Electronic Supplementary Information for:

Dual phosphorescent dinuclear transition metal complexes and their application as triplet photosensitizers for TTA upconversion and photodynamic therapy

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1.0 Molecular structure characterization data

Ru-2:

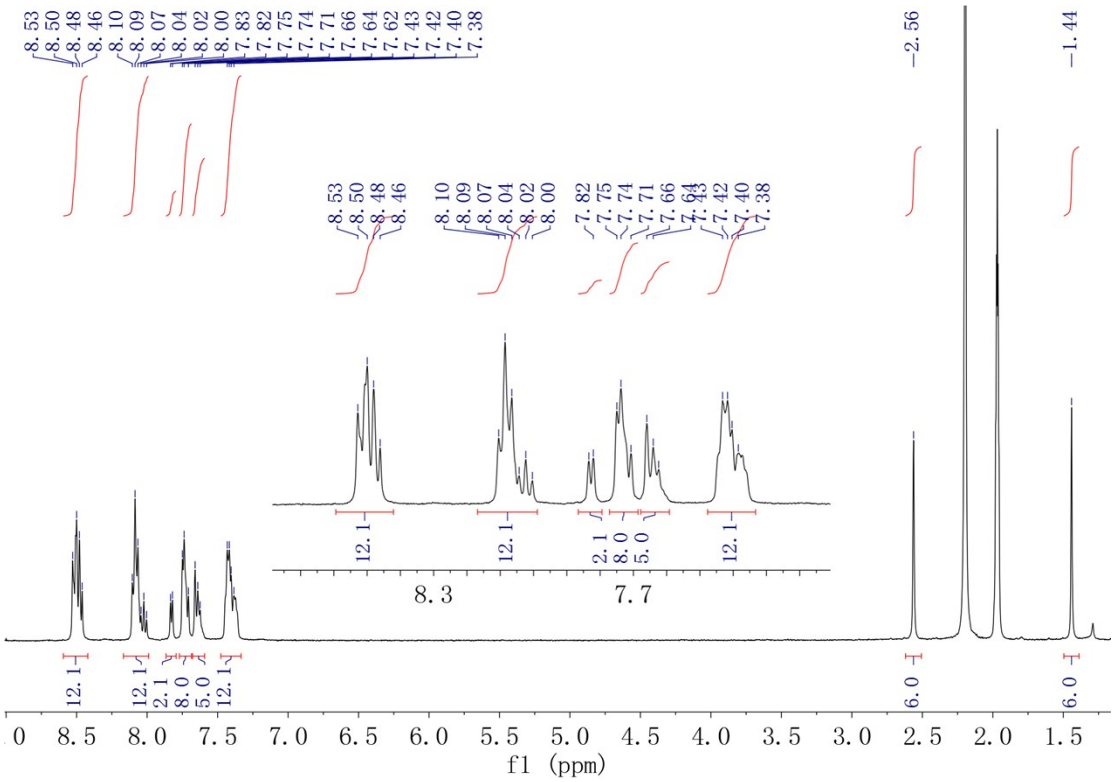


Figure S1. ^{1}H NMR spectra of **Ru-2** (400 MHz, CD_3CN), 20 °C.

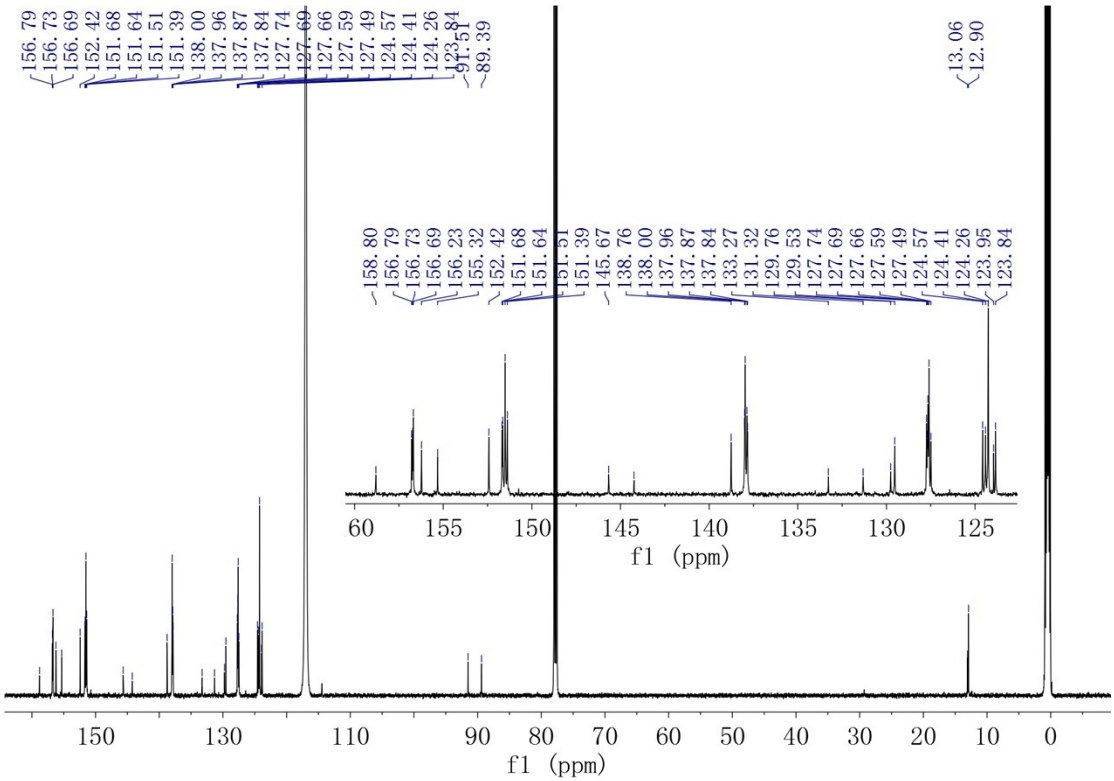


Figure S2. ^{13}C NMR spectra of **Ru-2** (150 MHz, CD_3CN), 20 °C.

