80	C81	1.208(9)
C16	C20	1.506(8)		C81	C82	1.434(9)
C17	C21	1.505(8)		C82	C83	1.370(10)
C22	C23	1.194(7)		C82	C87	1.388(9)
C23	C24	1.448(7)		C83	C84	1.397(9)
C24	C25	1.388(9)		C84	C85	1.388(9)
C24	C29	1.371(9)		C85	C86	1.390(9)
C25	C26	1.398(8)		C85	C88	1.536(8)
C26	C27	1.384(9)		C86	C87	1.380(8)
C27	C28	1.371(10)		C88	C89	1.539(11)
C27	C30	1.431(7)		C88	C90	1.524(10)
C28	C29	1.386(8)		C88	C91	1.511(10)
C30	C31	1.207(8)		Cl1	C1S	1.723(9)
C31	C32	1.438(8)		Cl2A	C1S	1.793(8)
C32	C33	1.397(9)		Cl2B	C1S	1.789(8)
C32	C37	1.393(10)		Cl3	C2S	1.752(7)
C33	C34	1.384(8)		Cl4	C2S	1.744(7)
C34	C35	1.379(10)		Cl5	C3S	1.749(5)

Table S20 continued. Selected bond lengths for **13**.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
C35	C36	1.411(10)		Cl6	C3S	1.733(5)
C35	C38	1.529(8)				

Table S21. Selected bond angles for **13**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Ir1	O2	88.11(15)		C35	C34	C33	122.4(6)
N1	Ir1	O1	88.47(16)		C34	C35	C36	117.2(5)
N1	Ir1	O2	94.25(16)		C34	C35	C38	120.3(6)
N1	Ir1	N2	173.11(17)		C36	C35	C38	122.5(6)
N2	Ir1	O1	95.31(16)		C37	C36	C35	120.7(7)
N2	Ir1	O2	91.63(16)		C36	C37	C32	121.4(7)
C7	Ir1	O1	91.44(18)		C35	C38	C40	111.7(6)
C7	Ir1	O2	175.08(17)		C39	C38	C35	110.1(5)
C7	Ir1	N1	80.84(19)		C39	C38	C40	107.2(6)
C7	Ir1	N2	93.29(19)		C41	C38	C35	108.2(6)
C57	Ir1	O1	175.51(18)		C41	C38	C39	111.8(7)
C57	Ir1	O2	89.84(18)		C41	C38	C40	108.0(7)
C57	Ir1	N1	95.67(19)		N2	C51	C52	122.3(5)
C57	Ir1	N2	80.75(19)		C51	C52	C53	119.1(5)
C57	Ir1	C7	90.9(2)		C52	C53	C62	120.8(5)
C1A	O1	Ir1	125.1(4)		C54	C53	C52	117.9(4)
C3A	O2	Ir1	124.9(4)		C54	C53	C62	121.3(5)
C1	N1	Ir1	124.5(4)		C53	C54	C55	120.6(5)
C1	N1	C5	119.0(4)		N2	C55	C54	120.3(5)
C5	N1	Ir1	116.5(3)		N2	C55	C56	113.6(4)
C51	N2	Ir1	124.3(3)		C54	C55	C56	126.1(5)
C51	N2	C55	119.7(4)		C57	C56	C55	115.4(4)
C55	N2	Ir1	115.6(3)		C61	C56	C55	123.7(4)
N1	C1	C2	122.0(5)		C61	C56	C57	120.9(5)
O1	C1A	C2A	126.9(5)		C56	C57	Ir1	114.3(4)
O1	C1A	C5A	115.6(6)		C58	C57	Ir1	127.8(4)
C2A	C1A	C5A	117.5(6)		C58	C57	C56	117.9(5)
C1	C2	C3	119.6(5)		C57	C58	C59	120.9(5)
C3A	C2A	C1A	128.1(6)		C60	C59	C58	120.4(5)
C2	C3	C12	119.5(5)		C59	C60	C61	120.2(5)
C4	C3	C2	117.6(5)		C60	C61	C56	119.7(5)
C4	C3	C12	122.9(5)		C63	C62	C53	119.7(4)
O2	C3A	C2A	126.8(6)		C63	C62	C67	122.0(4)
O2	C3A	C4A	114.8(6)		C67	C62	C53	118.3(5)
C2A	C3A	C4A	118.4(6)		C62	C63	C64	119.3(5)
C5	C4	C3	121.0(5)		C62	C63	C68	120.4(4)
N1	C5	C4	120.7(5)		C64	C63	C68	120.3(5)
N1	C5	C6	112.9(4)		C63	C64	C69	120.3(5)
C4	C5	C6	126.3(5)		C65	C64	C63	119.3(5)
C7	C6	C5	115.4(5)		C65	C64	C69	120.4(5)
C11	C6	C5	122.8(5)		C64	C65	C66	121.7(5)
C11	C6	C7	121.7(5)		C64	C65	C72	118.8(5)
C6	C7	Ir1	114.2(4)		C66	C65	C72	119.4(5)
C8	C7	Ir1	129.2(4)		C65	C66	C70	119.9(5)
C8	C7	C6	116.6(5)		C67	C66	C65	118.8(5)
C9	C8	C7	121.1(5)		C67	C66	C70	121.2(5)
C10	C9	C8	121.9(5)		C62	C67	C71	122.0(5)
C9	C10	C11	119.0(6)		C66	C67	C62	118.9(5)
C6	C11	C10	119.6(6)		C66	C67	C71	119.1(5)
C13	C12	C3	120.2(5)		C73	C72	C65	177.9(6)
C13	C12	C17	121.8(5)		C72	C73	C74	172.3(6)
C17	C12	C3	118.0(5)		C75	C74	C73	118.5(5)
C12	C13	C14	119.8(5)		C75	C74	C79	119.0(5)
C12	C13	C18	121.0(5)		C79	C74	C73	122.5(6)

Table S21 continued. Selected bond angles for **13**.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C14	C13	C18	119.2(5)		C74	C75	C76	121.1(6)
C13	C14	C19	121.3(5)		C77	C76	C75	119.9(7)
C15	C14	C13	118.7(5)		C76	C77	C78	119.0(6)
C15	C14	C19	119.9(5)		C76	C77	C80	119.1(6)
C14	C15	C16	121.6(5)		C78	C77	C80	121.9(6)
C14	C15	C22	119.9(5)		C79	C78	C77	120.7(6)
C16	C15	C22	118.5(5)		C74	C79	C78	120.1(6)
C15	C16	C20	119.9(5)		C81	C80	C77	175.9(8)
C17	C16	C15	119.3(5)		C80	C81	C82	177.6(8)
C17	C16	C20	120.7(5)		C83	C82	C81	119.8(6)
C12	C17	C21	121.7(5)		C83	C82	C87	119.4(6)
C16	C17	C12	118.7(5)		C87	C82	C81	120.8(6)
C16	C17	C21	119.6(5)		C82	C83	C84	120.3(7)
C23	C22	C15	176.0(7)		C85	C84	C83	120.9(7)
C22	C23	C24	177.4(7)		C84	C85	C86	117.9(6)
C25	C24	C23	120.2(6)		C84	C85	C88	121.8(6)
C29	C24	C23	120.7(6)		C86	C85	C88	120.2(6)
C29	C24	C25	119.2(5)		C87	C86	C85	121.2(6)
C24	C25	C26	120.2(6)		C86	C87	C82	120.3(6)
C27	C26	C25	120.1(6)		C85	C88	C89	112.4(6)
C26	C27	C30	119.4(6)		C90	C88	C85	110.0(5)
C28	C27	C26	118.8(5)		C90	C88	C89	107.9(7)
C28	C27	C30	121.8(6)		C91	C88	C85	108.6(6)
C27	C28	C29	121.4(7)		C91	C88	C89	108.7(6)
C24	C29	C28	120.3(6)		C91	C88	C90	109.1(7)
C31	C30	C27	176.3(7)		Cl1	C1S	Cl2A	109.3(4)
C30	C31	C32	176.9(8)		Cl1	C1S	Cl2B	113.0(4)
C33	C32	C31	120.4(6)		Cl2B	C1S	Cl2A	20.2(2)
C37	C32	C31	121.7(6)		Cl4	C2S	Cl3	111.3(4)
C37	C32	C33	117.9(6)		Cl6	C3S	Cl5	114.2(5)
C34	C33	C32	120.4(6)					

S4. Orbital contributions

Density functional theory (DFT) calculations were carried out using the Gaussian 09 package (Gaussian, Inc)[8], all results were displayed using GaussView[9] and GaussSum[10]. All calculations used the B3LYP level set employing a 6-31G(d)/LANL2DZ basis set, geometrically optimised in a DCM solvent field using the SCRF-PCM method.

