Electronic supplementary information (ESI)

Dinuclearization Strategy of Cationic Iridium(III) Complexes for Efficient and Stable Flexible Light-Emitting Electrochemical Cells

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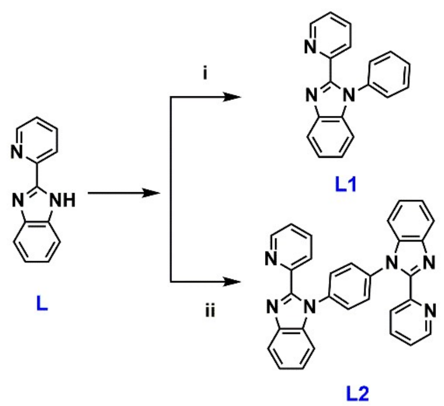
Experimental Section

Materials and solvents

The 2-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole, iodobenzene, 18-Crown-6, CuI, K_2CO_3, KOH, and DMPU were used as purchased. All other chemicals were analytical grade reagent and dried according to standard procedures. All air-sensitive reactions were carried out under an argon atmosphere. The cyclometalated iridium(III) μ-chlorobridged dimers of **(dfppz)$_2$Ir(μ-Cl)$_2$(dfppz)$_2$** was prepared as previously described.

Synthesis and characterization

Flash chromatography was performed by using silica gel 60 (200-300 mesh, HAIYANG). Analytical thin layer chromatography (TLC) was performed by using aluminum coated silica gel 60 F254 plates (Leading Chem). The NMR spectra were recorded on a Bruker Avance 500 (^{1}H: 500 MHz; ^{13}C: 150 MHz) with tetramethylsilane (TMS) as an internal standard. The coupling constants (*J*) and chemical shifts (δ) are expressed in Hz and ppm, respectively. Multiplicities are denoted as follows: s=singlet, d=doublet, t=triplet, m=multiplet. Mass spectra data was measured on matrix-assisted laser desorption-ionization time-of-flight (MALDI-TOF) mass spectrometry.



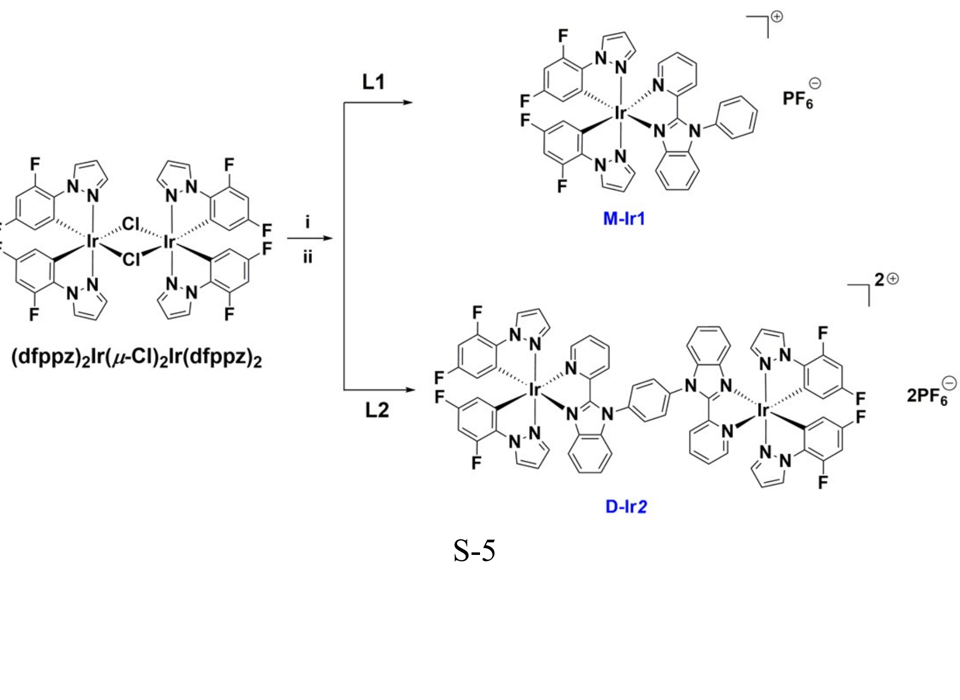
Scheme S1. Synthetic routes of **L1** and **L2**. (i) (ii) **L**, C_6H_5I, K_2CO_3, CuI, 18-crown-6, DMPU, 190°C.

Synthetic route of L1.

A mixture of 2-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole (0.43 g, 2.2 mmol), iodobenzene (0.41 g, 2.0 mmol), 18-Crown-6 (0.05 g, 0.2 mmol), CuI (0.05 g, 0.2 mmol) and K_2CO_3 (0.41 g, 3.0 mmol) in DMPU (5 mL) was heated at 190ºC under nitrogen for 12 h. After cooling to room temperature, the reaction mixture was diluted with a saturated aqueous NaCl solution, then extracted with dichloromethane. The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel eluting with dichloromethane and petroleum ether in volumetric ratio 10:1. A white solid was isolated in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$, δ [ppm]): 8.39 (d, J = 4.5 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.72-7.76 (m, 1H), 7.43-7.50 (m, 3H), 7.28-7.38 (m, 4H), 7.21-7.26 (m, 2H).

Synthetic route of L2

The reaction was carried out according to the procedure described for the synthesis of **L1**, using the following amounts of reagents: 1,4-dibromobenzene (0.24 g, 1.0 mmol), 2-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole (0.43 g, 2.2 mmol), 18-Crown-6 (0.05 g, 0.2 mmol), CuI (0.05 g, 0.2 mmol), K_2CO_3 (0.41 g, 3.0 mmol) and DMPU (5 mL). ^{1}H NMR (500 MHz, $CDCl_3$, δ [ppm]): 8.45 (d, J = 4.5 Hz, 2H), 8.27 (d, J = 7.0 Hz, 2H), 7.97 (d, J = 7.5 Hz, 2H), 7.84 (t, J = 7.5 Hz, 2H), 7.46 (s, 4H), 7.37-7.43 (m, 4H), 7.30-7.34 (m, 4H).



Scheme S2. Synthetic routes of **M-Ir1** and **D-Ir2**. (i) **L1**, **L2**, **L3**, or **L4**, ethylene glycol, 150°C, 12 h; (ii) aqueous NH_4PF_6 solution.

Synthetic route of complexes

The prior synthesized chloro-bridge di-iridium intermediate complex **[(dfppz)$_2$Ir(μ-Cl)]$_2$** and the respective ancillary N^N ligands **L1** and **L2** were transferred into a flask. Ethylene glycol was added via a cannula and the reaction mixture heated under reflux at 150°C for 24 h, to give a clear solution. After cooling to room temperature, the solution was transferred to another flask. An aqueous solution of NH_4PF_6 (2 g, 12.3 mmol) was added to the mixture resulting in an immediate precipitation of the desired product complex. The mixture was filtered and the residue was purified by column chromatography, using a dichloromethane:ethyl acetate (10:1) mixture to elude the desired purified complexes. Eluant was distilled off leading to slow precipitation crystallization of pure complexes. The purified complexes were then dried under vacuum.

M-Ir1: [(dfppz)$_2$Ir(μ-Cl)]$_2$ (0.6 g, 0.5 mmol), **L1** (0.27 g, 1.0 mmol), ethylene glycol (20 mL). Yellow powder (yield: 62%). ^{1}H NMR (500 MHz, d_6-DMSO) δ 8.68 (d, J = 2.7 Hz, 1H), 8.65 (d, J = 2.7 Hz, 1H), 8.15 (d, J = 4.9 Hz, 1H), 8.08 (td, J = 8.0, 1.6 Hz, 1H), 7.99 – 7.92 (m, 1H), 7.91 – 7.84 (m, 4H), 7.68 – 7.59 (m, 2H), 7.50 – 7.42 (m, 2H), 7.29 (ddd, J = 8.3, 7.3, 1.0 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.15 (dd, J = 13.3, 8.6 Hz, 2H), 6.81 (dt, J = 4.2, 2.7 Hz, 2H), 6.46 (d, J = 8.4 Hz, 1H), 5.79 (dd, J = 8.0, 2.4 Hz, 1H), 5.69 (dd, J = 8.0, 2.5 Hz, 1H). ^{13}C NMR (125 MHz, d_6-DMSO, ppm): δ 152.82, 152.78, 150.1, 150.0, 149.8, 149.7, 148.04, 148.0, 147.8, 147.7, 147.1, 140.7, 140.4, 140.3, 139.8, 138.4, 137.9, 134.73, 134.69, 134.2, 133.0, 132.9, 132.7, 132.6, 132.0, 131.5, 131.4, 129.3, 128.9, 128.6, 127.8, 127.68, 127.65, 127.6, 127.0, 126.2, 125.1, 116.7, 115.8, 115.6, 115.0, 114.8, 113.1, 110.03, 109.96, 100.3, 100.2, 100.11, 100.08, 100.01, 100.0, 99.9, 99.8. MS (MALDI-TOF) m/z: Calcd for $C_{36}H_{23}F_4IrN_7$: 822.2, Found 822.2 $[M]^+$.

D-Ir2: [(dfppz)$_2$Ir(μ-Cl)]$_2$ (0.59 g, 0.5 mmol), **L2** (0.21 g, 0.45 mmol), ethylene glycol (20 mL). Yellow powder (yield: 66%). ^{1}H NMR (500 MHz, d_6-DMSO) δ 8.74

– 8.64 (m, 4H), 8.39 (dd, *J* = 8.2, 5.3 Hz, 4H), 8.21 (dt, J = 13.0, 7.6 Hz, 4H), 7.79 – 7.53 (m, 9H), 7.51 – 7.33 (m, 5H), 7.31 – 7.23 (m, 2H), 7.19 (ddt, *J* = 11.6, 9.2, 2.3 Hz, 2H), 6.83 (ddt, *J* = 8.8, 5.3, 2.7 Hz, 4H), 6.51 (td, *J* = 8.3, 3.9 Hz, 2H), 5.80 (dd, *J* = 7.9, 2.2 Hz, 2H), 5.71 (d, *J* = 7.7 Hz, 2H). ^{13}C NMR (125 MHz, d_6-DMSO, ppm): δ 152.99, 152.96,152.8, 150.1, 150.0, 149.9, 149.7, 148.1, 148.0, 147.8, 147.7, 146.9, 140.74, 140.70, 140.6, 140.3, 140.2, 139.9, 139.8, 138.2, 138.1, 137.8, 136.6, 136.5, 134.6, 134.5, 133.1, 133.0, 132.8, 132.7, 131.8, 131.7, 131.6, 131.5, 129.6, 127.9, 127.7, 127.3, 127.1, 126.5, 125.6, 116.8, 115.8, 115.6, 115.0, 114.8, 113.7, 113.6, 110.1, 100.0, 100.4, 100.3, 100.20, 100.16, 100.0, 99.9. MS (MALDI-TOF) m/z: Calcd for $C_{66}H_{40}F_8Ir_2N_{14}$ 1566.2, Found 1711.2 (M-PF_6).