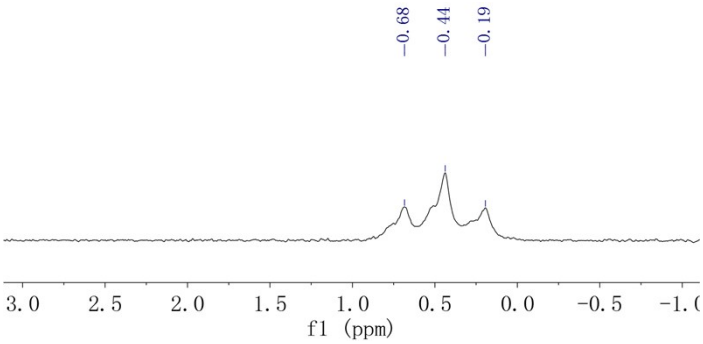


Figure S3. ^{11}B NMR spectrum of **Ru-2** (128 MHz, CD_3CN), 20 °C.

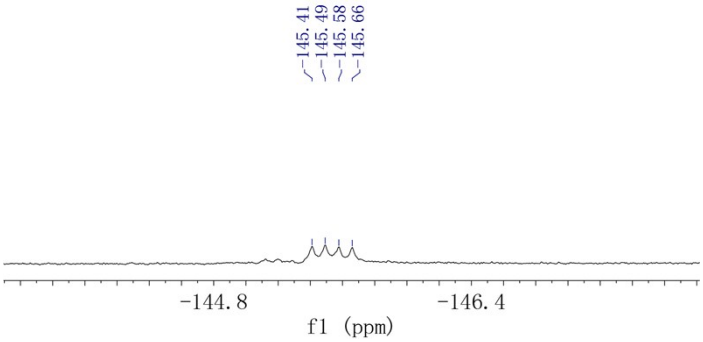


Figure S4. ^{19}F NMR spectra of **Ru-2** (376 MHz, CD_3CN), 20 °C.

Ir-2:

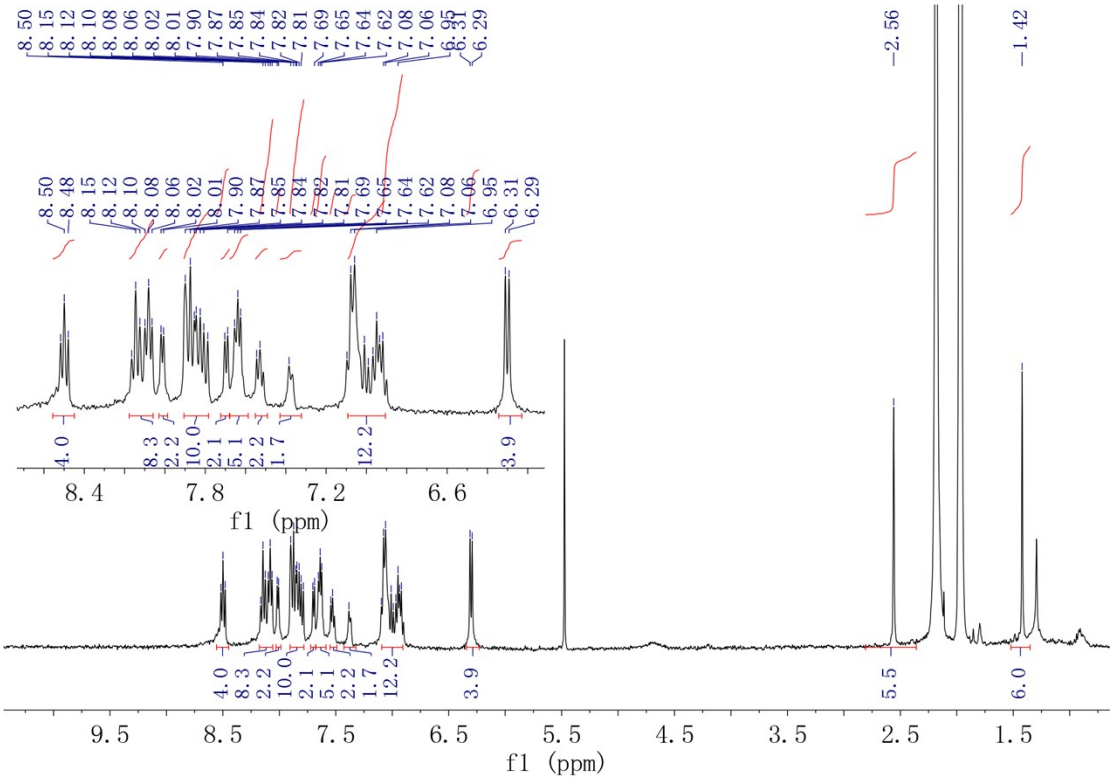


Figure S5. ^{1}H NMR spectra of **Ir-2** (400 MHz, CD_3CN), 20 °C.