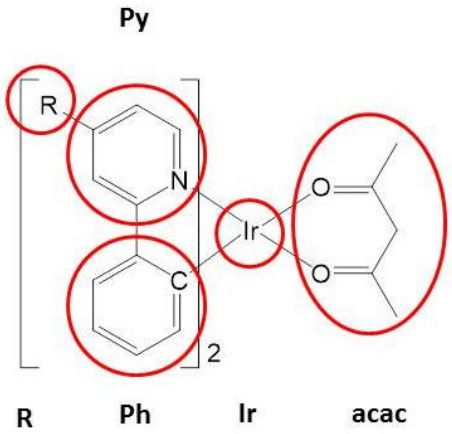

Figure S46. Molecular components of complexes **1-13, Ir(*o*TolPPy)$_2$(acac)**, and **Ir(PhPPy)$_2$(acac).**

Table S22. Orbital contributions for **1**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
199	L+10	0.49	11	1	84	4	0
198	L+9	0.32	7	1	86	5	2
197	L+8	0.11	0	0	0	4	96
196	L+7	0.10	0	0	0	4	96
195	L+6	0.07	0	0	3	2	95
194	L+5	0.06	0	0	5	1	94
193	L+4	-0.85	3	63	3	29	2
192	L+3	-0.88	1	34	7	55	3
191	L+2	-0.95	2	0	11	82	4
190	L+1	-1.41	4	1	25	68	2
189	LUMO	-1.44	4	1	29	64	2
188	HOMO	-5.08	45	5	44	6	0
187	H-1	-5.51	40	50	3	6	0
186	H-2	-5.96	67	5	13	14	1
185	H-3	-6.03	1	2	60	25	13
184	H-4	-6.11	1	0	1	1	98
183	H-5	-6.12	0	0	9	3	87
182	H-6	-6.30	15	39	41	5	0
181	H-7	-6.31	9	1	63	24	2
180	H-8	-6.48	1	2	8	4	84
179	H-9	-6.49	0	0	0	3	96
178	H-10	-6.51	15	14	46	12	13

Table S23. Orbital contributions for **2**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
179	L+10	0.58	1	0	37	41	21
178	L+9	0.49	0	0	41	39	20
177	L+8	0.43	10	1	68	4	16
176	L+7	0.40	0	0	2	7	91
175	L+6	0.39	3	0	12	7	77
174	L+5	0.23	8	2	84	2	5
173	L+4	-0.91	2	97	0	1	0
172	L+3	-1.07	2	0	27	68	3
171	L+2	-1.19	1	0	30	66	4
170	L+1	-1.93	5	1	10	65	20
169	LUMO	-1.94	4	1	9	66	21
168	HOMO	-5.17	44	5	45	6	0
167	H-1	-5.58	38	51	3	6	2
166	H-2	-6.02	63	5	11	15	6
165	H-3	-6.13	1	3	70	26	0
164	H-4	-6.33	16	43	29	7	5
163	H-5	-6.37	7	1	68	23	2
162	H-6	-6.52	8	8	64	13	7
161	H-7	-6.77	4	69	24	1	1
160	H-8	-7.14	13	6	8	23	50
159	H-9	-7.26	16	5	2	21	56
158	H-10	-7.33	9	38	37	4	12

Table S24. Orbital contributions for **3**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
219	L+10	0.47	10	1	85	4	0
218	L+9	0.30	6	1	86	5	1
217	L+8	-0.39	0	0	1	7	92
216	L+7	-0.39	0	0	1	4	94
215	L+6	-0.54	2	1	1	48	49
214	L+5	-0.55	2	0	4	44	49
213	L+4	-0.88	2	97	0	1	0
212	L+3	-1.11	2	1	30	51	16
211	L+2	-1.21	1	0	33	53	13
210	L+1	-1.91	3	0	6	47	43
209	LUMO	-1.92	3	1	6	47	44
208	HOMO	-5.12	45	5	45	6	0
207	H-1	-5.52	39	47	3	7	3
206	H-2	-5.92	56	4	7	15	18
205	H-3	-6.07	1	3	69	27	0
204	H-4	-6.20	7	32	6	10	46
203	H-5	-6.29	2	1	59	20	19
202	H-6	-6.38	3	9	64	6	18
201	H-7	-6.46	20	2	11	11	56
200	H-8	-6.63	17	21	30	8	24
199	H-9	-6.74	12	65	19	2	3
198	H-10	-7.24	0	0	0	0	100

Table S25. Orbital contributions for **4**.

Molecular Orbital		Energy (eV)	Molecular Components Contributions (%)				
			Ir	acac	Ph	Py	R
227	L+10	0.49	8	1	88	3	0
226	L+9	0.33	6	1	88	4	1
225	L+8	-0.29	0	0	1	2	97
224	L+7	-0.29	0	0	1	1	98
223	L+6	-0.67	2	1	1	57	39
222	L+5	-0.69	2	0	3	49	46
221	L+4	-1.07	2	68	9	17	5
220	L+3	-1.11	1	28	17	27	26
219	L+2	-1.19	1	0	28	47	24
218	L+1	-1.71	4	0	11	52	33
217	LUMO	-1.71	3	1	10	53	33
216	HOMO	-5.08	45	5	44	6	0
215	H-1	-5.49	46	38	5	9	3
214	H-2	-5.89	60	5	9	14	11
213	H-3	-6.05	1	2	72	25	0
212	H-4	-6.25	1	17	1	7	75
211	H-5	-6.27	2	1	42	15	41
210	H-6	-6.37	3	18	66	6	7
209	H-7	-6.38	15	2	26	15	43
208	H-8	-6.61	13	34	33	9	11
207	H-9	-6.80	14	62	19	3	2
206	H-10	-6.95	0	0	0	0	100

Table S26. Orbital contributions for **5**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
251	L+10	0.50	8	1	88	3	0
250	L+9	0.34	6	1	88	4	1
249	L+8	-0.04	0	0	3	3	94
248	L+7	-0.05	0	0	4	1	95
247	L+6	-0.88	1	1	3	29	66
246	L+5	-0.89	0	0	0	6	94
245	L+4	-0.91	1	1	7	53	37
244	L+3	-1.00	2	0	11	79	8
243	L+2	-1.07	2	93	1	3	0
242	L+1	-1.46	4	3	24	68	2
241	LUMO	-1.48	4	1	29	65	2
240	HOMO	-5.07	45	5	43	6	0
239	H-1	-5.50	46	40	5	8	0
238	H-2	-5.92	66	6	12	14	1
237	H-3	-6.04	1	2	70	25	2
236	H-4	-6.08	0	0	0	2	98
235	H-5	-6.09	0	0	0	2	98
234	H-6	-6.27	2	0	13	6	78
233	H-7	-6.28	0	0	4	0	96
232	H-8	-6.33	6	1	52	19	22
231	H-9	-6.35	5	31	55	6	3
230	H-10	-6.56	13	35	39	12	1

Table S26. Orbital contributions for **6**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
187	L+10	0.46	11	1	84	4	0
186	L+9	0.30	6	1	85	5	2
185	L+8	-0.24	0	0	0	0	100
184	L+7	-0.24	0	0	0	0	100
183	L+6	-0.33	2	0	2	37	60
182	L+5	-0.35	2	0	5	32	60
181	L+4	-0.89	2	97	0	1	0
180	L+3	-1.07	2	0	31	59	8
179	L+2	-1.18	1	0	34	58	7
178	L+1	-2.01	4	0	6	54	36
177	LUMO	-2.02	3	1	6	54	36
176	HOMO	-5.13	44	5	45	6	0
175	H-1	-5.51	39	43	3	8	7
174	H-2	-5.84	44	3	5	16	32
173	H-3	-6.08	2	26	22	20	30
172	H-4	-6.09	1	8	51	18	22
171	H-5	-6.27	5	1	57	17	20
170	H-6	-6.38	5	14	68	5	8
169	H-7	-6.47	29	2	18	16	35
168	H-8	-6.66	14	30	33	7	16
167	H-9	-6.77	19	57	15	3	6
166	H-10	-7.08	0	0	0	0	100