Single Crystal X-Ray Diffraction Analysis

Single crystal of complexes **M-Ir1** and **D-Ir2** were obtained by solvent diffusion method (from methanol to dichloromethane). The crystals were mounted on glass fiber and the data were collected on a on a Bruker Apex CCD II area-detector diffractometer. The structure was solved with the ShelXT structure solution program using the Intrinsic Phasing solution method and by using Olex2 as the graphical interface. Further details of the crystal structure determination have been deposited to the Cambridge Crystallographic Data Centre as supplementary publication. CCDC 2122653 (**M-Ir1**) and 2122652 (**D-Ir2**) contain the supplementary crystallographic data for this paper.

Theoretical Calculations

Theoretical calculations were carried out by using the Gaussian 09 program package. The optimization of the geometries of ground (S_0) and excited (T_1) states of the iridium(III) complexes **M-Ir1** and **D-Ir2** were carried out using density functional theory (DFT) at the B3LYP level. The ground-state structures were optimized based on their corrspoding single crystal structures. The iridium(III) atom was calculated by the Double-ξ quality basis set containing LANL2DZ, while a 6-31G** basis set was employed for C, H, N atoms. Solvent effects were considered by using the polarized continuum model (PCM) approach. The spin-orbit coupling constants of **M-Ir1** and

D-Ir2 were calculated using ORCA 5.0.2 under the conductor-like polarizable continuum model (C-PCM) in the Acetonitrile solvent with B3LYP functional and ZORA-def2-TZVP basis set.

Photophysical characterization

UV-vis absorption and Photoluminescent spectra of these complexes were measured at room temperature on a Cary 500 UV-Vis-NIR spectrophotometer and FL-4600 FL spectrophotometer in CH_3CN, respectively. In addition, the excited-state lifetimes and photoluminescence quantum yields (PLQYs) were monitored by an Edinburgh FLSP920 spectrofluorimeter. Absolute photoluminescence quantum efficiency at room temperature was measured using an integrating sphere.

Electrochemical characterization

Cyclic voltammetry was performed on an electrochemical workstation (BAS100W instrument) in CH_3CN solutions (1×10^{-3} M) at a scan rate of 100 mV s^{-1} using a glassy-carbon electrode as the working electrode, an aqueous saturated calomel electrode as the reference electrode, and a platinum-wire electrode as the auxiliary electrode. Tetrabutylammonium hexafluorophosphate (1×10^{-1} M) and ferrocene was selected as the supporting electrolyte and internal standard, respectively.

Device preparation

The rigid ITO/glass substrates and flexible ITO/PET substrates with a sheet resistance of 25±5 Ω/sq and 400±20 Ω/sq, respectively, were sonicated in acetone, ethanol, and deionized water for 30 min and then dried in an oven. The iridium(III) complexes were dissolved in CH_3CN solutions at 20 mg/ml. BMIM-PF_6 were dissolved in CH_3CN solutions at 10 mg/ml. To improve the wettability, plasma treatment of ITO was performed for 1 min. A thin film of PEDOT:PSS was spin-coated onto ITO/glass substrates and baked at 120ºC for 30 min. Then, the emissive layer of LEC was spin-coated on the top of the PEDOT:PSS layer. After spin-coating the emissive layers, the samples were baked at 70ºC for 1 h in a nitrogen glove box. Finally, an aluminum cathode was thermally evaporated in a vacuum chamber below 3×10^{-3} Pa. The EL spectra of the LECs were measured using a Hitachi F-4600 fluorescence spectrophotometer. The electrical and emission characteristics of the LECs were recorded with a Keithley 4200 semiconductor characterization system. The luminance was employed using a Topcon SR-3A spectroradiometer. The flexible devices were not encapsulated and were characterized inside the glovebox.

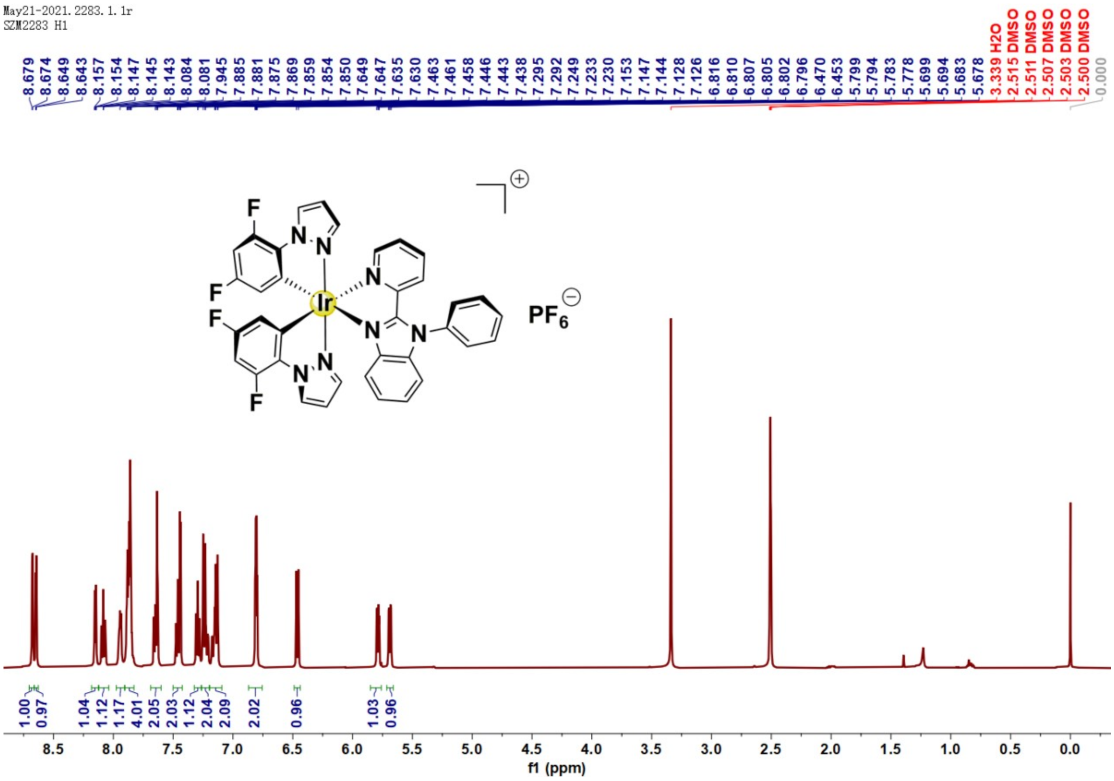


Fig. S1. ^{1}H NMR spectrum of **M-Ir1** in d_6-DMSO.

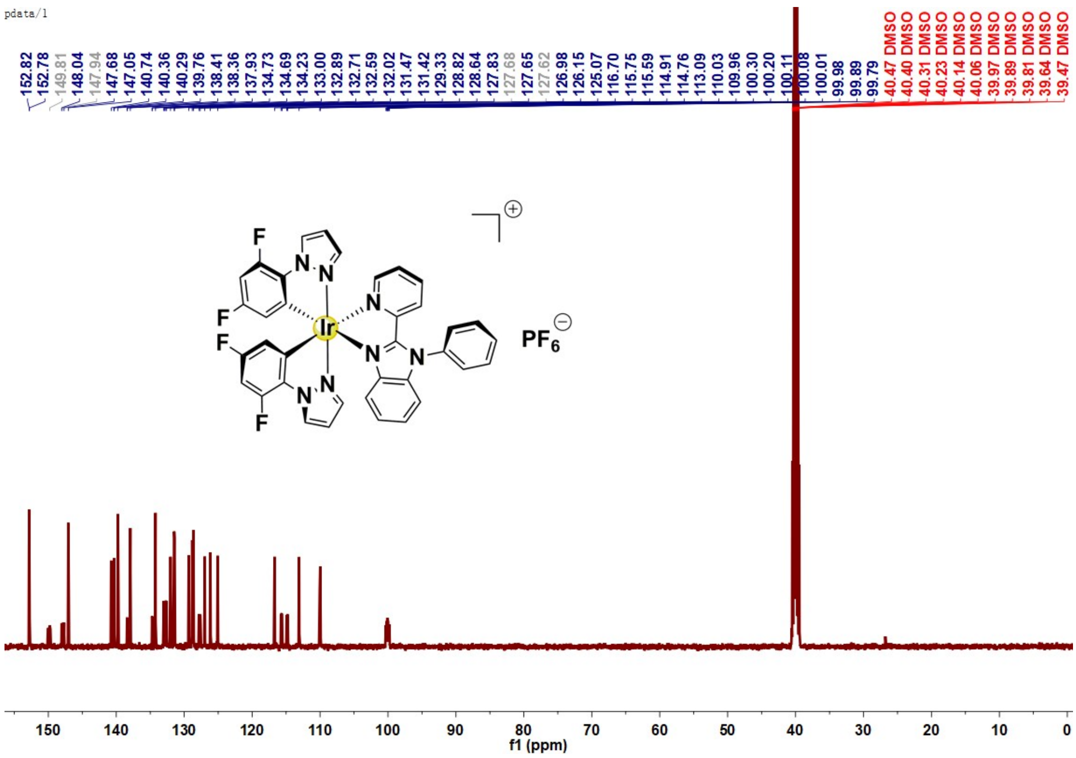


Fig. S2. ^{13}C NMR spectrum of **M-Ir1** in d_6-DMSO.