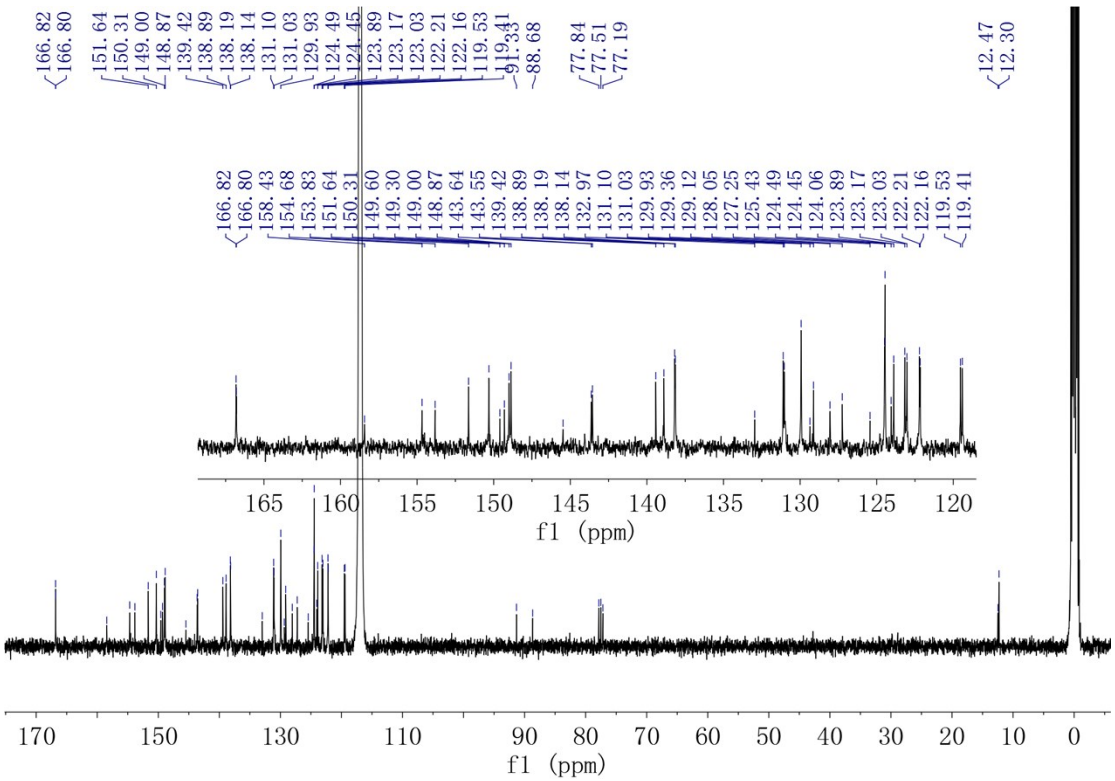


Figure S6. ^{13}C NMR spectra of **Ir-2** (100 MHz, CD_3CN), 20 °C.

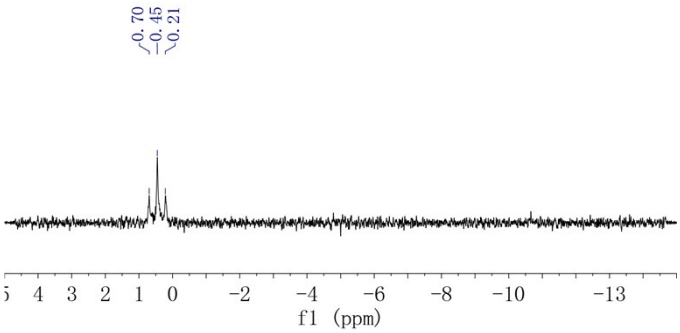


Figure S7. ^{11}B NMR spectrum of **Ir-2** (128 MHz, CD_3CN), 20 °C.

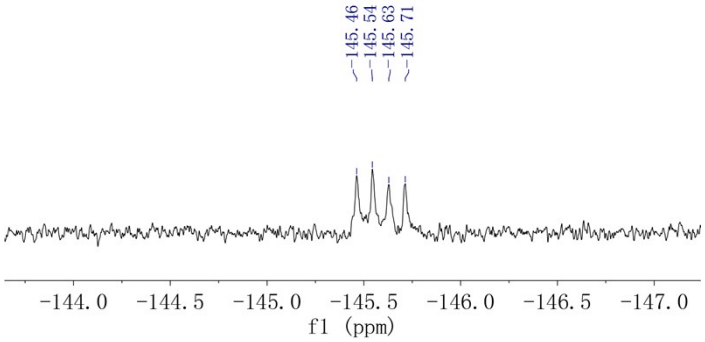


Figure S8. ^{19}F NMR spectrum of **Ir-2** (376 MHz, CD_3CN), 20 °C.

2.0 Stern–Volmer plots of triplet excited state lifetime quenching

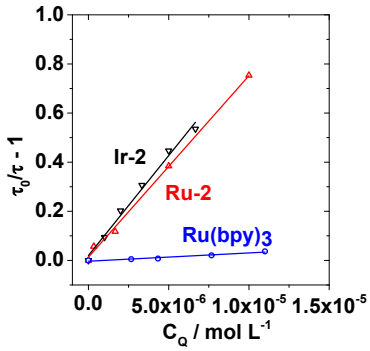


Figure S9. Stern–Volmer plots generated from triplet excited state lifetime (τ_T) quenching of complexes **Ru-2**, **Ir-2** and $Ru(bpy)_3$ measured with the increasing DPA concentration in CH_3CN. The lifetimes were measured with the nanosecond time-resolved transient absorption. c [Sensitizers] = 1.0×10^{-5} M, 20 °C.

3.0 Delayed fluorescence

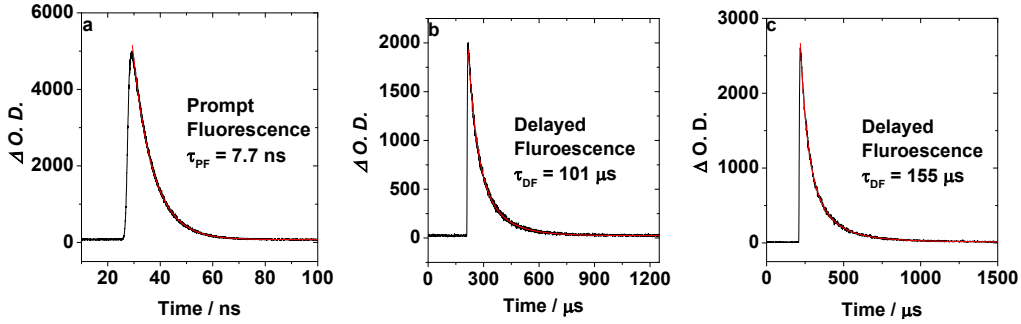


Figure S10. The delayed fluorescence decay of DPA observed in the TTA upconversion with **Ru-2** and **Ir-2** complexes as triplet photosensitizer and DPA as the triplet acceptor, the complexes were excited at 589 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and the emission was due to the upconverted emission of DPA monitored at 428 nm. (a) The prompt fluorescence decay of DPA determined in a different experiment (excited with picosecond 405 nm laser, the decay of the emission was monitored at 428 nm). (b) **Ir-2** as triplet photosensitizer; (c) **Ru-2** as triplet photosensitizer. In deaerated CH_3CN, 25 °C. c [Sensitizers] = 1.0×10^{-5} M, c [DPA] = 2×10^{-3} M.