Table S27. Orbital contributions for **7**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
239	L+10	-0.19	0	0	0	0	100
238	L+9	-0.19	0	0	0	0	100
237	L+8	-0.37	0	0	0	0	100
236	L+7	-0.37	0	0	0	0	100
235	L+6	-0.90	2	96	0	1	1
234	L+5	-0.97	1	1	14	62	22
233	L+4	-1.05	1	0	12	55	33
232	L+3	-1.31	2	1	19	33	46
231	L+2	-1.36	2	0	26	37	35
230	L+1	-2.25	3	0	3	37	57
229	LUMO	-2.26	2	0	3	37	57
228	HOMO	-5.15	44	5	45	6	0
227	H-1	-5.50	34	34	3	8	23
226	H-2	-5.66	12	1	1	9	77
225	H-3	-5.77	4	22	1	4	70
224	H-4	-6.08	49	4	14	10	23
223	H-5	-6.11	1	3	71	25	0
222	H-6	-6.33	14	37	36	5	8
221	H-7	-6.36	8	1	64	22	5
220	H-8	-6.51	8	8	55	12	17
219	H-9	-6.75	3	67	25	1	4
218	H-10	-6.89	10	1	2	12	75

Table S28. Orbital contributions for **8**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
227	L+10	-0.18	0	0	0	0	100
226	L+9	-0.18	0	0	0	0	100
225	L+8	-0.36	0	0	1	2	97
224	L+7	-0.36	0	0	1	3	96
223	L+6	-0.80	2	5	3	54	36
222	L+5	-0.84	2	0	4	50	44
221	L+4	-0.87	1	92	1	5	1
220	L+3	-1.17	2	1	28	41	29
219	L+2	-1.25	1	0	32	45	21
218	L+1	-1.95	3	0	5	39	53
217	LUMO	-1.96	2	0	5	40	53
216	HOMO	-5.10	45	5	45	6	0
215	H-1	-5.49	37	40	3	7	12
214	H-2	-5.71	16	1	1	9	73
213	H-3	-5.81	1	15	1	4	80
212	H-4	-6.06	48	4	15	9	23
211	H-5	-6.06	1	3	70	27	0
210	H-6	-6.32	13	34	44	5	3
209	H-7	-6.33	11	1	62	24	3
208	H-8	-6.52	16	15	50	12	7
207	H-9	-6.73	7	69	23	1	1
206	H-10	-7.01	0	0	0	0	100

Table S29. Orbital contributions for **9**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
279	L+10	-0.39	0	0	1	5	94
278	L+9	-0.39	0	0	1	3	96
277	L+8	-0.51	1	0	1	28	70
276	L+7	-0.51	1	0	2	25	71
275	L+6	-0.88	2	97	0	1	0
274	L+5	-1.04	1	0	23	55	21
273	L+4	-1.14	1	0	23	54	22
272	L+3	-1.50	2	1	11	35	51
271	L+2	-1.51	2	0	14	36	47
270	L+1	-2.13	2	0	2	22	74
269	LUMO	-2.14	1	0	2	23	73
268	HOMO	-5.12	44	5	45	6	0
267	H-1	-5.47	27	26	2	6	39
266	H-2	-5.55	4	0	0	3	93
265	H-3	-5.62	12	25	1	2	60
264	H-4	-5.98	58	5	10	12	15
263	H-5	-6.07	1	3	69	27	0
262	H-6	-6.27	12	38	16	7	28
261	H-7	-6.31	4	1	63	22	11
260	H-8	-6.41	1	3	55	6	35
259	H-9	-6.49	12	1	5	7	76
258	H-10	-6.62	15	17	27	7	33

Table S30. Orbital contributions for **10**.

Molecular Orbital		Energy (eV)	Molecular Components Contributions (%)				
			Ir	acac	Ph	Py	R
235	L+10	-0.17	0	0	0	0	100
234	L+9	-0.17	0	0	0	0	100
233	L+8	-0.25	0	0	1	1	98
232	L+7	-0.25	0	0	1	2	97
231	L+6	-0.82	2	1	7	69	21
230	L+5	-0.88	2	0	6	62	29
229	L+4	-1.07	2	89	3	5	1
228	L+3	-1.21	1	7	20	31	41
227	L+2	-1.26	1	0	28	38	33
226	L+1	-1.76	3	0	7	41	48
225	LUMO	-1.76	3	1	7	42	48
224	HOMO	-5.07	45	5	44	6	0
223	H-1	-5.47	43	34	4	9	10
222	H-2	-5.70	14	1	1	6	77
221	H-3	-5.78	3	7	1	3	87
220	H-4	-5.97	52	5	12	10	21
219	H-5	-6.03	1	3	71	25	0
218	H-6	-6.31	9	1	64	25	1
217	H-7	-6.35	5	30	59	6	1
216	H-8	-6.56	13	34	38	11	4
215	H-9	-6.79	10	63	21	3	3
214	H-10	-6.90	0	0	0	1	99

Table S31. Orbital contributions for **11**.

Molecular Orbital		Energy (eV)	Molecular Components Contributions (%)				
			Ir	acac	Ph	Py	R
287	L+10	-0.30	0	0	0	0	100
286	L+9	-0.30	0	0	0	0	100
285	L+8	-0.56	1	0	0	31	67
284	L+7	-0.57	1	0	2	26	70
283	L+6	-0.88	2	97	0	1	0
282	L+5	-1.00	1	0	20	54	24
281	L+4	-1.10	1	0	20	56	23
280	L+3	-1.49	3	1	14	45	38
279	L+2	-1.50	3	0	18	44	34
278	L+1	-2.03	1	0	2	17	79
277	LUMO	-2.03	1	0	2	18	79
276	HOMO	-5.11	44	5	45	6	0
275	H-1	-5.48	25	25	2	5	42
274	H-2	-5.54	2	0	0	2	95
273	H-3	-5.60	14	25	2	2	57
272	H-4	-5.99	61	5	11	13	11
271	H-5	-6.07	1	3	69	27	0
270	H-6	-6.28	12	36	18	7	27
269	H-7	-6.31	4	1	61	22	12
268	H-8	-6.40	1	3	47	5	45
267	H-9	-6.45	10	1	6	6	78
266	H-10	-6.59	17	16	32	9	26

Table S32. Orbital contributions for **12**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
259	L+10	-0.04	0	0	3	2	94
258	L+9	-0.05	0	0	4	1	95
257	L+8	-0.13	0	0	0	0	100
256	L+7	-0.13	0	0	0	0	100
255	L+6	-0.87	3	84	1	11	1
254	L+5	-0.91	1	13	9	72	5
253	L+4	-0.99	2	0	11	82	5
252	L+3	-1.27	0	0	1	2	97
251	L+2	-1.27	0	0	0	2	98
250	L+1	-1.44	4	1	24	68	3
249	LUMO	-1.48	4	1	28	64	3
248	HOMO	-5.10	45	5	44	6	0
247	H-1	-5.53	39	50	3	6	1
246	H-2	-5.63	0	0	0	1	99
245	H-3	-5.63	0	0	0	1	98
244	H-4	-5.98	67	5	13	14	1
243	H-5	-6.05	1	3	68	27	2
242	H-6	-6.25	2	0	8	4	86
241	H-7	-6.27	0	0	4	0	96
240	H-8	-6.31	14	38	40	6	2
239	H-9	-6.33	8	1	56	21	14
238	H-10	-6.52	16	16	54	13	1

Table S33. Orbital contributions for **13**.