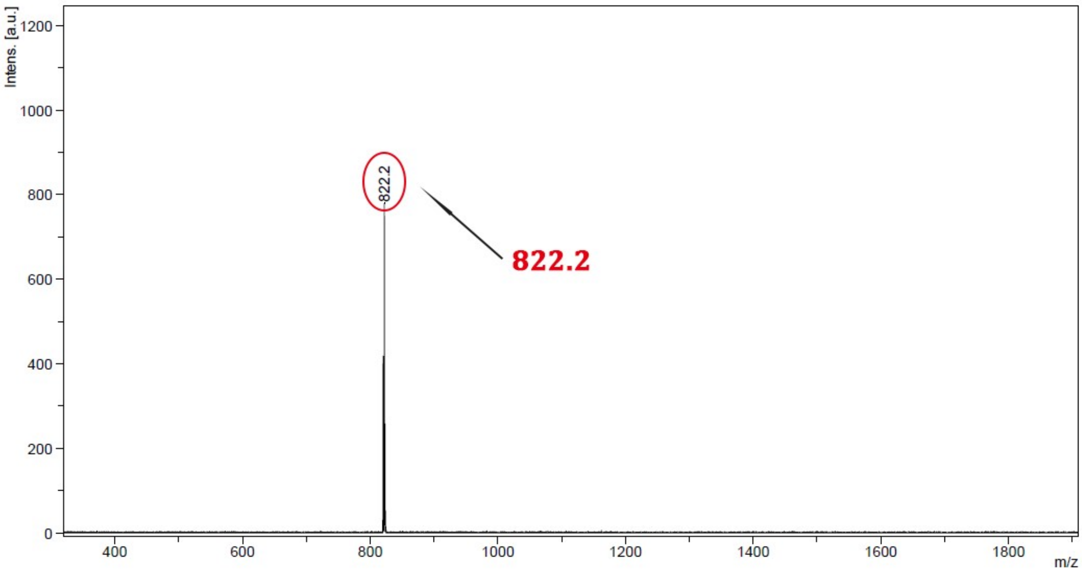


Fig. S3. Copy of the MALDI-TOF MS spectrum for **M-Ir1** (positive mode).

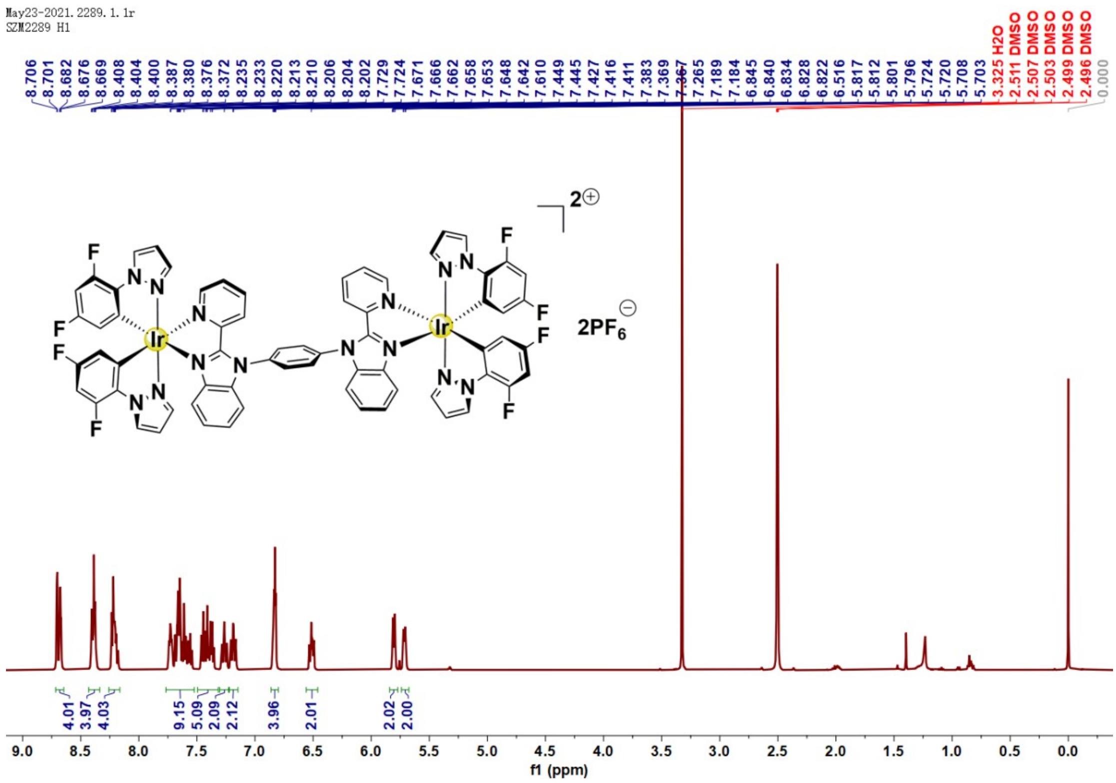


Fig. S4. ^{1}H NMR spectrum of **D-Ir2** in d_6-DMSO.

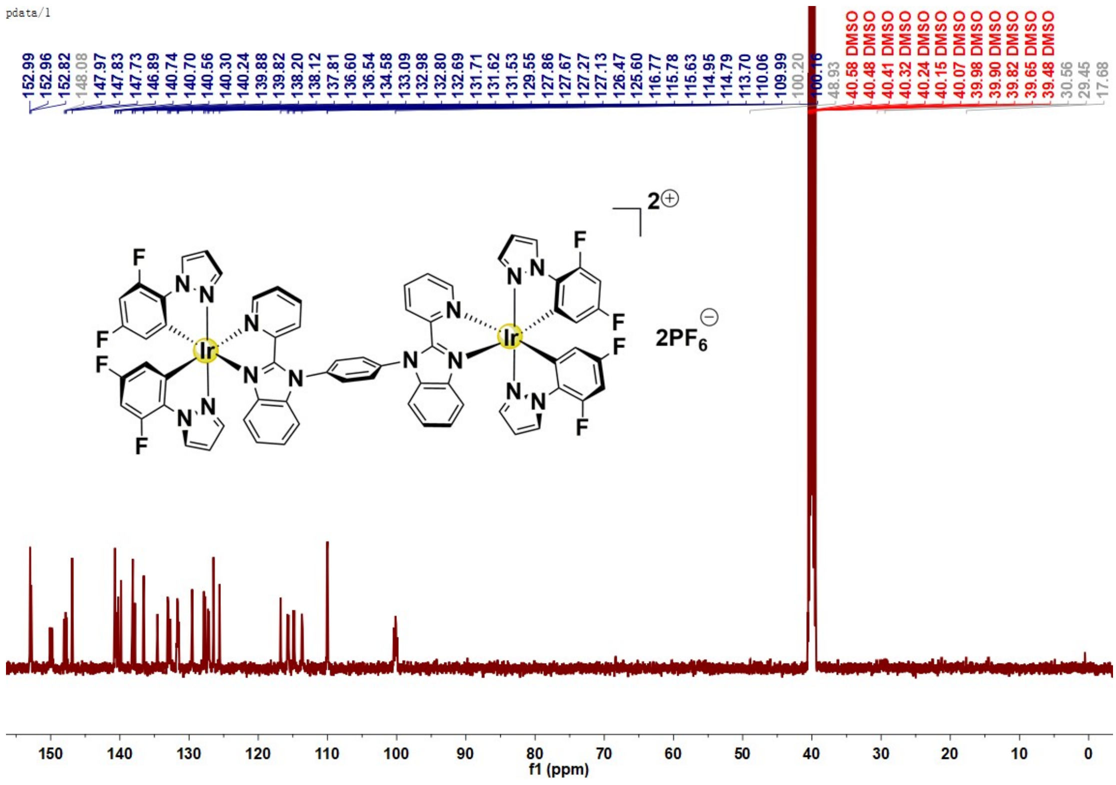


Fig. S5. ^{13}C NMR spectrum of **D-Ir2** in d_6-DMSO.

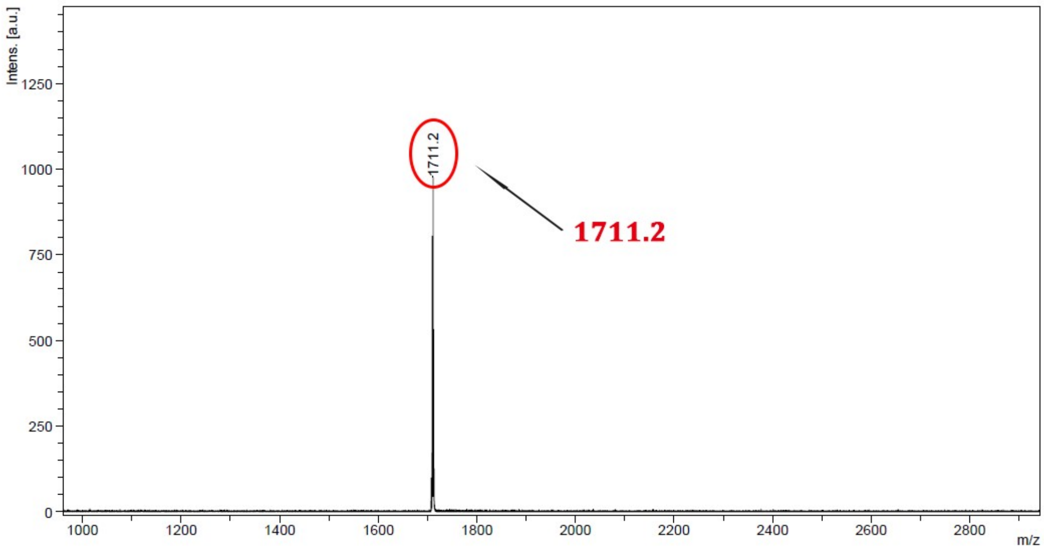


Fig. S6. Copy of the MALDI-TOF MS spectrum for **D-Ir2** (positive mode).

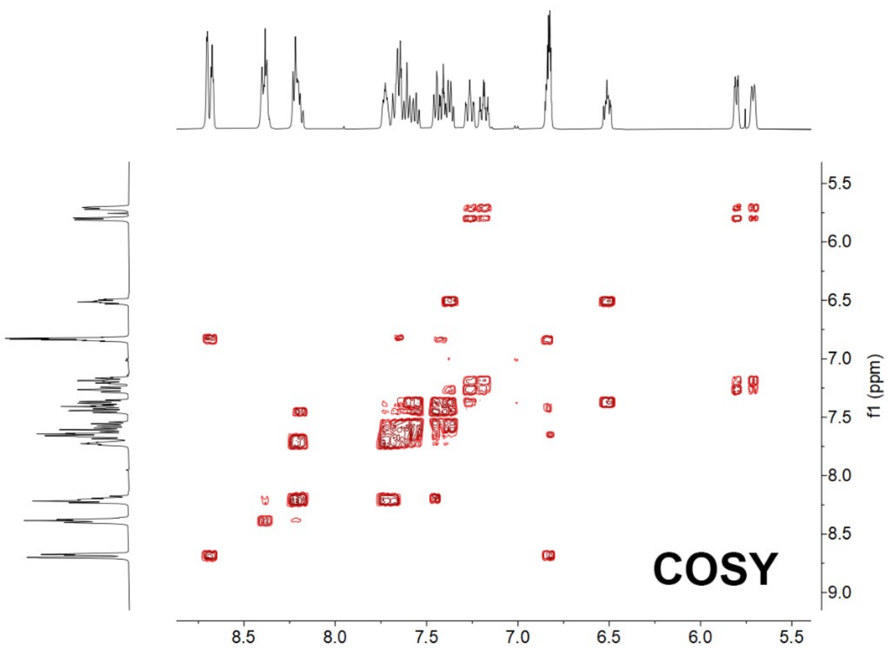


Fig. S7. 2D COSY NMR spectrum of complex **D-Ir2** in d_6-DMSO.