4.0 Intermolecular triplet energy transfer

Bimolecular quenching constant (k_q):

$$k_q = K_{sv}/\tau_0 \qquad \text{(S1)}$$

K_{sv} Stern-Volmer quenching constant; τ_0 is the triplet state lifetime of the triplet energy donor.

Quenching efficiency (f_Q):

$$f_Q = k_q/k_0 \qquad \text{(S2)}$$

$$k_0 = \frac{4\pi N}{1000}(R_f + R_q)(D_f + D_q) \qquad \text{(S3)}$$

where k_0 is the diffusion-controlled bimolecular quenching rate constant; N is Avogadro's number; R is the collision radius, the sum of the molecule radii of the energy donor (R_f) and the energy quencher (R_q); D is the diffusion coefficients, the sum of the energy donor(D_f) and energy quencher (D_q). Diffusion coefficients can be obtained by the Stokes-Einstein eq. (S4).

$$D = kT/6\pi\eta R \qquad \text{(S4)}$$

where k is Boltzmann's constant, η is the solvent viscosity, R is the molecule radius. The radius of **Ir-2** or **Ru-2** is 15.6 Å and the radius of **1** is 5.7 Å. According to eq. (S6), the diffusion coefficients of donor and acceptor were 3.8 ×10^{-6} cm^{-2} s^{-1} and 1.0 ×10^{-5} cm^{-2} s^{-1}.

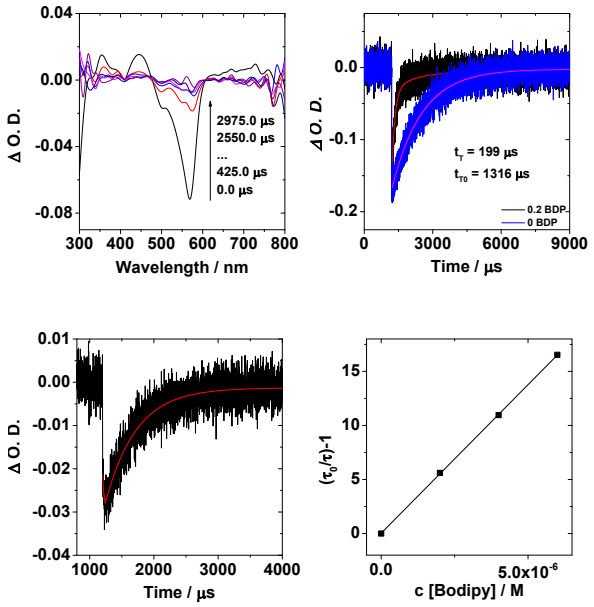


Figure S11. Nanosecond time-resolved transient absorption spectra and decay traces of the mixture of **Ru-2** and **1**. (a) the molar ratio is 1:0.2 (**Ru-2**:**1**) ; (b) the decay trace at 575 nm and (c) at 500 nm; (d) triplet lifetime quenching Stern-Volmer plot of **Ru-2** with the increasing concentration of **1**, λ_{ex} = 570 nm, c[**Ru-2**] = 1.0 × 10^{-5} M, in deaerated CH_3CN at 25 °C.

Table S1. The triplet energy transfer rate constant (k_{ET}) and triplet energy transfer efficiency (Φ_{ET}) for TTET in the mixture of **Ru-2** and **1**. [a]

Ru-2:**1**	k_{ET} /s^{-1}	Φ_{ET} (%)
1:0.2	3.7×10^4	94.7
1:0.4	11.2×10^4	96.6
1:0.6	37.9×10^4	98.5

[a]In deaerated CH_3CN at 25 °C.

5.0 TTA upconversion photos

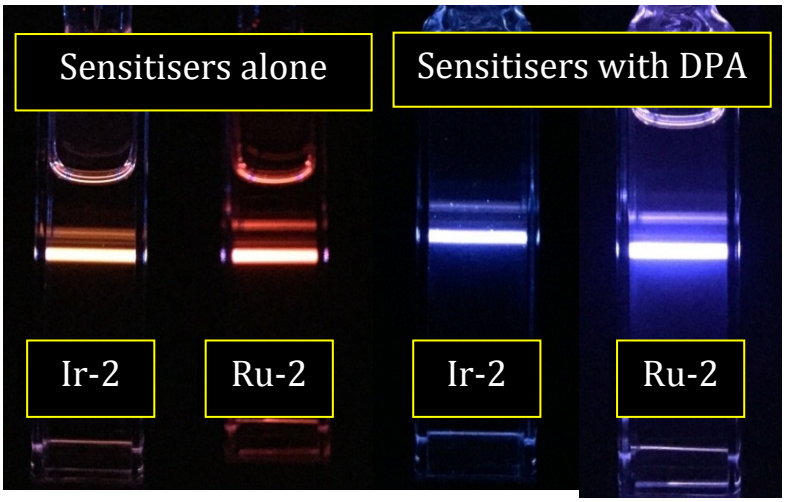


Figure S11. Upconversion with **Ir-2**, **Ru-2** as triplet sensitizers excited with yellow laser, λ_{ex} = 589 nm, 5.0 mW. In deaerated CH_3CN, 25 °C. c [Sensitizers] = 1.0×10^{-5} M, c [DPA] = 1.25×10^{-3} M for **Ir-2**, c [DPA] = 1.67×10^{-3} M for **Ru-2**.

6.0 Computational details

Table S2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main Configurations and CI coefficients of the Low-lying Electronic Excited States of the complex **Ru-2** calculated by TDDFT/B3LYP/GENECP/LANL2DZ, CH_3CN as the solvent (PCM model) based on the optimized Ground State Geometries.