Molecular Orbital		Energy (eV)	Molecular Components Contributions (%)				
			Ir	acac	Ph	Py	R
311	L+10	-0.27	0	0	0	0	100
310	L+9	-0.27	0	0	0	0	100
309	L+8	-0.66	0	0	0	2	98
308	L+7	-0.67	0	0	0	1	99
307	L+6	-0.88	2	88	1	8	1
306	L+5	-0.92	1	9	10	75	5
305	L+4	-1.00	2	0	11	82	5
304	L+3	-1.45	4	1	24	68	2
303	L+2	-1.49	4	1	29	64	2
302	L+1	-1.82	0	0	0	1	99
301	LUMO	-1.82	0	0	0	1	99
300	HOMO	-5.11	45	5	44	6	0
299	H-1	-5.47	1	1	0	1	98
298	H-2	-5.48	0	0	0	1	99
297	H-3	-5.54	39	50	3	6	2
296	H-4	-5.99	67	5	13	14	1
295	H-5	-6.06	1	3	68	27	2
294	H-6	-6.28	3	0	16	7	74
293	H-7	-6.30	1	4	9	0	86
292	H-8	-6.30	0	1	0	1	97
291	H-9	-6.30	0	0	0	1	99
290	H-10	-6.32	13	34	34	5	13

Table S34. Orbital contributions for **Ir(PhPPy)$_2$(acac)**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
167	L+10	0.49	10	1	84	4	0
166	L+9	0.36	4	1	74	14	8
165	L+8	0.09	2	0	9	32	57
164	L+7	0.08	4	1	22	22	52
163	L+6	-0.25	0	0	1	2	97
162	L+5	-0.25	0	0	1	2	97
161	L+4	-0.87	2	97	0	1	0
160	L+3	-0.98	1	0	24	65	9
159	L+2	-1.10	1	0	26	63	10
158	L+1	-1.67	4	1	14	60	21
157	LUMO	-1.67	4	1	12	62	22
156	HOMO	-5.09	45	4	45	6	0
155	H-1	-5.50	40	47	3	7	2
154	H-2	-5.92	64	5	9	15	7
153	H-3	-6.05	1	3	69	27	0
152	H-4	-6.26	15	46	23	8	7
151	H-5	-6.30	5	1	67	24	2
150	H-6	-6.44	5	6	67	12	10
149	H-7	-6.72	3	68	26	1	2
148	H-8	-6.84	11	2	2	16	69
147	H-9	-6.94	18	7	3	12	60
146	H-10	-7.03	0	0	0	0	100

Table S35. Orbital contributions for **Ir(*o*TolPPy)$_2$(acac)**.

Molecular Orbital		**Energy (eV)**	**Molecular Components Contributions (%)**				
			Ir	acac	Ph	Py	R
175	L+10	0.49	10	1	84	4	0
174	L+9	0.34	5	1	80	9	5
173	L+8	0.02	1	0	4	24	70
172	L+7	0.02	2	0	12	18	67
171	L+6	-0.15	0	0	1	1	98
170	L+5	-0.15	0	0	1	2	97
169	L+4	-0.86	2	97	0	1	0
168	L+3	-0.94	1	0	21	68	10
167	L+2	-1.05	1	0	22	66	10
166	L+1	-1.57	4	1	16	65	15
165	LUMO	-1.57	4	1	18	63	14
164	HOMO	-5.09	45	5	44	6	0
163	H-1	-5.51	40	49	3	7	2
162	H-2	-5.94	65	5	10	15	6
161	H-3	-6.04	1	3	68	27	0
160	H-4	-6.27	15	44	28	7	6
159	H-5	-6.29	7	1	66	25	2
158	H-6	-6.45	5	6	61	12	15
157	H-7	-6.68	4	1	1	5	89
156	H-8	-6.70	0	47	22	1	30
155	H-9	-6.73	9	25	7	2	58
154	H-10	-6.85	4	1	1	7	88

S5. Photophysical Data

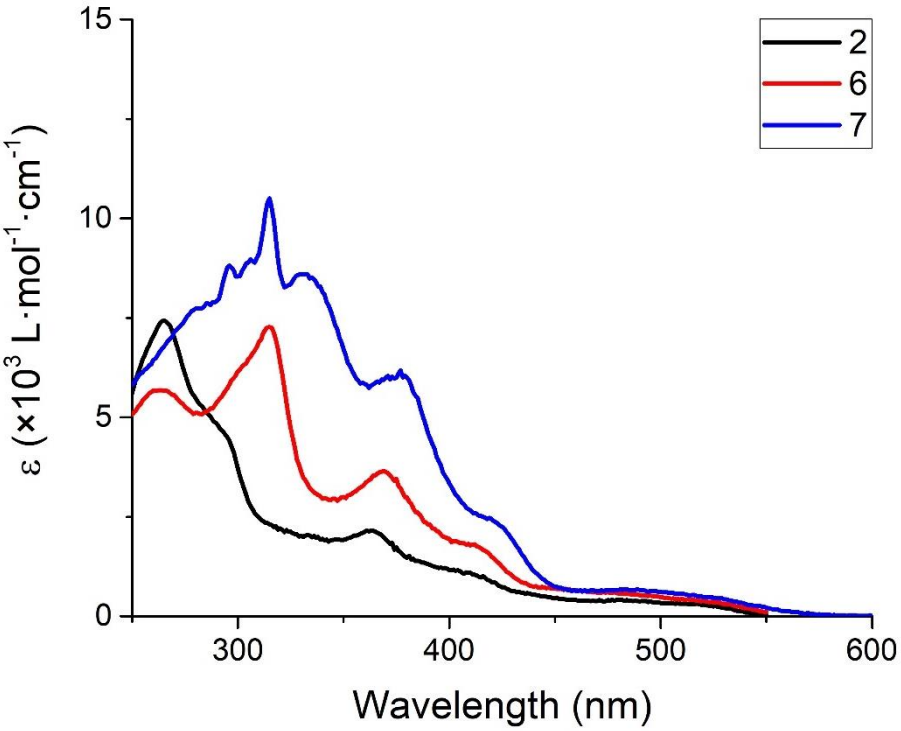

Figure S47. UV-Visible absorbance spectra of **2**, **6**, and **7** recorded in DCM.

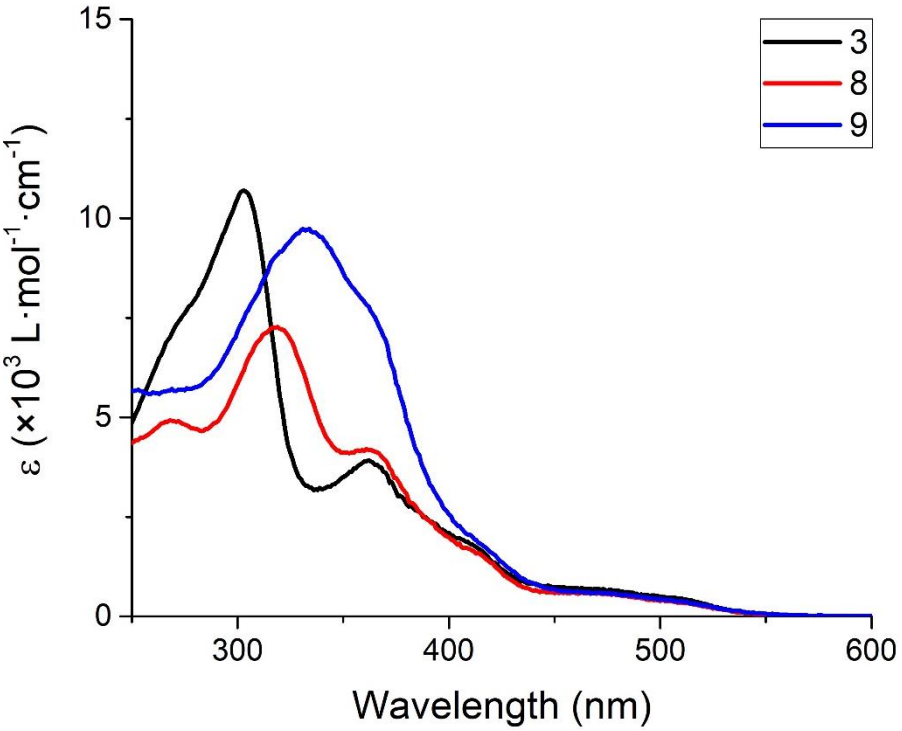

Figure S48. UV-Visible absorbance spectra of **3**, **8**, and **9** recorded in DCM.