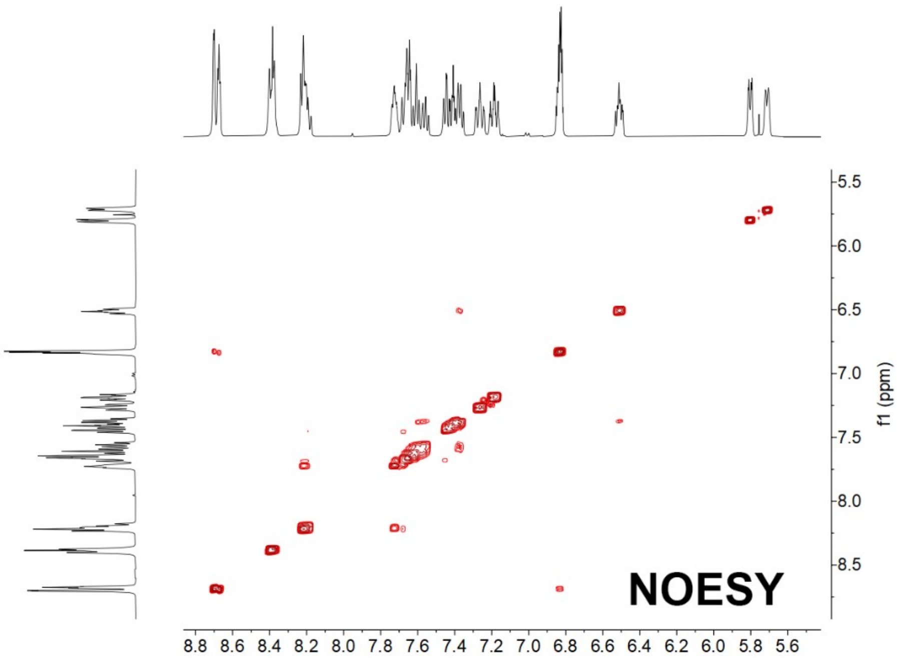


Fig. S8. 2D NOESY NMR spectrum of complex **D-Ir2** in d_6-DMSO.

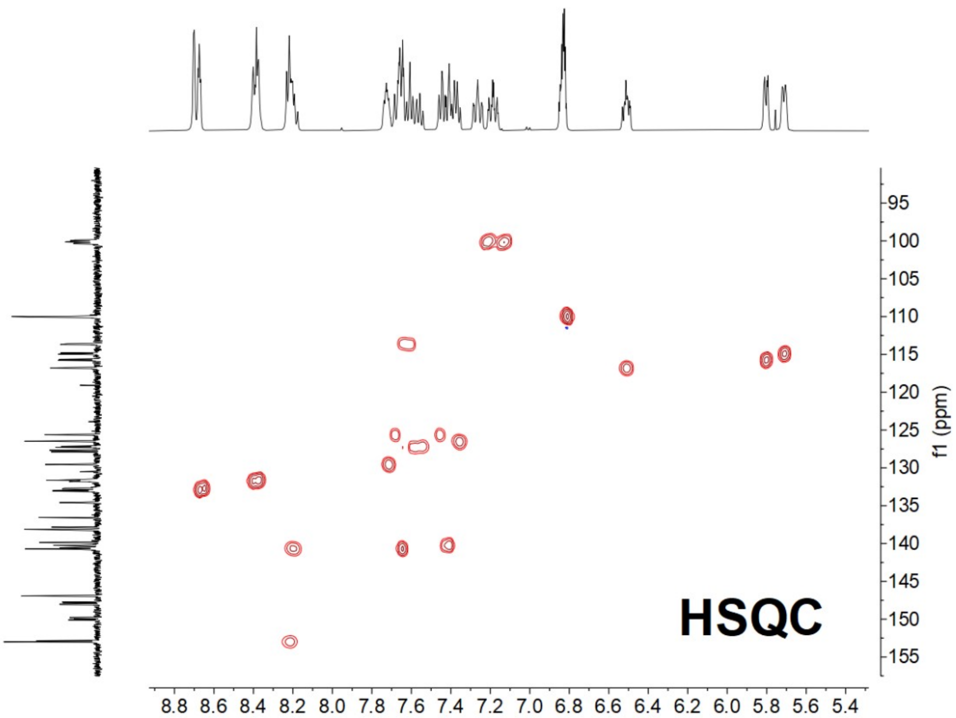


Fig. S9. 2D HSQC NMR spectrum of complex **D-Ir2** in d_6-DMSO.

Table S1. Crystal Data and Structure Refinement for **M-Ir1** and **D-Ir2**

	M-Ir1	**D-Ir2**
Empirical formula	$C_{36}H_{23}F_{10}IrN_7P$	$C_{66}H_{40}F_{20}Ir_2N_{14}P_2$
Formula weight	966.78	1815.64
Temperature (K)	173.0	173.01
Crystal system	Triclinic	Triclinic
space group	P-1	P-1
a/Å	10.9140(4)	10.5106(4)
b/Å	13.7335(5)	17.8993(7)
c/Å	16.7474(6)	20.5010(8)
α/°	67.455(2)	86.048(2)
β/°	88.131(2)	79.912(2)
γ/°	73.286(2)	84.680(2)
V/Å^3	2211.87(14)	3775.5(3)
Z	2	2
ρ calc (g/cm^3)	1.452	1.597
μ/mm^{-1}	6.847	7.992
R_{int}	0.0526	0.0416
Goodness of fit on F^2	1.042	1.031
R_1^a, wR_2^b[I>2σ(I)]	0.0911, 0.2145	0.0473, 0.1188
R_1, wR_2 (all data)	0.1093, 0.2283	0.0582, 0.1256

^{a} $R_1 = \Sigma||Fo|-|Fc||/\Sigma|Fo|$. ^{b} $wR_2 = \{\Sigma[w(Fo^2-Fc^2)^2]/\Sigma[w(Fo^2)^2]\}^{1/2}$

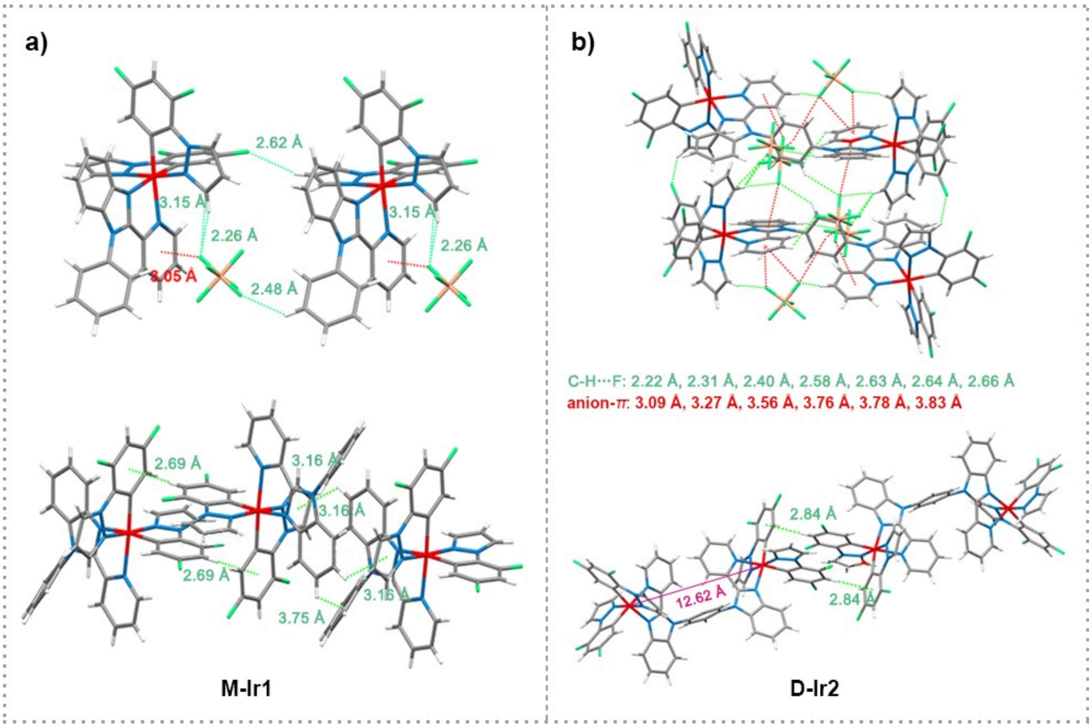


Fig. S10. Hydrogen bonding, anion-π, and intramolecular CH···π interactions in the crystal structure of a) **M-Ir1** and b) **D-Ir2**.

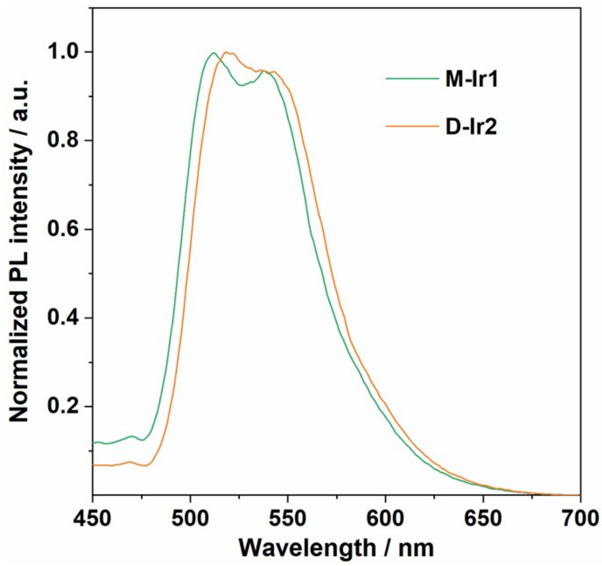


Fig. S11. PL spectra of iridium(III) phosphors in CH_3CN (10^{-5} M) at 77 K.