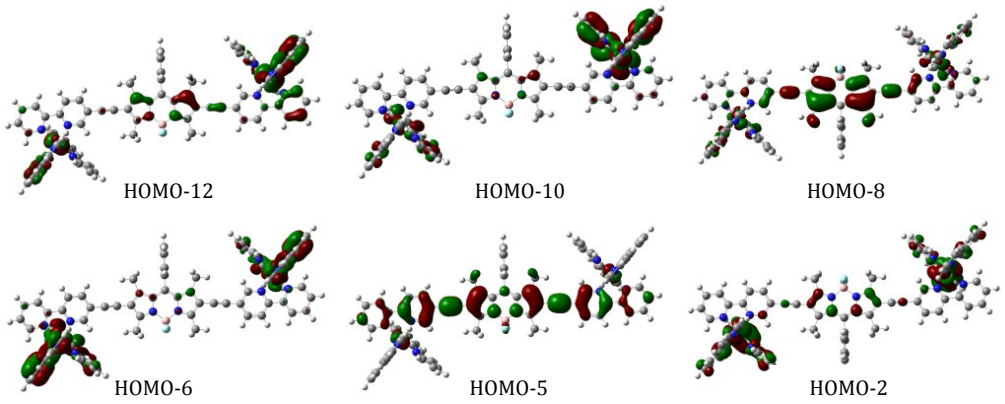
	Electronic transition	TD-SCF/B3LYP/GEN				
		Energy [a] **(eV/nm)**	***f*** [b]	**Composition** [c]	**CI** [d]	**Character** [e]
Singlet	$S_0 \rightarrow S_1$	2.2832/543	1.9522	H→L	0.6870	ILCT
	$S_0 \rightarrow S_{13}$	2.8414/436	0.1570	H-2→L	0.3727	MLCT
				H→L+2	0.3765	LL'CT
	$S_0 \rightarrow S_{23}$	3.0333/409	0.1767	H-3→L+1	0.2336	L'LCT
				H-3→L+3	0.2442	LL'CT
				H→L+6	0.2810	L'LCT
Triplet	$S_0 \rightarrow T_1$	1.5504/800	0.0000[f]	H-8→L	0.2329	ILCT
				H→L	0.6212	ILCT
				H→L+2	0.1924	LLCT
	$S_0 \rightarrow T_2$	2.1295/585	0.0000[f]	H-8→L	0.4356	ILCT
				H→L	0.2738	ILCT
				H-1→L+1	0.1729	MLCT
				H→L+2	0.2715	LLCT
	$S_0 \rightarrow T_3$	2.1570/575	0.0000[f]	H-7→L	0.3821	MLCT
				H-1→L	0.2574	MLCT
				H→L+1	0.3444	LLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values. [e] L stands for BODIPY localized ligand and L' stands for bipyridine localized ligand. [f] No spin-orbital coupling effect was considered, thus the *f* values are zero.

Table S3. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main Configurations and CI coefficients of the Low-lying Electronic Excited States of the complex **Ir-2** calculated by TDDFT/B3LYP/GENECP/LANL2DZ, CH_3CN as the solvent (PCM model) based on the optimized Ground State Geometries.

	Electronic transition	TD-SCF/B3LYP/GEN				
		Energy [a] (eV/nm)	*f* [b]	Composition [c]	CI [d]	Character [e]
Singlet	$S_0 \rightarrow S_1$	2.2837/543	1.9723	H-2 –L	0.11933	MLCT
				H-L	0.67951	ILCT
	$S_0 \rightarrow S_{11}$	2.8767/ 431	0.2980	H-8-L	0.23264	MLCT
				H-L+2	0.58867	ILCT
	$S_0 \rightarrow S_{19}$	3.1523/393	0.2372	H-10-L	0.33818	L'LCT
				H-8-L	0.23258	MLCT
				H-5-L+1	0.24395	ILCT
Triplet	$S_0 \rightarrow T_1$	1.5467/802	0.0000 [f]	H-8-L	0.21184	MLCT
				H-2-L	0.19874	MLCT
				H-L	0.59488	ILCT
	$S_0 \rightarrow T_2$	2.1266/583	0.0000 [f]	H-12-L	0.15212	L'LCT
				H-8-L	0.39479	MLCT
				H-5-L+2	0.23322	ILCT
				H-L	0.29387	ILCT
				H-L+2	0.28617	ILCT
	$S_0 \rightarrow T_3$	2.1648/ 573	0.0000 [f]	H-8-L	0.22045	MLCT
				H-2-L	0.50778	MLCT
				H-1-L+1	0.29611	L'LCT; MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strengths. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values. [e] L stands for BODIPY localized ligand and L' stands for bipyridine localized ligand. [f] No spin-orbital coupling effect was considered, thus the *f* values are zero.



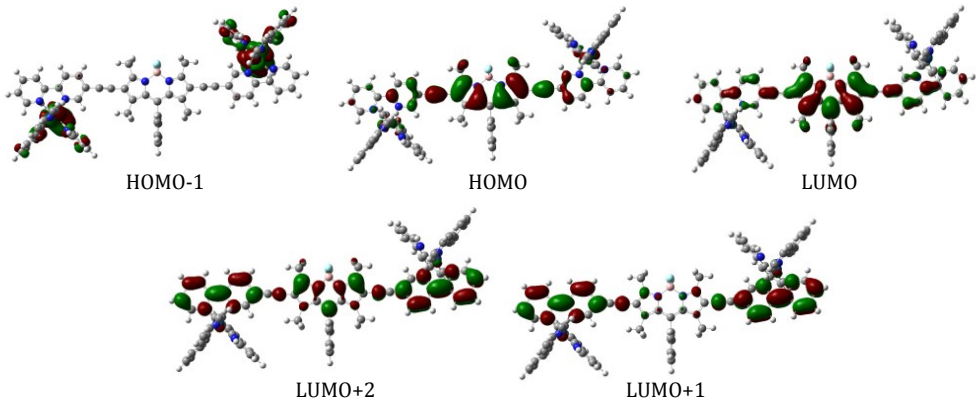


Figure S12. Electron density maps of the frontier molecular orbital of the complex **Ir-2**, based on ground state optimized geometry by the TDDFT calculations at the TDDFT/B3LYP/GENECP/LANL2DZ level with Gaussian 09W.