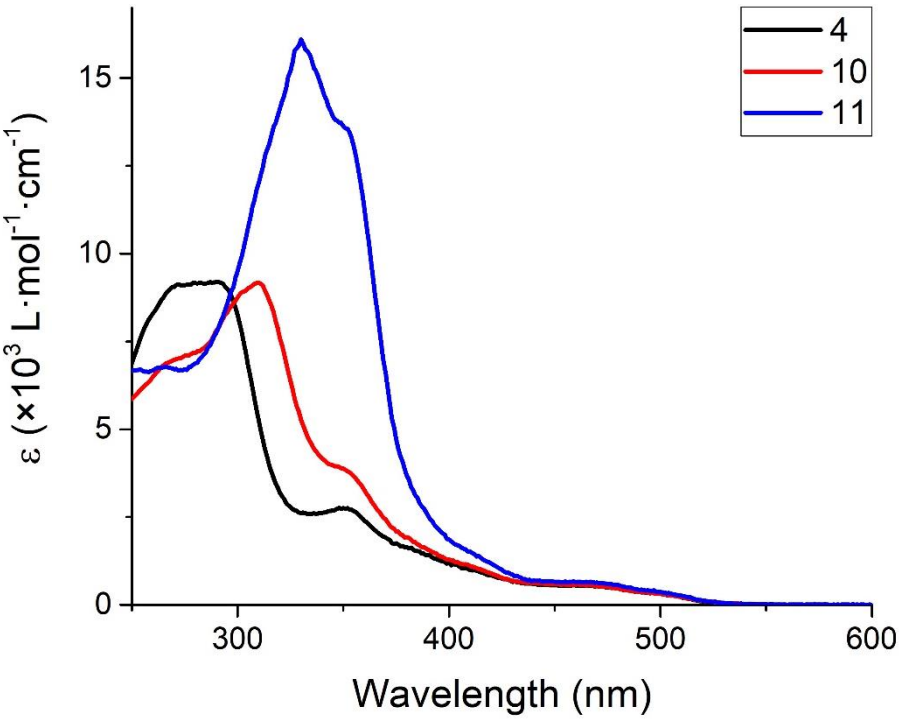

Figure S49. UV-Visible absorbance spectra of **4**, **10**, and **11** recorded in DCM.

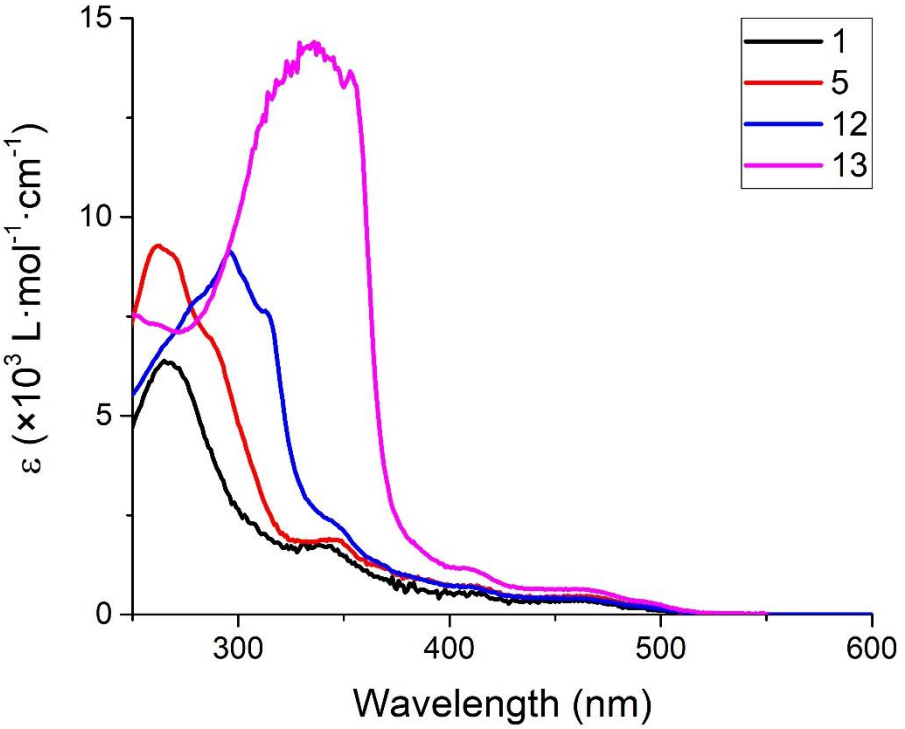

Figure S50. UV-Visible absorbance spectra of **1**, **5**, **12** and **13** recorded in DCM.

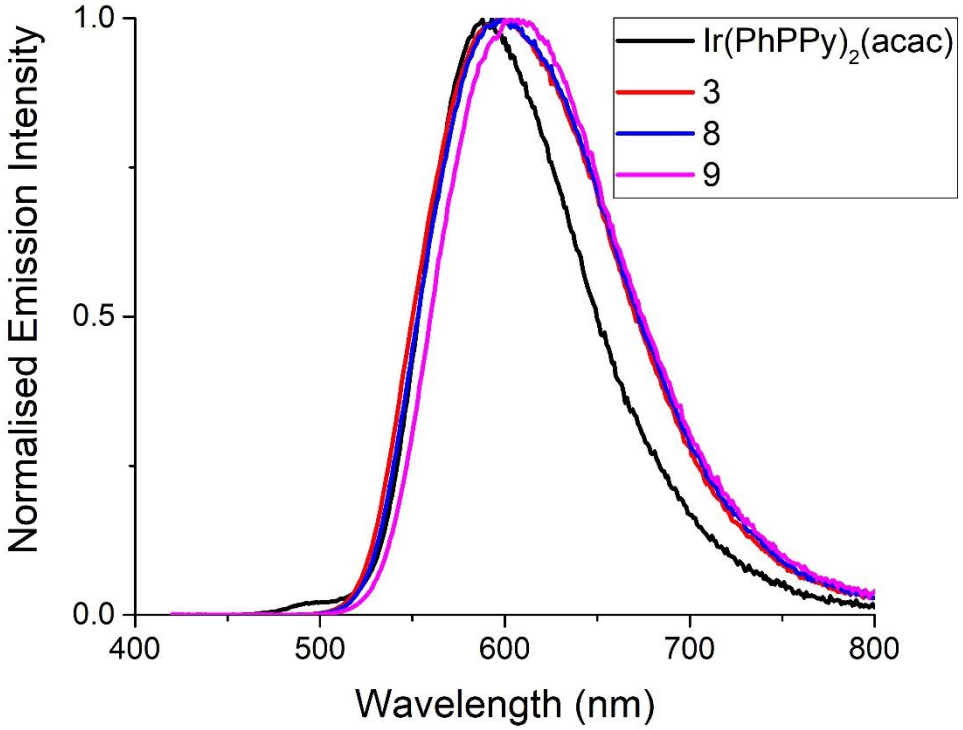

Figure S51 Emission spectra of complexes Ir(PhPPy)$_2$(acac), **3**, **8** and **9** recorded in DCM.

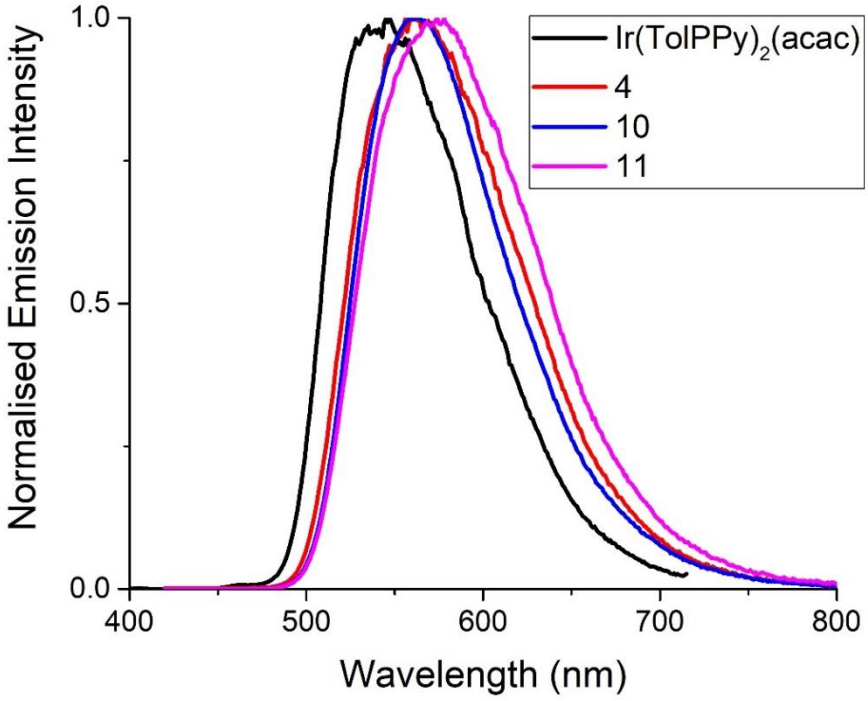

Figure S52 Emission spectra of complexes Ir(TolPPy)$_2$(acac), **4**, **10** and **11** recorded in DCM.