Table S2. Calculated energy levels, transition nature of the lowest triplet excited state (T_1) of all phosphors

Phosphors	State	eV	Assignment	Character [a]
MIr-1	T_1	2.17	HOMO-1→LUMO (90%)	^{3}LC/^{3}MLCT
DIr-2	T_1	2.10	HOMO-2→LUMO (87%)	^{3}LC/^{3}MLCT

[a] MLCT and ILCT denote metal to ligand charge transfer and intraligand charge transfer, respectively.

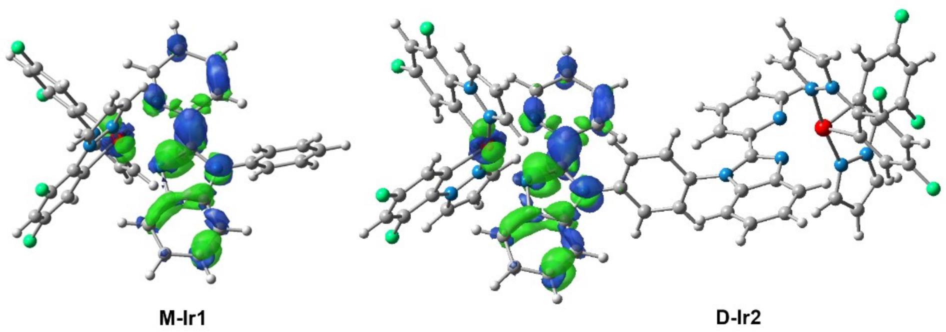


Fig. S12. Electron density difference maps (EDDMs) of the lowest energy singlet-triplet electronic transition of all complexes in their lowest-lying triplet state geometries. Blue indicates a decrease in charge density, while green indicates an increase.

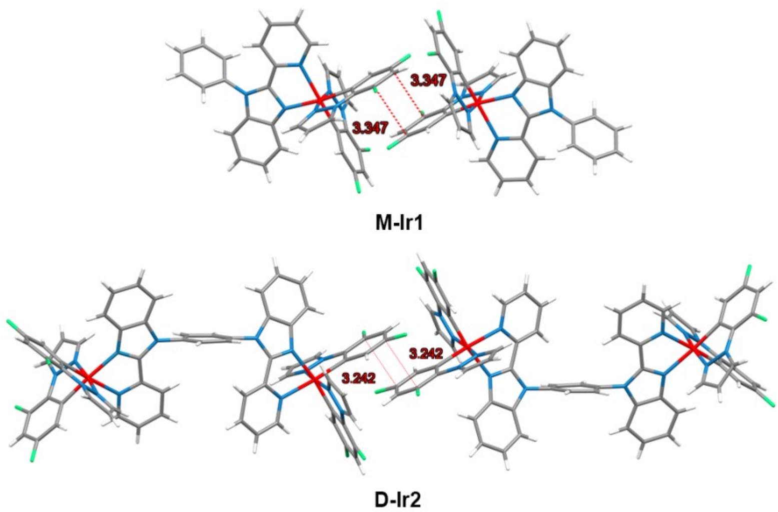


Fig. S13. The π-π interactions in the crystal structure of a) **M-Ir1** and b) **D-Ir2**.

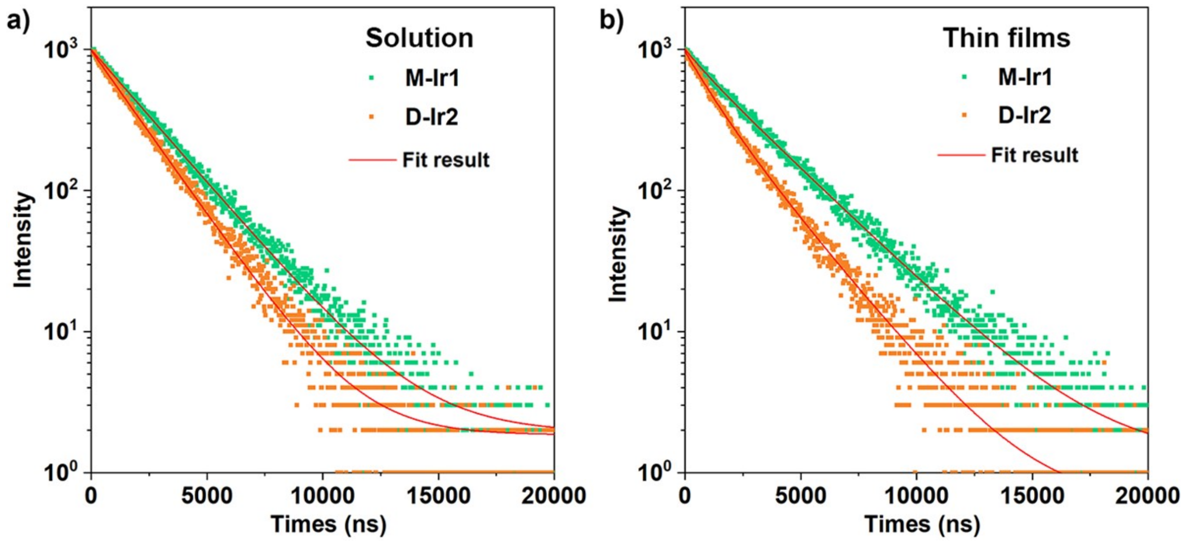


Fig. S14. Emission lifetime decay curves recorded in CH_3CN solution with a concentration of 10^{-5} M and thin films at room temperature.

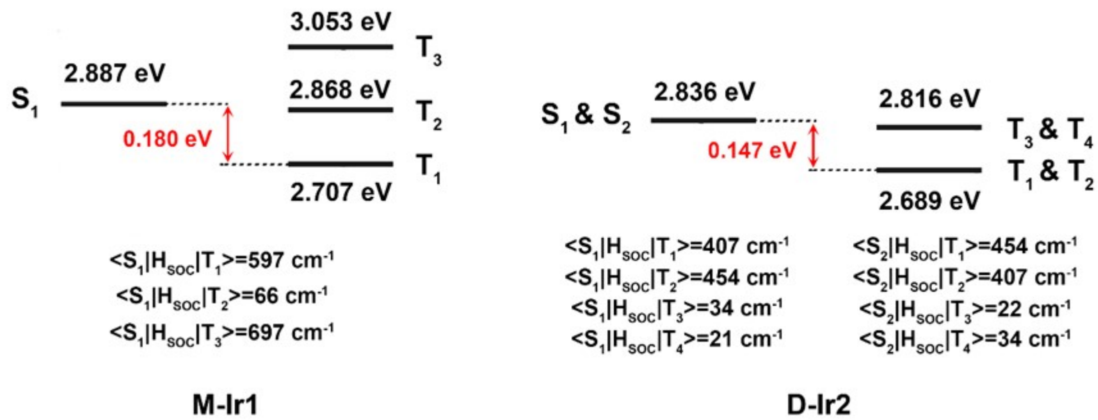


Fig. S15. The energy level diagrams and spin-orbit coupling (SOC) constant for **M-Ir1** and **D-Ir2**.

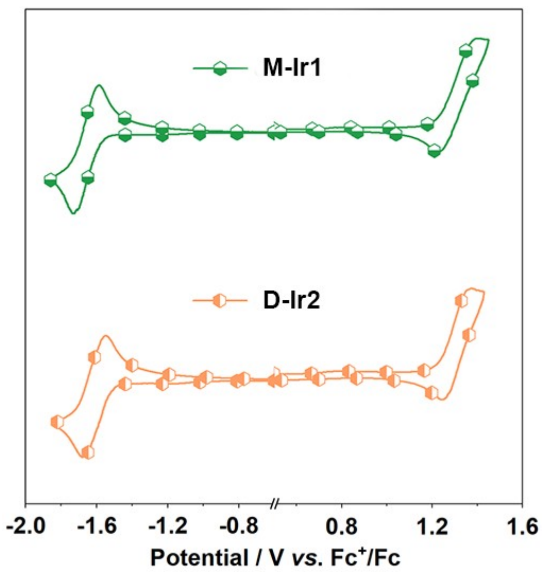


Fig. S16. Cyclic voltammograms of complexes **M-Ir1** and **D-Ir2** in acetonitrile solution (10^{-3} M).

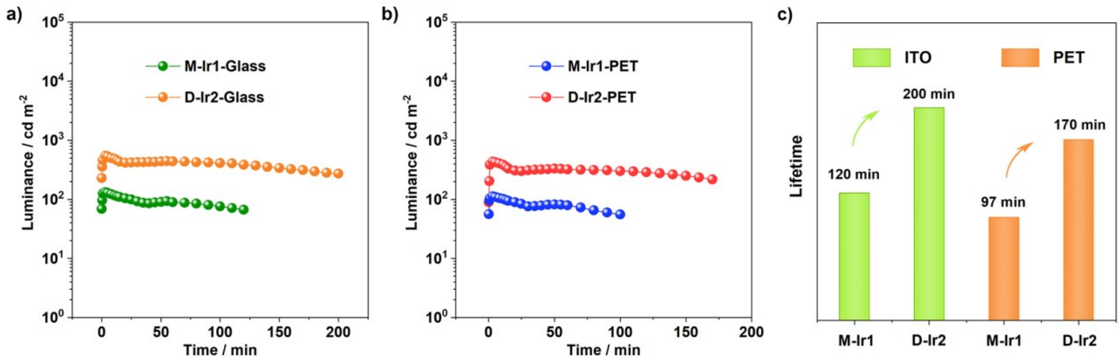


Fig. S17. Lifetime test of devices based on a) **M-Ir1-Glass** and **D-Ir2-Glass**, b) **M-Ir1-PET** and **D-Ir2-PET** under a constant current density of 5 mA cm^{-2}. c) Statistical histogram of a lifetime for rigid and flexible devices based on **M-Ir1** and **D-Ir2** under a constant current density of 5 mA cm^{-2}.