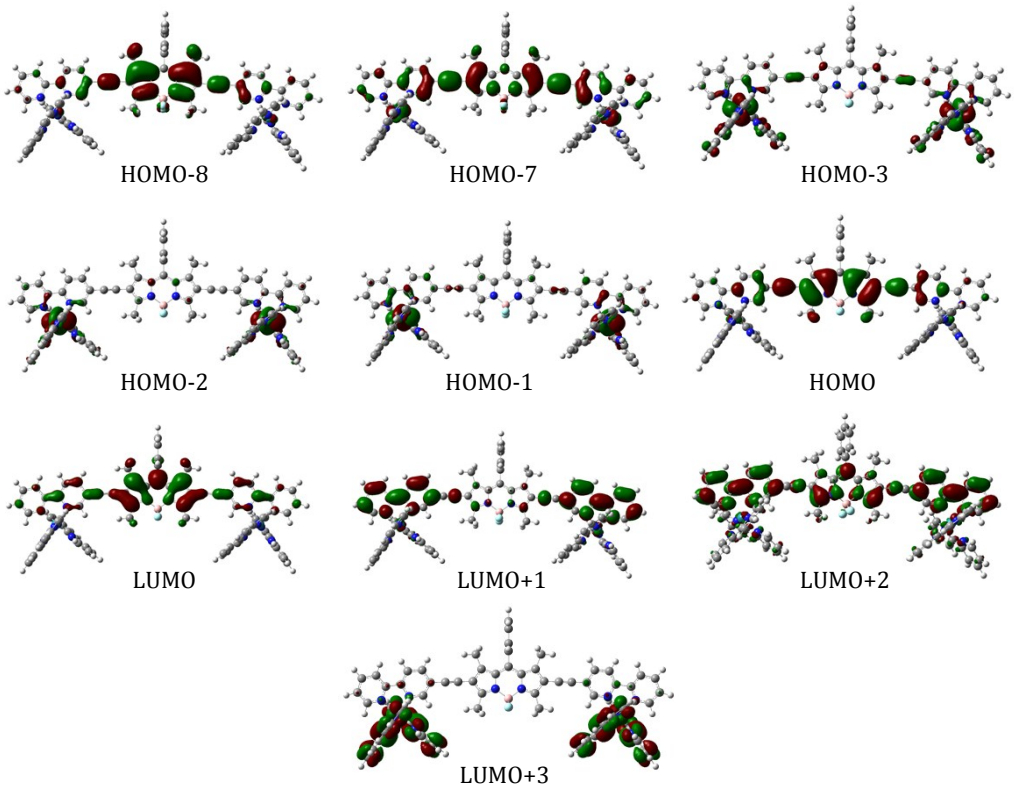


Figure S13. Electron density maps of the frontier molecular orbital of the complex **Ru-2**, based on ground state optimized geometry by the TDDFT calculations at the TDDFT/B3LYP/GENECP/LANL2DZ level with Gaussian 09W.

7.0 The x-y-z coordinates of the triplet optimized geometries of complexes

Complex Ru-2 (DFT/B3LYP/GENECP/LANL2DZ)
Charge = 4 Multiplicity = 1

C	3.34019	3.39785	-0.08063
C	1.30692	2.3319	-0.07522
C	1.93809	3.57467	-0.11244
C	2.37678	1.3765	-0.01983
C	2.36611	-0.02944	0.02229
C	3.5661	-0.76303	0.04608
C	3.81159	-2.17608	0.07896
C	5.2004	-2.2994	0.07412
C	5.79203	-1.01602	0.04391
N	3.59013	2.07428	-0.02585
N	4.79994	-0.10291	0.02852
B	5.00822	1.43793	0.0212
F	5.74345	1.81909	-1.10139
F	5.67351	1.83522	1.18637
C	-0.17072	2.08506	-0.09098
H	-0.46747	1.44683	-0.92859
H	-0.50747	1.58821	0.82453
H	-0.70819	3.0318	-0.17844
C	7.23472	-0.63438	0.01627
H	7.86938	-1.49862	0.21827
H	7.50405	-0.22487	-0.96416
H	7.43656	0.14273	0.75858
C	2.82099	-3.29903	0.11213
H	2.21455	-3.33009	-0.79899
H	3.3419	-4.25455	0.20366
H	2.1292	-3.20539	0.95439
C	1.0591	-0.75364	0.03048
C	0.40843	-1.02711	1.24287
C	0.47154	-1.16267	-1.17277
C	-0.81225	-1.6983	1.2471
H	0.86131	-0.71797	2.1802
C	-0.75607	-1.82639	-1.1645
H	0.97049	-0.95729	-2.11518
H	-1.30667	-1.90813	2.1917
H	-1.20935	-2.13008	-2.10351
C	-1.40907	-2.09926	0.04325
C	4.427	4.4202	-0.11583
H	5.18416	4.1978	0.64073
H	4.92847	4.41401	-1.0907
H	4.02473	5.41884	0.06081
H	-2.35339	-2.60237	0.04906
C	1.24557	4.94825	-0.18529
C	0.76688	5.89769	-0.23564
C	0.06963	7.2881	-0.30377
C	-0.38035	7.79883	-1.52509
C	-0.11582	8.05633	0.87042
H	-0.25234	7.22674	-2.43342
C	-0.99164	9.04046	-1.55663
H	0.2112	7.69632	1.8106
N	-0.71531	9.25837	0.80912
C	-1.13746	9.75431	-0.34627
H	-1.34213	9.44921	-2.48339
C	-1.78608	11.12263	-0.27467
N	-1.88108	11.65492	0.93834