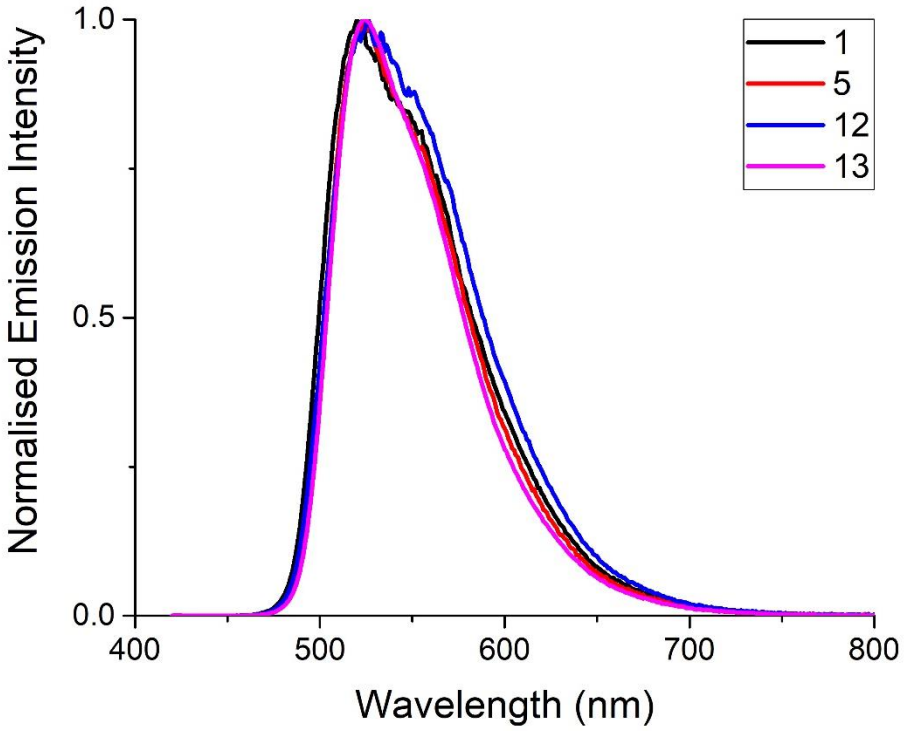

Figure S53 Emission spectra of complexes **1**, **5**, **12** and **13** recorded in DCM.

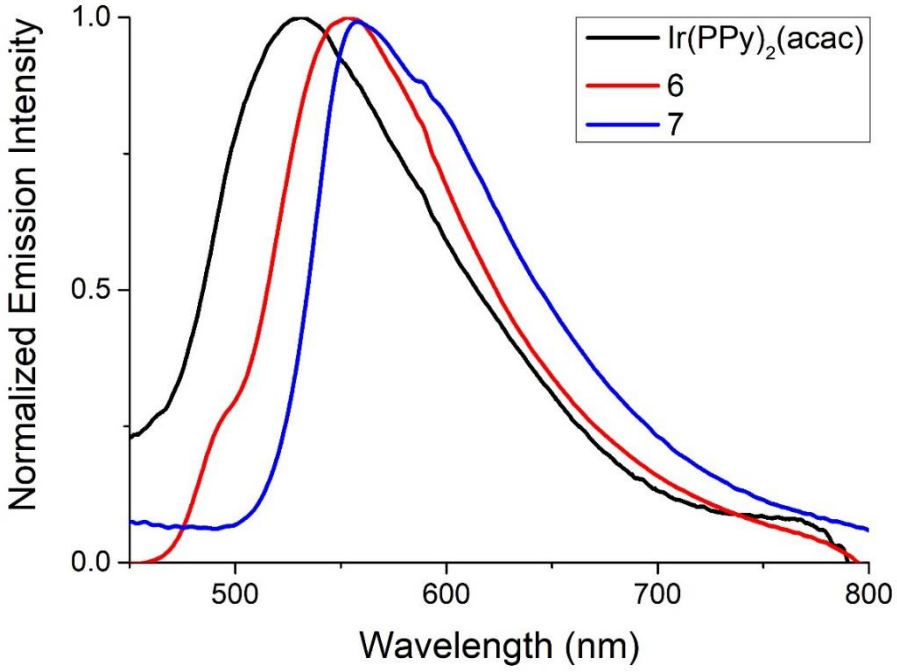

Figure S54 Emission spectra of complexes $Ir(PPy)_2(acac)$, **6**, and **7** recorded in PBiBM films.

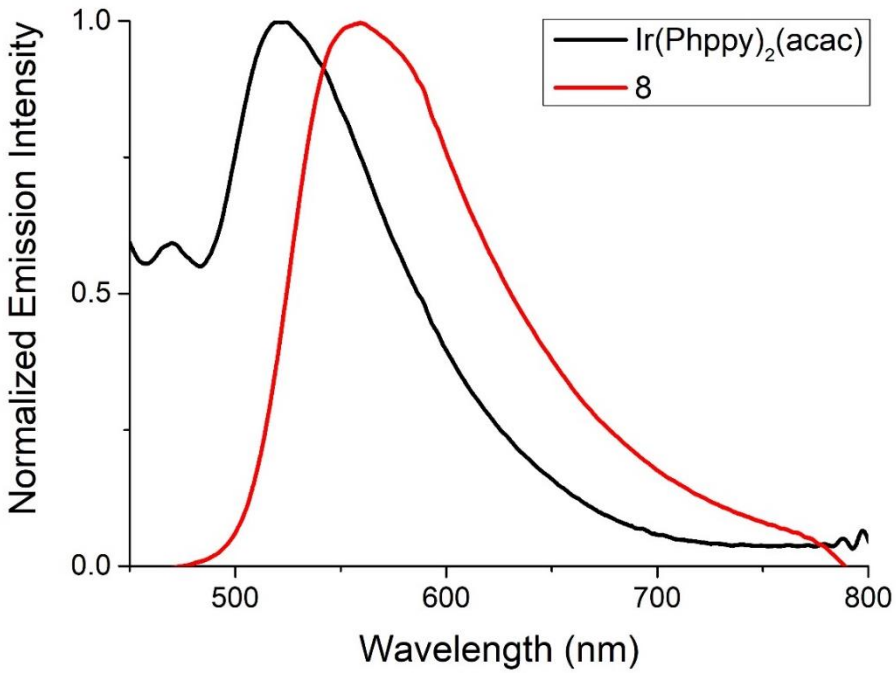

Figure S55 Emission spectra of complexes Ir(PhPPy)$_2$(acac) and **8** recorded in PBiBM films.