Coordinates of all optimized geometrical structures

M-Ir1 in S_0 state

N	-0.73041500	-1.84002500	0.55315900
N	-1.37314300	0.60391300	-0.23080600
N	-3.58269700	0.34740600	-0.18935200
C	-2.36987500	-0.23848800	0.02053200
C	-2.06277300	-1.59953200	0.45792300
C	-0.31247900	-3.04894800	0.94050800
H	0.76186100	-3.18625600	0.99981000
C	-3.33822000	1.64661500	-0.59695100
C	-1.19127200	-4.07747500	1.25646800
H	-0.80050300	-5.04043600	1.56627800
C	-2.55561100	-3.83786400	1.16608300
H	-3.27408400	-4.61507000	1.40604800
C	-2.99996800	-2.58424700	0.76165300
H	-4.05935300	-2.37873300	0.68567500
C	-1.93909600	1.79681300	-0.61913900
C	-4.20916500	2.67945900	-0.94190400
H	-5.28578100	2.54666100	-0.91955200
C	-1.36264100	3.01461300	-0.99952000

H	-0.28568400	3.13983900	-1.02554200
C	-3.62399900	3.88001100	-1.31393700
H	-4.25991100	4.71550400	-1.59126000
C	-2.22444500	4.04398000	-1.34265500
H	-1.81281500	5.00306000	-1.64288300
Ir	0.60419700	-0.19172400	0.07014800
N	0.81937900	-0.93364500	-1.81458600
N	0.62341900	0.60915500	1.94238300
C	2.34294700	-1.19549300	0.27786300
C	1.70165700	1.46799300	-0.26314000
F	5.05586900	-2.21464900	2.46314300
F	3.52278300	3.51375500	-2.64410600
C	2.76696500	-1.84998800	-0.89848200
F	4.30848700	-3.23172700	-2.04918000
N	1.92934800	-1.68069000	-2.01887900
C	2.27782700	1.90927600	-1.45823600
H	2.17888300	1.33940400	-2.37716600
C	3.14392300	-1.33184700	1.41566000
H	2.87935900	-0.85151300	2.35287100
C	1.88829000	2.26749600	0.88453700
N	1.29942300	1.77480700	2.06613900
C	2.98328000	3.10481300	-1.48350300
F	2.75024900	4.21328200	1.92383700
C	0.16564400	-0.87731000	-2.97344000
H	-0.75843200	-0.32238700	-3.04907300
C	3.93107400	-2.60960600	-0.91936400
C	4.30233500	-2.09551000	1.35720400
C	4.72295200	-2.74730300	0.20801800
H	5.62918600	-3.34122400	0.18309500
C	3.15832900	3.90554800	-0.36492200
H	3.71120600	4.83680600	-0.40486400
C	0.15082900	0.29894300	3.14813700
H	-0.42434300	-0.60507500	3.29002100
C	2.59804800	3.46124400	0.82070300
C	0.86611700	-1.60142700	-3.94582000
H	0.59485400	-1.74372900	-4.98125500
C	0.52878700	1.28291500	4.06986400
H	0.30088400	1.31732900	5.12476300
C	1.98382800	-2.09852700	-3.30446600
H	2.79875600	-2.70700600	-3.66148800
C	1.25907400	2.20657500	3.34789300
H	1.74375100	3.12184200	3.64648800
C	-4.89600900	-0.20619900	-0.04948400
C	-5.56469300	-0.07378400	1.16541100

C	-5.49125600	-0.82976900	-1.14386000
C	-6.84940000	-0.59614400	1.28863600
H	-5.07805400	0.42545400	1.99799300
C	-6.77613500	-1.34838800	-1.00812500
H	-4.94823400	-0.90943500	-2.08089700
C	-7.45254800	-1.23372800	0.20551900
H	-7.37877500	-0.50252200	2.23215000
H	-7.24860800	-1.84059100	-1.85294100
H	-8.45490300	-1.63986800	0.30664100

D-Ir2 in S_0 state

Ir	-6.49036631	-0.32568448	-0.02524645
Ir	6.49036055	-0.32577828	0.02532092
N	4.95324880	1.18221745	0.08516026
N	-4.95329884	1.18234768	-0.08563403
N	-4.62188218	-1.44169495	-0.03091130
N	4.62187282	-1.44179114	0.03002257
N	-2.80336630	1.74820310	-0.06580956
N	6.59954304	-0.09825273	-1.99514814
N	2.80333863	1.74808742	0.06445599
N	-6.62273678	-0.59019340	-2.04145830
N	7.62633942	0.66350588	-2.43808124
N	7.42107458	-1.60762573	2.44004041
N	6.62205149	-0.59037495	2.04155880
N	-6.59881061	-0.09829343	1.99526899
N	-7.62549030	0.66334238	2.43867325
N	-7.42188607	-1.60743937	-2.43970283
C	-4.88357916	2.55700674	-0.09686473
C	-3.47395602	-0.71825202	-0.05801607
C	-3.70670532	0.72532187	-0.06685934
C	-3.11168661	4.25930482	-0.09017024
C	7.74327283	-1.90559522	0.09731279
C	3.70666525	0.72520465	0.06580218
C	3.47391586	-0.71836877	0.05652310
C	3.52674152	2.92835784	0.08322536
C	-5.88553000	3.53431072	-0.12184688
C	4.88353956	2.55687930	0.09649153
C	-3.52677169	2.92847219	-0.08415260
C	8.46438261	1.19813948	-1.43943022
C	-1.37485057	1.70614781	-0.03318077
C	8.93344771	1.34696794	0.91146213
C	3.11166900	4.25919570	0.08927073
C	-3.34194060	-3.46029027	-0.04846180
C	-4.55100962	-2.77614577	-0.02589204

C	8.32971510	-2.60396521	-0.96246006
C	4.11526824	5.21562702	0.11228284
C	9.54636249	2.02863529	-1.70862339
C	2.22707034	-1.33872082	0.07953968
C	-2.16354642	-2.72734444	-0.07889323
C	-8.93384972	1.34703728	-0.91032474
C	0.72332477	1.71631561	-1.19969575
C	5.88549084	3.53416805	0.12206209
C	5.92849263	-0.51517192	-3.06720893
C	8.03579137	-2.34296869	1.40685836
C	10.00894501	2.16971633	0.60458932
C	-0.66652648	1.71729514	-1.23275888
C	0.66649560	1.71638233	1.23132024
C	2.16349451	-2.72745737	0.07574349
C	10.33999523	2.53257109	-0.69222224
C	-10.00933798	2.16962401	-0.60298052
C	-6.14201168	-0.01499719	-3.14221849
C	-8.32928202	-2.60399136	0.96307384
C	-9.15965553	-3.68586074	0.70134827
C	-9.45121124	-4.12408590	-0.58129124
C	-8.87294005	-3.43037790	-1.63071823
C	-8.03618757	-2.34287483	-1.40633714
C	-7.74323663	-1.90554964	-0.09687105
C	6.53338895	-0.01387378	-4.22618296
C	6.14090496	-0.01525551	3.14217602
C	-7.60977183	0.73115500	3.78988569
C	8.87251083	-3.43044638	1.63148115
C	6.63789474	-0.67296009	4.27389079
C	9.45118182	-4.12407786	0.58222429
C	-7.45082482	-1.68036625	-3.79024374
C	-9.54596619	2.02828283	1.71005722
C	9.16004876	-3.68580749	-0.70049604
C	8.12559715	0.84866725	-0.11508377
C	1.37482253	1.70608195	0.03173678
C	-5.47844982	4.85875072	-0.12909677
C	5.47842347	4.85861027	0.12932437
C	-2.22712943	-1.33860039	-0.08217095
C	-0.72334800	1.71546257	1.19825514
C	-8.12559641	0.84869501	0.11588414
C	4.55100685	-2.77624227	0.02458832
C	7.44952971	-1.68062227	3.79058840
C	-4.11528474	5.21575209	-0.11260492
C	-8.46395567	1.19798865	1.44038656
C	7.61125009	0.73129346	-3.78930164

C	-5.92720853	-0.51512541	3.06702026
C	-10.34000269	2.53225834	0.69398968
C	3.34191757	-3.46038928	0.04601361
C	-6.53162833	-0.01389388	4.22627168
C	-6.63939427	-0.67265377	-4.27378783
H	2.06075214	4.52879284	0.07800844
H	3.84420714	6.26713496	0.11850481
H	6.22802347	5.64416458	0.14944286
H	6.93446451	3.25940534	0.13867552
H	1.31881904	-0.75170920	0.10532389
H	1.19909805	-3.22546377	0.09787338
H	3.33920865	-4.54485748	0.04157162
H	5.49820861	-3.30432323	0.00132296
H	1.19973550	1.72322816	2.17653523
H	-1.30023686	1.72204554	2.11747793
H	-1.19976858	1.72480275	-2.17796758
H	1.30021518	1.72350079	-2.11891244
H	-2.06076172	4.52888691	-0.07932298
H	-3.84421286	6.26725741	-0.11879325
H	-6.22805469	5.64431207	-0.14876204
H	-6.93451859	3.25957874	-0.13802160
H	-5.49819813	-3.30422424	-0.00204977
H	-3.33923718	-4.54475955	-0.04435289
H	-1.19915198	-3.22531727	-0.10194828
H	-1.31889232	-0.75158910	-0.10845674
H	-8.03473334	-2.43030442	-4.29845370
H	-6.43600399	-0.44402248	-5.30930503
H	-5.47709682	0.83340632	-3.06591016
H	-5.05908922	-1.14835176	2.95090980
H	-6.22494048	-0.17356158	5.24921616
H	-8.35330884	1.29269101	4.33172887
H	8.35497072	1.29291624	-4.33079957
H	6.22718260	-0.17356530	-5.24926761
H	5.06039128	-1.14850068	-2.95151738
H	11.18245684	3.17807074	-0.91169645
H	8.73313126	1.11240911	1.95249617
H	5.47598417	0.83312521	3.06566740
H	6.43412319	-0.44439037	5.30934652
H	8.03325916	-2.43058722	4.29896452
H	10.10197130	-4.97087863	0.76664780
H	8.15032994	-2.31861707	-1.99472583
H	-8.73387152	1.11261800	-1.95145528
H	-11.18248070	3.17760831	0.91384133
H	-10.10203088	-4.97090343	-0.76552912

H	-8.14955898	-2.31867230	1.99528856
F	-9.71023646	-4.34439448	1.73484760
F	-9.13542255	-3.83091393	-2.88619786
F	-10.76862986	2.64383216	-1.60476451
F	-9.83917717	2.36097963	2.97838585
F	9.71101912	-4.34426700	-1.73383517
F	9.13455644	-3.83103875	2.88703522
F	10.76784233	2.64388090	1.60669138
F	9.83993484	2.36158029	-2.97680376