C	-2.2501	11.79159	-1.41759
C	-2.433	12.85657	1.12248
C	-2.83535	13.05768	-1.25866
H	-2.17009	11.36323	-2.39337
C	-2.92801	13.60214	0.02647
H	-2.49374	13.25435	2.10495
H	-3.2004	13.59234	-2.11489
H	-3.37048	14.57079	0.19238
N	0.17941	10.99	2.68524
C	0.14227	11.92109	3.63211
C	1.25683	10.83167	1.91538
C	-1.13705	11.99379	4.43423
C	1.22504	12.78626	3.86362
C	2.39328	11.65891	2.08039
H	1.25455	10.07711	1.16757
C	-1.31292	12.90734	5.48745
C	2.37309	12.64695	3.07083
H	1.19172	13.53696	4.62408
H	3.25514	11.51836	1.45039
C	-2.5335	12.9051	6.17756
H	-0.54484	13.59618	5.76757
C	-3.26043	11.10838	4.72165
H	3.21681	13.29319	3.2258
C	-3.52311	11.99377	5.7944
H	-2.69691	13.59297	6.98613
H	-4.00047	10.40974	4.41808
H	-4.47489	11.95966	6.29718
C	-3.32244	7.57455	3.35755
C	-4.43359	8.85647	1.777
C	-2.04556	7.40836	4.14966
C	-4.40099	6.68198	3.47584
C	-5.56584	8.00918	1.8339
H	-4.43152	9.69499	1.12491
C	-1.8649	6.36531	5.07386
N	-1.10148	8.31458	3.92297
C	-5.54539	6.90939	2.69822
H	-4.36705	5.84518	4.14025
H	-6.42434	8.21909	1.21856
C	-0.64527	6.2846	5.76088
H	-2.6278	5.6395	5.2579
C	0.0697	8.26413	4.55877
H	-6.38599	6.24462	2.76893
C	0.33777	7.24611	5.50504
H	-0.47681	5.49496	6.46921
H	0.8041	9.00299	4.35277
H	1.28858	7.2199	6.01011
C	5.99696	-3.61729	0.0905
C	6.54755	-4.52825	0.10182
C	7.35572	-5.85895	0.11283
C	7.58009	-6.54472	1.31047
C	7.8775	-6.39177	-1.09014
H	7.18702	-6.15743	2.24011
C	8.30707	-7.72262	1.29112
H	7.72255	-5.89787	-2.01348

N	8.578	-7.53946	-1.07819
C	8.80295	-8.19201	0.05436
H	8.49046	-8.26192	2.19906
C	9.61471	-9.46597	-0.07299
N	9.98384	-9.79583	-1.30534
C	9.96357	-10.24551	1.04043
C	10.70302	-10.8963	-1.53819
C	10.72023	-11.40912	0.83012
H	9.66839	-9.97703	2.0318
C	11.09907	-11.74148	-0.47471
H	10.98238	-11.13204	-2.53495
H	11.00068	-12.02566	1.66287
H	11.67965	-12.62603	-0.67985
N	10.4717	-7.64979	-3.00708
C	11.21601	-8.14971	-3.98737
C	10.93012	-6.67433	-2.22164
C	10.57694	-9.24981	-4.80388
C	12.51817	-7.68576	-4.2396
C	12.23041	-6.14659	-2.40555
H	10.30921	-6.29608	-1.44705
C	11.22993	-9.855	-5.89114
C	13.03083	-6.6612	-3.43126
H	13.11657	-8.09176	-5.02704
H	12.58571	-5.3593	-1.7626
C	10.5615	-10.86863	-6.59245
H	12.21428	-9.5626	-6.18861
C	8.69116	-10.57011	-5.07949
H	14.02252	-6.28554	-3.6014
C	9.27367	-11.23333	-6.18608
H	11.03631	-11.35012	-7.42693
H	7.71403	-10.8342	-4.75796
H	8.72595	-12.00752	-6.69645
C	5.70135	-8.78353	-3.58897
C	6.23627	-10.44862	-2.06666
C	6.21923	-7.59214	-4.3622
C	4.36929	-9.21977	-3.68525
C	4.91558	-10.95607	-2.10375
H	6.96392	-10.91	-1.44537
C	5.40862	-6.85994	-5.24625
N	7.49412	-7.28001	-4.1594
C	3.97329	-10.33105	-2.92744
H	3.66193	-8.72846	-4.31856
H	4.6526	-11.81148	-1.50472
C	5.97113	-5.76532	-5.91811
H	4.38388	-7.1156	-5.41122
C	8.0578	-6.24389	-4.78164
H	2.96181	-10.68804	-2.98213
C	7.31429	-5.45034	-5.6878
H	5.37409	-5.18393	-6.59571
H	9.07901	-6.0199	-4.59546
H	7.78467	-4.61732	-6.1824
Ru	8.53938	-8.53053	-2.77455
Ru	-1.59154	9.81337	2.47811
N	6.5823	-9.39053	-2.80141

N	9.35226	-9.608	-4.43434
N	-3.3606	8.61417	2.53139
N	-2.08792	11.1338	4.08643

Complex Ir-2 (DFT/B3LYP/GENECP/LANL2DZ)

Charge = 2 Multiplicity = 1

C	3.34019	3.39785	-0.08063
C	1.30692	2.3319	-0.07522
C	1.93809	3.57467	-0.11244
C	2.37678	1.3765	-0.01983
C	2.36611	-0.02944	0.02229
C	3.5661	-0.76303	0.04608
C	3.81159	-2.17608	0.07896
C	5.2004	-2.2994	0.07412
C	5.79203	-1.01602	0.04391
N	3.59013	2.07428	-0.02585
N	4.79994	-0.10291	0.02852
B	5.00822	1.43793	0.0212
F	5.74345	1.81909	-1.10139
F	5.67351	1.83522	1.18637
C	-0.17072	2.08506	-0.09098
H	-0.46747	1.44683	-0.92859
H	-0.50747	1.58821	0.82453
H	-0.70819	3.0318	-0.17844
C	7.23472	-0.63438	0.01627
H	7.86938	-1.49862	0.21827
H	7.50405	-0.22487	-0.96416
H	7.43656	0.14273	0.75858
C	2.82099	-3.29903	0.11213
H	2.21455	-3.33009	-0.79899
H	3.3419	-4.25455	0.20366
H	2.1292	-3.20539	0.95439
C	1.0591	-0.75364	0.03048
C	0.40843	-1.02711	1.24287
C	0.47154	-1.16267	-1.17277
C	-0.81225	-1.6983	1.2471
H	0.86131	-0.71797	2.1802
C	-0.75607	-1.82639	-1.1645
H	0.97049	-0.95729	-2.11518
H	-1.30667	-1.90813	2.1917
H	-1.20935	-2.13008	-2.10351
C	-1.40907	-2.09926	0.04325
C	4.427	4.4202	-0.11583
H	5.18416	4.1978	0.64073
H	4.92847	4.41401	-1.0907
H	4.02473	5.41884	0.06081
H	-2.35339	-2.60237	0.04906
C	1.24557	4.94825	-0.18529
C	0.76688	5.89769	-0.23564
C	0.06963	7.2881	-0.30377
C	-0.38035	7.79883	-1.52509
C	-0.11582	8.05633	0.87042
H	-0.25234	7.22674	-2.43342
C	-0.99164	9.04046	-1.55663