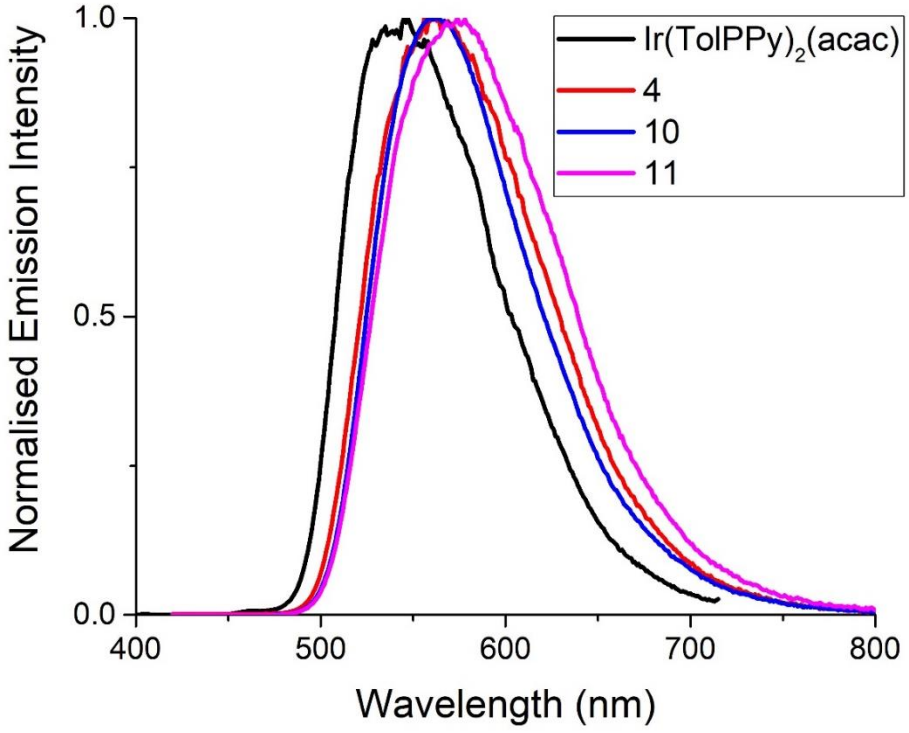

Figure S56 Emission spectra of complexes Ir(TolPPy)$_2$(acac), **10**, and **11** recorded in PBiBM films.

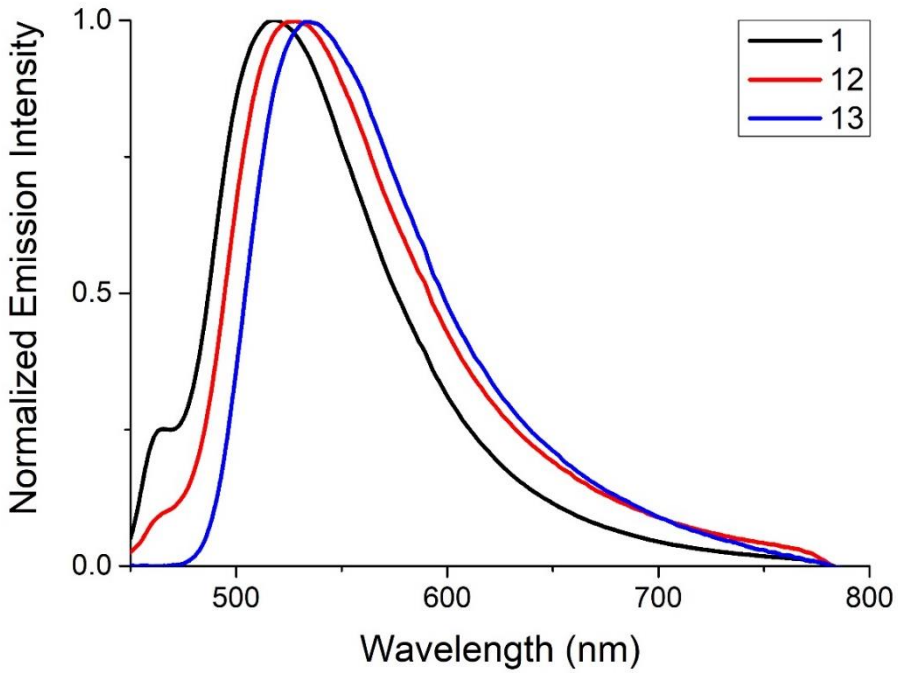

Figure S57 Emission spectra of complexes **1**, **12**, and **13** recorded in PBiBM films.

S6 Triplet Energy Determination of BPEB

The triplet state of 1,4-bis(phenylethynyl)benzene was (BPEB) studied in argon saturated benzene solution using the pulse radiolysis-energy transfer method.[11-13] Here, the substrate triplet states (^{3}S*) are selectively produced by pulse radiolysis of benzene solutions in the presence of relatively high concentrations of biphenyl or other sensitizers (A), as indicated in the reaction sequence

$^1Bz^* \rightarrow {}^3Bz^*$

$^1Bz^* + A \rightarrow Bz + {}^1A^*$

$^1A^* \rightarrow {}^3A^*$

$^3Bz^* + A \rightarrow Bz + {}^3A^*$

$^3A^* + S \rightarrow A + {}^3S^*$

and subject to the kinetically demanded concentration ratio [Bz] >> [A] >> [S]. Using biphenyl (10 mM) as sensitizer, new absorptions were seen to grow-in within a few microseconds by a second-order process, with near diffusion-controlled rates in the range 5-9 $\times 10^9$ $M^{-1}s^{-1}$, and decayed by a first order process. The transient absorption was quenched by the presence of oxygen, in agreement with the assignment to the triplets. As discussed in detail elsewhere,[14] alternative assignments of the transient absorptions to positively or negatively charged species are unlikely under our reaction conditions. The molar extinction coefficient was obtained by the energy transfer method.[11, 15] Spectral and kinetic data are given in Table 36.

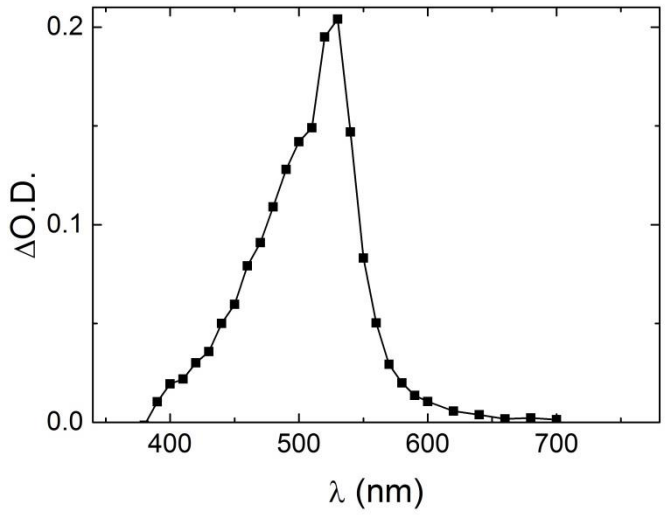

Figure S58. Triplet-singlet difference spectrum observed following pulse radiolysis of argon saturated solutions of BPEB in benzene in the presence of biphenyl (10 mM).

Table S36 Spectral and kinetic data for triplet state of BPEB formed by pulse radiolysis of argon saturated benzene solution in the presence of biphenyl (10 mM) sensitizer

λ_{max} / nm	ε_{max} /10^4 $M^{-1}cm^{-1}$	τ / μs [a]	Φ_Δ [b]
530	11.2 ± 0.7	150	0.23

a. Triplet lifetime from pulse radiolysis experiments

b. Singlet oxygen yield from time resolved phosphorescence.

Triplet energies were determined by studying the sensitisation with a variety of donors as described elsewhere.[12-13] Data are presented in Table 37. Energies of the lowest singlet state in benzene solution were determined from the onset of the ground state absorption, and area also given. From these, the energy between the lowest excited singlet and triplet states was calculated.

Table S37 Energies of lowest excited state of BPEB

E_{S1} / eV	E_{T1} / eV [a]	$\Delta E(S_1 - T_1)$ / eV
3.44	2.56	0.88

a. Estimated error ± 0.05 eV

Experimental

Pulse radiolysis experiments were carried out at the Free Radical Research Facility, Daresbury, UK using 200 ns - 2 μs high energy electron pulses from a 12 MeV linear accelerator, which were passed through a solution 2.5 cm optical path length quartz cuvette attached to a flow system. All solutions were bubbled with argon for about 30 minutes before experiments. The experimental set up has been described elsewhere.[16] Optical spectra, normalized for the radiation dose, were recorded using a spectrometer consisting of a xenon arc lamp, monochromator, photomultiplier and appropriate filters. Signals were then directed to a computer for analysis. The general spectrometer design is similar to that given in reference 17. Triplet states were generated by pulse radiolysis of argon saturated solutions of BPEB and biphenyl (10 mM) in benzene. Triplet state molar absorption coefficients were determined using the method of Bensasson and Land,[11] using argon saturated solutions of biphenyl (10 mM) in benzene as standard, taking the value ε = 27 100 $M^{-1}cm^{-1}$ at 367 nm for its triplet extinction coefficient.