M-Ir1 in MC state

Ir	0.48613000	-0.22969600	0.08384400
N	1.23014400	2.33763500	1.77719600
C	1.68339000	1.36953500	-0.38893300
N	1.20618800	-1.78681400	-1.90040800
N	0.23301900	1.44213100	1.89276200
C	2.28845300	1.47893800	-1.64690100
H	2.18431200	0.69459700	-2.39068700
C	3.00838100	-1.87221200	-0.37334800
C	0.54293300	2.47664500	3.86279000
H	0.43204400	2.76869600	4.89701400
C	-0.18718300	1.51140500	3.15327700
H	-0.99255500	0.87189000	3.48986600
N	2.52150500	-1.98624300	-1.69550500
C	2.28027500	-1.11031900	0.55800100
C	2.61631600	3.54468300	0.15525100
C	3.21781300	3.65600500	-1.08576000
H	3.79743100	4.53403200	-1.34627700
C	3.17533000	-2.21585100	-2.86214000
H	4.23920500	-2.39037300	-2.89016600
C	4.17835400	-2.52217000	0.02109900
C	3.03277500	2.60461400	-1.96831500
C	1.86782100	2.42664600	0.52074000
C	2.23364700	-2.16120700	-3.86949700
H	2.40298800	-2.30472000	-4.92692800
F	4.84876300	-3.27777700	-0.86470900
F	2.75814600	4.56416600	1.01929000
F	3.60161700	2.68319500	-3.18242000
F	4.41771200	-1.55374000	3.46446700
C	3.95593800	-1.66672000	2.20863400
C	4.68031000	-2.42863100	1.30667000
H	5.59442100	-2.93991800	1.58566400
C	2.78091700	-1.01545200	1.86321500
H	2.26739900	-0.42854400	2.61958200

C	1.44500900	2.98457200	2.94890800
H	2.20960400	3.73824000	3.04729100
C	1.02260000	-1.88504500	-3.21441300
H	0.03111200	-1.76054000	-3.63016600
N	-0.86849500	-1.92337800	0.45194000
N	-1.49011100	0.50913400	-0.40123600
N	-3.69909400	0.25896900	-0.33512300
C	-2.48903100	-0.33833000	-0.16362800
C	-2.18832000	-1.71348100	0.22728700
C	-0.44744300	-3.14032800	0.80906800
H	0.61901700	-3.24808200	0.97582900
C	-3.45499400	1.56754500	-0.71927700
C	-1.31655700	-4.21298700	0.95614800
H	-0.92919700	-5.18193800	1.25103500
C	-2.66876600	-4.01175100	0.70975200
H	-3.37706600	-4.82912700	0.80085800
C	-3.11443300	-2.74853200	0.33869600
H	-4.16253300	-2.57762800	0.13146900
C	-2.05659900	1.71217700	-0.75824700
C	-4.32596500	2.61393600	-1.01804300
H	-5.40273800	2.48644700	-0.97977500
C	-1.47877600	2.93475700	-1.11665000
H	-0.40151600	3.05452000	-1.15731700
C	-3.73976100	3.82083000	-1.36839400
H	-4.37546700	4.66682800	-1.61215400
C	-2.34027800	3.97760000	-1.41851400
H	-1.92834200	4.94162400	-1.70177900
C	-5.00658000	-0.26851500	-0.08338800
C	-5.46854800	-0.34407800	1.22920300
C	-5.79890500	-0.66468800	-1.15817100
C	-6.74361900	-0.84873700	1.46723700
H	-4.83292600	-0.01583300	2.04634100
C	-7.07502800	-1.16257100	-0.90692500
H	-5.41349600	-0.59013300	-2.17057900
C	-7.54452600	-1.25822100	0.40206800
H	-7.11169800	-0.91762300	2.48657300
H	-7.70063200	-1.47821900	-1.73648700
H	-8.53927900	-1.65060400	0.59279100

D-Ir2 in MC state

Ir	-6.55695500	-0.31804000	-0.03283200
N	-7.98066200	1.20534500	-2.02948500
C	-8.17390600	0.83746100	0.31691700
N	-6.43666900	-1.04710600	1.86663600

N	-6.91869900	0.37494100	-1.91249400
C	-8.83403200	1.07203900	1.52675700
H	-8.50381400	0.60531000	2.44981200
C	-7.94225500	-2.62682000	1.02443200
C	-7.13375800	0.98464400	-4.05051000
H	-6.96144200	1.07538900	-5.11260500
C	-6.39546400	0.23244800	-3.12875900
H	-5.52988100	-0.39747600	-3.27696400
N	-7.19296500	-2.14169200	2.11470500
C	-7.81766400	-1.88739100	-0.17113400
C	-9.77254000	2.33060500	-0.76266100
C	-10.41993100	2.57304400	0.43697600
H	-11.27500600	3.23738500	0.48387000
C	-7.05733000	-2.52333000	3.40545900
H	-7.58525200	-3.37848800	3.79515500
C	-8.74811400	-3.75776700	1.08989100
C	-9.92804900	1.92628700	1.56069000
C	-8.67574400	1.47943500	-0.83499400
C	-6.18023100	-1.64056600	4.00492400
H	-5.84835500	-1.65262300	5.03231800
F	-8.84284600	-4.45135600	2.23680200
F	-10.22516300	2.94100100	-1.87086400
F	-10.54356000	2.14363900	2.73501600
F	-10.02837300	-3.86936500	-2.25846000
C	-9.34144200	-3.46090400	-1.17856300
C	-9.46448400	-4.19739700	-0.01033000
H	-10.09090300	-5.07982100	0.04934400
C	-8.54364200	-2.32887300	-1.28145900
H	-8.49696500	-1.80480400	-2.23126200
C	-8.13533000	1.59047700	-3.31721000
H	-8.93195800	2.25417000	-3.61140600
C	-5.81750200	-0.73236900	3.00290600
H	-5.15732000	0.12227200	3.04240700
N	-4.72893200	-1.38996700	-0.52182600
N	-4.99089600	1.14711900	0.17812500
N	-2.84326800	1.70878700	0.04971400
C	-3.76424900	0.71025500	-0.08320800
C	-3.56754200	-0.69130900	-0.45199800
C	-4.69309300	-2.68343400	-0.85564100
H	-5.65028500	-3.19195300	-0.89735300
C	-3.53362200	2.85063200	0.41961100
C	-3.50721500	-3.34952500	-1.13837400
H	-3.53277800	-4.39967300	-1.40747400
C	-2.31448400	-2.64362300	-1.06335600

H	-1.36705100	-3.12946600	-1.27472800
C	-2.34166300	-1.29823100	-0.71413500
H	-1.42090700	-0.73483100	-0.64687500
C	-4.88917400	2.48241000	0.49631800
C	-3.09068600	4.14571700	0.68449400
H	-2.04126900	4.41376800	0.62030000
C	-5.86018100	3.42481300	0.85501400
H	-6.90720300	3.15090600	0.92349600
C	-4.06402100	5.06841300	1.03615200
H	-3.77007300	6.09107700	1.25285300
C	-5.42510900	4.71322000	1.12069000
H	-6.15023900	5.47082400	1.40252100
Ir	6.41332900	-0.29555700	0.01533000
N	7.88532000	1.51306000	2.15870000
C	8.11676900	0.83180700	-0.15102900
N	6.67282000	-1.87962900	-2.10469800
N	6.64113900	1.00146800	2.12417500
C	8.80683700	0.92318100	-1.36542400
H	8.49349200	0.35000300	-2.23332900
C	8.24326600	-2.66163800	-0.51495900
C	7.17941000	1.51439700	4.24347500
H	7.12051300	1.64480000	5.31429900
C	6.20457000	0.99186200	3.38085000
H	5.21526800	0.61588100	3.60592700
N	7.85794500	-2.47168200	-1.86195100
C	7.74781900	-1.78865000	0.47119800
C	9.69356000	2.42523600	0.77605600
C	10.37809000	2.52247200	-0.42242000
H	11.23783100	3.17522600	-0.51954600
C	8.52487300	-2.74054200	-3.01181400
H	9.49615700	-3.20978600	-3.00539900
C	9.07876700	-3.71991100	-0.15664700
C	9.90955400	1.75728800	-1.47789500
C	8.58723600	1.59127500	0.93518800
C	7.73048800	-2.29974200	-4.05078500
H	7.94767400	-2.36035300	-5.10747300
F	9.51519600	-4.56772400	-1.10285100
F	10.11715100	3.17617800	1.80672800
F	10.55436600	1.82907900	-2.65342400
F	9.34265300	-3.25955300	3.38764000
C	8.98123100	-3.07134800	2.10813700
C	9.47313300	-3.94262400	1.15036700
H	10.12664600	-4.76960100	1.40274200
C	8.13676900	-2.01531400	1.79827400

H	7.79254900	-1.37176100	2.60254900
C	8.24446900	1.83588200	3.42547700
H	9.21092300	2.25746800	3.64981700
C	6.59114800	-1.76443500	-3.42812500
H	5.71629000	-1.31098600	-3.87586200
N	4.52335500	-1.42367500	0.11164600
N	4.88355500	1.14328100	-0.47769400
N	2.73270200	1.69953400	-0.55935500
C	3.63411700	0.69145000	-0.40094200
C	3.39413200	-0.73263000	-0.17661200
C	4.45063400	-2.73757400	0.34090300
H	5.38671200	-3.23726300	0.56650500
C	3.45677400	2.86557800	-0.76486700
C	3.25061500	-3.43425000	0.28726900
H	3.23845600	-4.50019200	0.48584700
C	2.09234500	-2.73965000	-0.03728800
H	1.13947700	-3.25447700	-0.10818500
C	2.16061200	-1.37196600	-0.27624000
H	1.27123800	-0.81853800	-0.54743400
C	4.81307900	2.49922200	-0.71062800
C	3.04320300	4.18018600	-0.97217100
H	1.99274900	4.44951400	-1.00581700
C	5.81629300	3.45917500	-0.88004800
H	6.86509100	3.18491800	-0.84721100
C	4.04793100	5.12201800	-1.13604400
H	3.77704000	6.16019100	-1.30313900
C	5.41051600	4.76708700	-1.09267700
H	6.16075200	5.54016400	-1.22923300
C	1.31140200	1.66878000	-0.41148900
C	0.76369200	1.53626700	0.86288000
C	0.50669900	1.82383900	-1.53799800
C	-0.61786600	1.52966200	1.00965500
H	1.41239700	1.43727800	1.72725800
C	-0.87594800	1.83467200	-1.38810600
H	0.95876300	1.93502300	-2.51834800
C	-1.42414700	1.67248300	-0.11774600
H	-1.07016900	1.42057300	1.99021700
H	-1.52558600	1.95784900	-2.24869500

M-Ir1 in T_1 state

N	-0.72568600	-1.80662800	0.64953500
N	-1.31995300	0.65397000	-0.18128700
N	-3.57849000	0.38450800	-0.14297800
C	-2.38469000	-0.25563400	0.08949900