H	0.2112	7.69632	1.8106
N	-0.71531	9.25837	0.80912
C	-1.13746	9.75431	-0.34627
H	-1.34213	9.44921	-2.48339
C	-1.78608	11.12263	-0.27467
N	-1.88108	11.65492	0.93834
C	-2.2501	11.79159	-1.41759
C	-2.433	12.85657	1.12248
C	-2.83535	13.05768	-1.25866
H	-2.17009	11.36323	-2.39337
C	-2.92801	13.60214	0.02647
H	-2.49374	13.25435	2.10495
H	-3.2004	13.59234	-2.11489
H	-3.37048	14.57079	0.19238
Ir	-1.59154	9.81337	2.47811
N	0.17941	10.99	2.68524
C	0.14227	11.92109	3.63211
C	1.25683	10.83167	1.91538
C	-1.13705	11.99379	4.43423
C	1.22504	12.78626	3.86362
C	2.39328	11.65891	2.08039
H	1.25455	10.07711	1.16757
C	-1.31292	12.90734	5.48745
C	-2.08792	11.1338	4.08643
C	2.37309	12.64695	3.07083
H	1.19172	13.53696	4.62408
H	3.25514	11.51836	1.45039
C	-2.5335	12.9051	6.17756
H	-0.54484	13.59618	5.76757
C	-3.26043	11.10838	4.72165
H	3.21681	13.29319	3.2258
C	-3.52311	11.99377	5.7944
H	-2.69691	13.59297	6.98613
H	-4.00047	10.40974	4.41808
H	-4.47489	11.95966	6.29718
C	-3.3606	8.61417	2.53139
C	-3.32244	7.57455	3.35755
C	-4.43359	8.85647	1.777
C	-2.04556	7.40836	4.14966
C	-4.40099	6.68198	3.47584
C	-5.56584	8.00918	1.8339
H	-4.43152	9.69499	1.12491
C	-1.8649	6.36531	5.07386
N	-1.10148	8.31458	3.92297
C	-5.54539	6.90939	2.69822
H	-4.36705	5.84518	4.14025
H	-6.42434	8.21909	1.21856
C	-0.64527	6.2846	5.76088
H	-2.6278	5.6395	5.2579
C	0.0697	8.26413	4.55877
H	-6.38599	6.24462	2.76893
C	0.33777	7.24611	5.50504
H	-0.47681	5.49496	6.46921
H	0.8041	9.00299	4.35277

H	1.28858	7.2199	6.01011
C	5.99696	-3.61729	0.0905
C	6.54755	-4.52825	0.10182
C	7.35572	-5.85895	0.11283
C	7.58009	-6.54472	1.31047
C	7.8775	-6.39177	-1.09014
H	7.18702	-6.15743	2.24011
C	8.30707	-7.72262	1.29112
H	7.72255	-5.89787	-2.01348
N	8.578	-7.53946	-1.07819
C	8.80295	-8.19201	0.05436
H	8.49046	-8.26192	2.19906
C	9.61471	-9.46597	-0.07299
N	9.98384	-9.79583	-1.30534
C	9.96357	-10.24551	1.04043
C	10.70302	-10.8963	-1.53819
C	10.72023	-11.40912	0.83012
H	9.66839	-9.97703	2.0318
C	11.09907	-11.74148	-0.47471
H	10.98238	-11.13204	-2.53495
H	11.00068	-12.02566	1.66287
H	11.67965	-12.62603	-0.67985
Ir	8.53938	-8.53053	-2.77455
N	10.4717	-7.64979	-3.00708
C	11.21601	-8.14971	-3.98737
C	10.93012	-6.67433	-2.22164
C	10.57694	-9.24981	-4.80388
C	12.51817	-7.68576	-4.2396
C	12.23041	-6.14659	-2.40555
H	10.30921	-6.29608	-1.44705
C	11.22993	-9.855	-5.89114
C	9.35226	-9.608	-4.43434
C	13.03083	-6.6612	-3.43126
H	13.11657	-8.09176	-5.02704
H	12.58571	-5.3593	-1.7626
C	10.5615	-10.86863	-6.59245
H	12.21428	-9.5626	-6.18861
C	8.69116	-10.57011	-5.07949
H	14.02252	-6.28554	-3.6014
C	9.27367	-11.23333	-6.18608
H	11.03631	-11.35012	-7.42693
H	7.71403	-10.8342	-4.75796
H	8.72595	-12.00752	-6.69645
C	6.5823	-9.39053	-2.80141
C	5.70135	-8.78353	-3.58897
C	6.23627	-10.44862	-2.06666
C	6.21923	-7.59214	-4.3622
C	4.36929	-9.21977	-3.68525
C	4.91558	-10.95607	-2.10375
H	6.96392	-10.91	-1.44537
C	5.40862	-6.85994	-5.24625
N	7.49412	-7.28001	-4.1594
C	3.97329	-10.33105	-2.92744
H	3.66193	-8.72846	-4.31856

H	4.6526	-11.81148	-1.50472
C	5.97113	-5.76532	-5.91811
H	4.38388	-7.1156	-5.41122
C	8.0578	-6.24389	-4.78164
H	2.96181	-10.68804	-2.98213
C	7.31429	-5.45034	-5.6878
H	5.37409	-5.18393	-6.59571
H	9.07901	-6.0199	-4.59546
H	7.78467	-4.61732	-6.1824