Singlet oxygen ($^1\Delta_g$) yield and lifetime was obtained by direct measurement of the phosphorescence at 1270 nm following irradiation of an aerated solution of BPEB in benzene with a frequency tripled pulse (355 nm) from a Nd:YAG laser, as described in detail elsewhere.[18-19] The quantum yield of singlet oxygen formation was determined by comparison of the initial emission intensity for optically matched solutions at the excitation

wavelength (A_{355} = 0.5) with 1*H*-phenalen-1-one taken as standard, using Φ_{Δ} = 0.93 in benzene solution.[20]

S7 Polarised microscopy

Samples of thin polymer films were mounted onto SuperFrost microscope slides capped with a 170 μm coverslip for imaging. The microscope is built on a Zeiss AxioVert 200M chassis and is equipped with a variable pulse sequence generator, which allows both CW and time-resolved operation and comprises an even number of polished-Al mirrors (Thor Labs) after selection of the polarised light of interest that are used to guide the emitted light to the detector. It is important to note that the transmission/DIC imaging de Sénarmont compensator of the microscope has been eliminated.[21] The absence of this component is a vital requirement, as such a rotatable optical element consists of two broad quarter-wave plates, and the linear polariser would severely limit chiroptical selection. The excitation source was a 365 nm UV LED (Nichia, 24 V, 1.2 W, collimated and scrambled to 1" diameter, focused to the back focal plane (BFP) of Zeiss x10/0.25NA A-Plan air objective) in an epi-fluorescence configuration to the applied 2D-CCD detector (Ocean Optics Maya2000 Pro,[22] 400-800 nm detection window, 200 μm slit). The imaging sequence was comprised of a full-filed-of-view spectroscopic collection of a baseline and red corrected average of 10000 spectra with a rolling 7.2 ms parallel illumination and light collection sequence set at 100 Hz.

The microscope is fitted with a 395 nm dichroic mirror to allow epifluorescence detection combined with a 420 nm long pass emission filter (placed in front of the detector). The unavoidable aperture restriction, due to the nature epi-fluorescence detection, has been compensated for with a pair of variable irises and a beam expander lens pair, in a linear arrangement between the 10x objective and the filter cube, thereby eliminating light loss in the detection arm. The final optical element in the set-up is a pair of linear polarisers that allow selection and differentiation of vertically and horizontally polarised linear light. In this

proof of concept instrument, (Figure S59) we have employed a pair of optical polarisers (1”; 40000:1 extinction ratio, Thor Labs.) in a relative 90° orientation.

The Polarisation Ratio (PR) was determined using the full integer of the respective red (Ocean Optics Cal 2000 blackbody radiator) and baseline (undoped virgin polymer film) corrected individual averaged emission spectra as a function of polarisation orientation of the emitted light. All final Polarisation Ratios are an average of triplicate measurements of 5 individual Fields of View per slide (3 x 5 x 10000 spectral acquisitions). The self-polarization of the apparatus was corrected by measuring the emission of solutions containing $Ir(ppy)_2(acac)$ (λ_{emis} = 520 nm) and $Ir(PhPPy)_2(acac)$ (λ_{emis} = 560 nm) in dichloromethane. The emission was recorded with a perpendicular and parallel ratio to determine the correction factor, $f = \frac{I_{\parallel}}{I_{\perp}}$, where $I_{\parallel}$ is the perpendicular emission intensity and $I_{\perp}$ is the perpendicular emission intensity. The correction factor for this apparatus was determined to be $f_{520\,nm} = 1.739$ and $f_{560\,nm} = 1.698$.

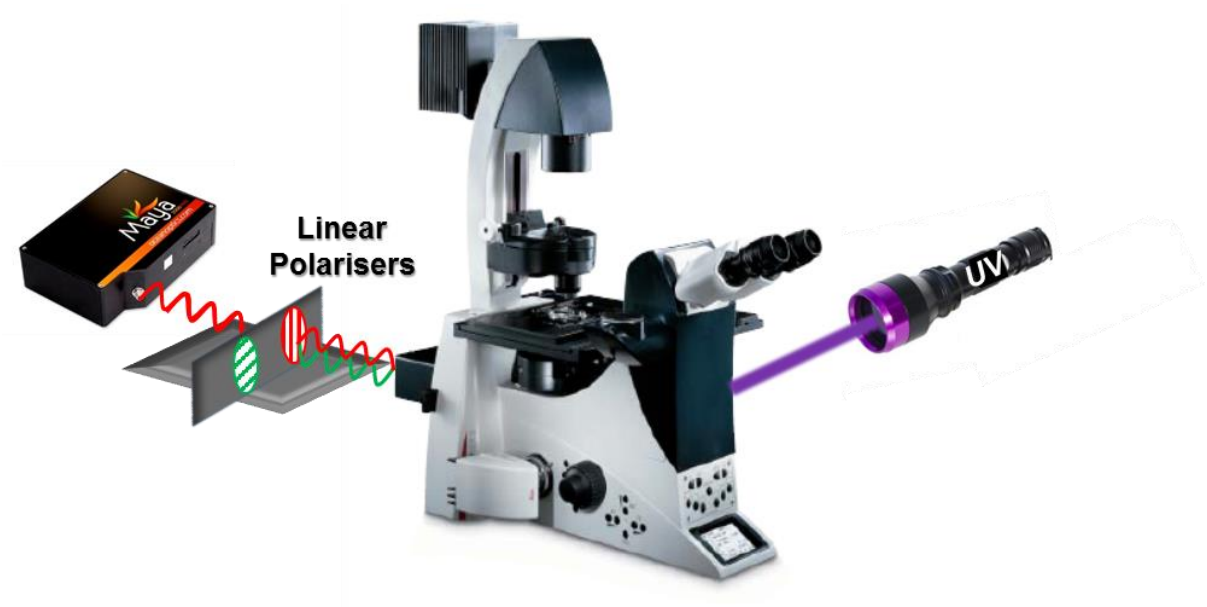

Figure S59 Schematic diagram of the Polarisation Microscope used to determine PR (polarisation ratio).

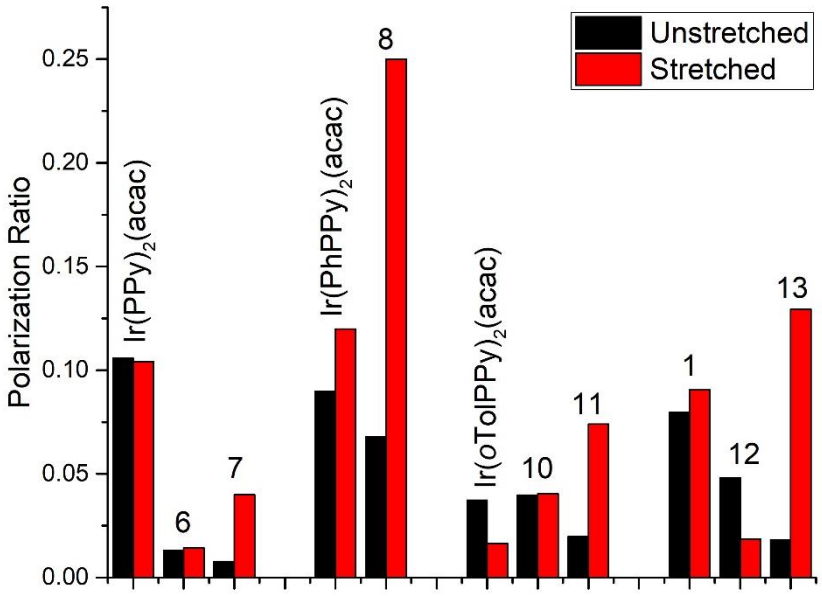

Figure S60 Polarization of complexes in film, unstretched and stretched.

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