C	-2.09076500	-1.54102300	0.53282300
C	-0.33282100	-3.00673700	1.06652800
H	0.74057700	-3.15506500	1.13724200
C	-3.29685300	1.68810000	-0.54447800
C	-1.21562300	-4.02879400	1.40434200
H	-0.82889700	-4.98432600	1.73901500
C	-2.59899100	-3.78122400	1.30020000
H	-3.31597900	-4.55444900	1.55868900
C	-3.03962000	-2.55595600	0.87033100
H	-4.09900800	-2.34946200	0.78758200
C	-1.87563500	1.81700300	-0.55495900
C	-4.12725100	2.72429600	-0.88241100
H	-5.20690300	2.62215700	-0.87040900
C	-1.27746800	3.04283900	-0.92423800
H	-0.19864400	3.14488000	-0.94086000
C	-3.50925100	3.94418900	-1.24935600
H	-4.13960900	4.78453200	-1.52359700
C	-2.11783400	4.09419800	-1.26778100
H	-1.68894900	5.04835300	-1.55645200
Ir	0.57783800	-0.17946900	0.09358000
N	0.69831200	-0.96609800	-1.78796200
N	0.71877000	0.61997800	1.95273900
C	2.31201800	-1.22496400	0.23924400
C	1.71033800	1.45276900	-0.30516700
F	5.10217600	-2.25419900	2.31619400
F	3.47618100	3.44064200	-2.77279300
C	2.66736400	-1.90557400	-0.94264400
F	4.13386900	-3.32867500	-2.14000600
N	1.78133600	-1.74032800	-2.02591000
C	2.23622200	1.87738300	-1.52810000
H	2.06458700	1.31722400	-2.44239800
C	3.16003700	-1.35489600	1.34211300
H	2.94659600	-0.85524200	2.28218000
C	1.98871700	2.23664200	0.83333300
N	1.44548600	1.75908400	2.04339900
C	2.98527400	3.04525600	-1.58681000
F	2.98261200	4.13962900	1.83344200
C	-0.01075800	-0.92284600	-2.91449500
H	-0.92607300	-0.35043300	-2.95928600
C	3.81784800	-2.68417500	-1.00454400
C	4.30146700	-2.14002800	1.24410300
C	4.65761500	-2.81700700	0.08793700
H	5.55222600	-3.42626000	0.03147200
C	3.25185100	3.83129700	-0.47579400

H	3.83784000	4.74058900	-0.54225200
C	0.29812100	0.32028600	3.18169900
H	-0.30339300	-0.56185700	3.34908100
C	2.74048200	3.40233300	0.73708400
C	0.62659800	-1.68508700	-3.90036700
H	0.30244500	-1.84607300	-4.91767000
C	0.76082300	1.28386800	4.08306600
H	0.58930200	1.32274600	5.14839700
C	1.76385700	-2.19041600	-3.30131300
H	2.54747800	-2.82542100	-3.68117100
C	1.48753200	2.18403800	3.32557100
H	2.01998700	3.07960800	3.60190700
C	-4.90201600	-0.14081800	-0.04204300
C	-5.62276700	0.04421500	1.13668100
C	-5.46154600	-0.80251900	-1.13418600
C	-6.91903000	-0.45654300	1.22526200
H	-5.16487800	0.56773400	1.97081200
C	-6.75754200	-1.30120800	-1.03412400
H	-4.88152200	-0.92617700	-2.04405300
C	-7.48421900	-1.12986000	0.14331900
H	-7.48637100	-0.32031400	2.14124700
H	-7.19997100	-1.82177100	-1.87836300
H	-8.49525200	-1.52023200	0.21701800

D-Ir2 in T_1 state

Ir	6.46532755	-0.33319310	-0.00602823
Ir	-6.49755328	-0.26243884	-0.09245706
N	-4.90595464	1.17383566	0.11950654
N	5.01774680	1.09536926	-0.48894363
N	4.67223189	-1.52650173	-0.17542877
N	-4.72974599	-1.28421870	-0.84449883
N	2.80922441	1.59484985	-0.77774070
N	-6.23723268	-0.79961189	1.85466175
N	-2.74940350	1.69746117	-0.02694472
N	6.16075980	-0.21708236	2.01186762
N	-7.12290850	-0.26394058	2.72611080
N	-7.91751417	-0.55817066	-2.58883914
N	-6.99875224	0.24340088	-2.00097007
N	7.01751332	-0.51359170	-1.94863525
N	8.13658943	0.16265457	-2.30189467
N	6.84201878	-1.11858652	2.75490261
C	4.92845439	2.40618974	-0.76219258
C	3.51114938	-0.81330553	-0.45939101
C	3.69552497	0.56530042	-0.53957519

C	3.17989635	4.05874306	-1.20040178
C	-7.83472646	-1.71568875	-0.50684973
C	-3.70327753	0.74743603	-0.24849327
C	-3.56159608	-0.59394777	-0.81259760
C	-3.39190669	2.79690394	0.51661435
C	5.94249842	3.38538745	-0.85933138
C	-4.75360472	2.45352487	0.60294756
C	3.56044113	2.76733984	-0.94569977
C	-8.09230375	0.59015025	2.16384407
C	1.40278421	1.58637430	-0.59607156
C	-8.95820204	1.59109038	0.15978674
C	-2.90191976	4.03403690	0.93272407
C	3.43208215	-3.57681060	-0.21899073
C	4.60872196	-2.84931528	-0.05731869
C	-8.26008045	-2.76996212	0.30684559
C	-3.83463773	4.92629663	1.43923672
C	-9.06521803	1.24348921	2.91163843
C	-2.37794277	-1.15115076	-1.28969035
C	2.25541462	-2.88071977	-0.54892773
C	8.67677055	1.57358158	1.03096760
C	-0.51908221	1.15334272	0.78708449
C	-5.68395390	3.36590643	1.11435518
C	-5.41267134	-1.57333986	2.55823601
C	-8.37861303	-1.63587245	-1.80675314
C	-9.91694871	2.22552769	0.93826405
C	0.85733281	1.13329590	0.60816779
C	-0.79648742	2.10685549	-1.42832794
C	-2.39730562	-2.44358676	-1.80144480
C	-9.99610436	2.07647749	2.31465604
C	9.81237249	2.34026777	0.80438443
C	5.46644893	0.54506964	2.85509401
C	8.46395689	-2.69988986	-0.12025134
C	9.19976711	-3.69264567	0.51393456
C	9.19018927	-3.88142736	1.88718508
C	8.40325174	-3.02370979	2.63627521
C	7.65564668	-2.01675300	2.03546801
C	7.66769097	-1.83738990	0.63756224
C	-5.77198243	-1.53728852	3.91105618
C	-6.69252816	1.19784668	-2.87780125
C	8.41763282	-0.05088787	-3.60607666
C	-9.29626433	-2.57612730	-2.26118906
C	-7.42667518	1.00993507	-4.05513587
C	-9.71552173	-3.62215993	-1.45681090
C	6.58256947	-0.93300690	4.06938935

C	9.87993514	1.69589867	-1.46912094
C	-9.17951089	-3.68987062	-0.17993302
C	-8.01095407	0.75993058	0.76542177
C	-1.33614684	1.63562018	-0.23435093
C	5.55758854	4.69128107	-1.12954780
C	-5.20223603	4.59779065	1.52722243
C	2.28528214	-1.51338948	-0.67038048
C	0.58062527	2.07117782	-1.61476979
C	8.11148886	0.84741918	-0.02007289
C	-4.73912190	-2.52617486	-1.33801009
C	-8.19659622	-0.11573793	-3.83640734
C	4.20894901	5.02607751	-1.29293077
C	8.74515327	0.91564721	-1.27773503
C	-6.86434852	-0.69492138	3.98227625
C	6.58651390	-1.15893706	-3.03273956
C	10.43503228	2.42565043	-0.43178377
C	-3.59452069	-3.14568676	-1.82432635
C	7.44247409	-0.89454884	-4.10606068
C	5.70237249	0.12664265	4.16953541
H	-1.84813905	4.28279464	0.86185259
H	-3.50300506	5.90399564	1.77601838
H	-5.89514034	5.33101728	1.92921796
H	-6.73671610	3.11352381	1.17963063
H	-1.45605500	-0.58592349	-1.26860826
H	-1.48308650	-2.89052673	-2.17901729
H	-3.65584185	-4.15611072	-2.21321784
H	-5.69825031	-3.03276261	-1.33753337
H	-1.45004859	2.48145743	-2.20975360
H	1.01594942	2.41024329	-2.54922894
H	1.50757546	0.77358752	1.39950381
H	-0.96003279	0.80870729	1.71714669
H	2.14092697	4.34289220	-1.32417136
H	3.93493993	6.05679928	-1.49535073
H	6.31329599	5.46566453	-1.21281818
H	6.98194758	3.11374813	-0.71774129
H	5.54520765	-3.35076984	0.16725687
H	3.44691048	-4.65458019	-0.10603315
H	1.32707707	-3.41888960	-0.71519614
H	1.39312493	-0.96655422	-0.94697504
H	7.03534189	-1.55585764	4.82345130
H	5.28755555	0.54277145	5.07537864
H	4.84771544	1.34776246	2.48035170
H	5.69808187	-1.77220761	-2.98138921
H	7.36430397	-1.26773679	-5.11624686

H	9.27403343	0.40463377	-4.07611830
H	-7.46507371	-0.37610025	4.81857581
H	-5.29867725	-2.05679762	4.73080026
H	-4.61720455	-2.11086625	2.06188838
H	-10.75229765	2.58052218	2.90517893
H	-8.95792438	1.76093347	-0.91256686
H	-5.97498339	1.96317372	-2.61907618
H	-7.40186788	1.61537512	-4.94886554
H	-8.90921732	-0.62464501	-4.46486440
H	-10.43140546	-4.35070102	-1.81931123
H	-7.88506524	-2.88871886	1.31896873
H	8.24254654	1.56022850	2.02609583
H	11.32053744	3.03061780	-0.58856584
H	9.76986654	-4.66342380	2.36376568
H	8.52112206	-2.61551614	-1.20121604
F	9.95718406	-4.51272616	-0.23225472
F	8.36983753	-3.18255324	3.96940158
F	10.33669178	3.03752504	1.82531829
F	10.45897136	1.75538398	-2.67951081
F	-9.57245072	-4.69680067	0.61802245
F	-9.79482444	-2.48348259	-3.50555211
F	-10.81336190	3.02542078	0.33685227
F	-9.11613589	1.07448965	4.24372142