Phosphorescent [3+2+1] Coordinated Ir(III) Cyano Complexes in Achieving Efficient Phosphors and Their Application into OLED Devices

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Iridium complexes, phosphorescent phosphors, N-Heterocyclic carbene, OLEDs

Contents:

1. X-ray crystallography

Diffraction data for complexes **thpy-Br**, **TaBt-CN** and **dfppy-OCN** were collected on a Bruker D8 VENTURE diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) at 100 K. Lattice determination and data collection were performed with using a Bruker D8 VENTURE diffractometer. Intensities integration, absorption correction and computing data reduction were performed wit using the built-in SADABS-2016/2 (Bruker, 2016/2) and SAINT V8.38A (Bruker AXS, 2016) program. The structures were solved by intrinsic phasing method employing SHELXT[1] and refined by full-matrix least squares on F^2 SHELXL[2] using the OLEX2 program suite.[3] The positions of the H atoms were calculated based on riding modes, and the H atoms were refined with their thermal parameters equal to 1.2 times those of the associated C atoms (1.5 times for H atoms in the methyl groups), and they were included in the calculation of final R indices. In the final stages of the least-square refinements, all non-hydrogen atoms were refined anisotropically. The ORTEP of complexes **thpy-Br**, **TaBt-CN** and **dfppy-OCN** were interpreted by employing the PLATON program. CCDC 2068837−2068839 contain the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/structures.

Table S1. Crystal data of complexes **thpy-Br**, **TaBt-CN** and **dfppy-OCN**.

Complex	thpy-Br	TaBt-CN	dfppy-OCN
Formula	$C_{31}H_{37}BrIrN_5OS_2$	$C_{36}H_{33}IrN_6S_2$	$C_{34}H_{34}F_2IrN_7O$
Fw	831.88	806.00	786.88
T/K	100	100	100
Crystal system	triclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/n$	$P2_1/c$
a/Å	8.437	8.4348(6)	8.448(10)
b/Å	13.500	12.8004(9)	19.35(2)
c/Å	15.212	29.548(2)	19.23(2)
α/deg	64.91	90	90
β/ deg	89.28	97.833(3)	95.01(2)
γ/ deg	86.97	90	90
V/Å^3	1566.9	3160.5(4)	3132(7)
Z	2	4	4
ρ_{calc} / g·cm^{-3}	1.763	1.694	1.669
μ/mm^{-1}	5.702	4.394	4.315
F(000)	820.0	1600.0	1560.0
Crystal size/mm^3	0.08 × 0.04 × 0.02	0.12 × 0.06 × 0.02	0.04 × 0.02 × 0.01
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ (min to max)	5.42 to 52.868	4.228 to 56.814	4.252 to 53.624
Index ranges	-10 ≤ h ≤ 10, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19	-11 ≤ h ≤ 11, -12 ≤ k ≤ 17, -39 ≤ l ≤ 39	-10 ≤ h ≤ 10, -19 ≤ k ≤ 24, -24 ≤ l ≤ 24
Reflections collected	27001	28647	28360
Independent reflections	6427 [0.0828, 0.0804]	7889 [0.0911, 0.0878]	6668 [0.0732, 0.0773]
Data/restraints/parameters	6427/0/350	7889/6/409	6668/18/404
Goodness-of-fit on F^2	1.039	1.038	1.037
Final R indexes [I ≥2σ (I)]	0.0457, 0.0951	0.0512, 0.1160	0.0368, 0.0707
Final R indexes [all data]	0.0696, 0.1047	0.0716, 0.1249	0.0697, 0.0788
Largest diff. peak/hole / e Å^{-3}	3.56/-2.29	2.37/-1.96	1.01/-1.02

[a] $R_1 = \sum||F_o| - |F_c|| / \sum|F_o|$; [b] $wR_2 = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2}$

Table S2. Selected Bond Length (Å) and Angles (deg).

Complexes		**thpy-Br**	**TaBt-CN**	**dfppy-OCN**
Bond Length (Å)	Ir1-C1	2.060(7)	2.048(5)	2.057(5)
	Ir1-C4	1.973(7)	1.976(5)	1.968(5)
	Ir1-C10	2.048(7)	2.042(6)	2.052(5)
	Ir1-C21	2.016(8)	2.072(6)	2.018(6)
	Ir1-N5	2.175(6)	2.192(4)	2.133(4)
	Ir1-X[a]	2.6029(9)	2.024(6)	2.143(5)
Bond Angles (deg)	C4-Ir1-N5	173.7(3)	172.07(19)	173.07(18)
	C21- Ir1-N5	78.6(3)	77.95(19)	78.87(18)
	C1-Ir1-C4	77.9(3)	78.0(2)	77.16(19)
	C4-Ir1-C10	78.1(3)	77.9(2)	78.0(2)
	C1-Ir1-C10	156.0(3)	155.7(2)	154.76(19)
	C21-Ir1-X[a]	173.4(2)	173.6(2)	172.35(17)
	C4-Ir1-X[a]	91.6(2)	92.2(2)	93.27(18)

[a] X represent the atoms which are coordinated to the iridium center of the monodentate ligand (X = Br1 for **thpy-Br**; X = C36 for **TaBt-CN**; X = O1 for **dfppy-OCN**).

2. Photophysical measurements

UV-vis absorption spectra were recorded on a Hewlett-Packard 8453 diode array spectrophotometer. Photo-excitation and steady-state emission spectra were obtained on a SPEX Fluorolog-3 Model FL3-21 spectrofluorometer. Excited state lifetime measurements of solution samples were performed with a Quanta Ray DCR-3 pulsed Nd:YAG laser system (pulse output 355 nm, 8 ns). The emission signals were detected by a Hamamatsu R928 photomultiplier tube and recorded on a Tektronix TDS 350 oscilloscope, and analysed by using a program for the exponential fits. Emission quantum yields (ϕ) are recorded on the absolute PL quantum yield spectrometer C11345 (Quantum-QY Hamamastu). Errors for λ values (± 1 nm), τ (± 10 %), ϕ (± 10 %) were estimated. Solution samples for measurements were degassed on a high-vacuum line in a two-compartment cell that consisted of a pyrex bulb (10 mL) and a quartz cuvette (path length: 1 cm) and was sealed from the atmosphere by a Bibby Rotaflo HP6 Teflon Stopper. The solutions were rigorously degassed by five successive freeze/pump/thaw cycles. The thin films (2 wt% in PMMA) of samples are prepared by dropping the mixed solution of PMMA and samples in CH_2Cl_2 on quartz glass plate (1 cm × 1 cm) and air dry. Emission spectra for glassy state (in a 77K DMF/MeOH/EtOH solution, v/v/v = 1/1/4) and solid state samples were recorded by placing the sample in 5 mm diameter quartz tubes. Low temperature (77 K) emission spectra were obtained by placing the quartz tubes in a liquid nitrogen Dewar flask equipped with quartz windows.

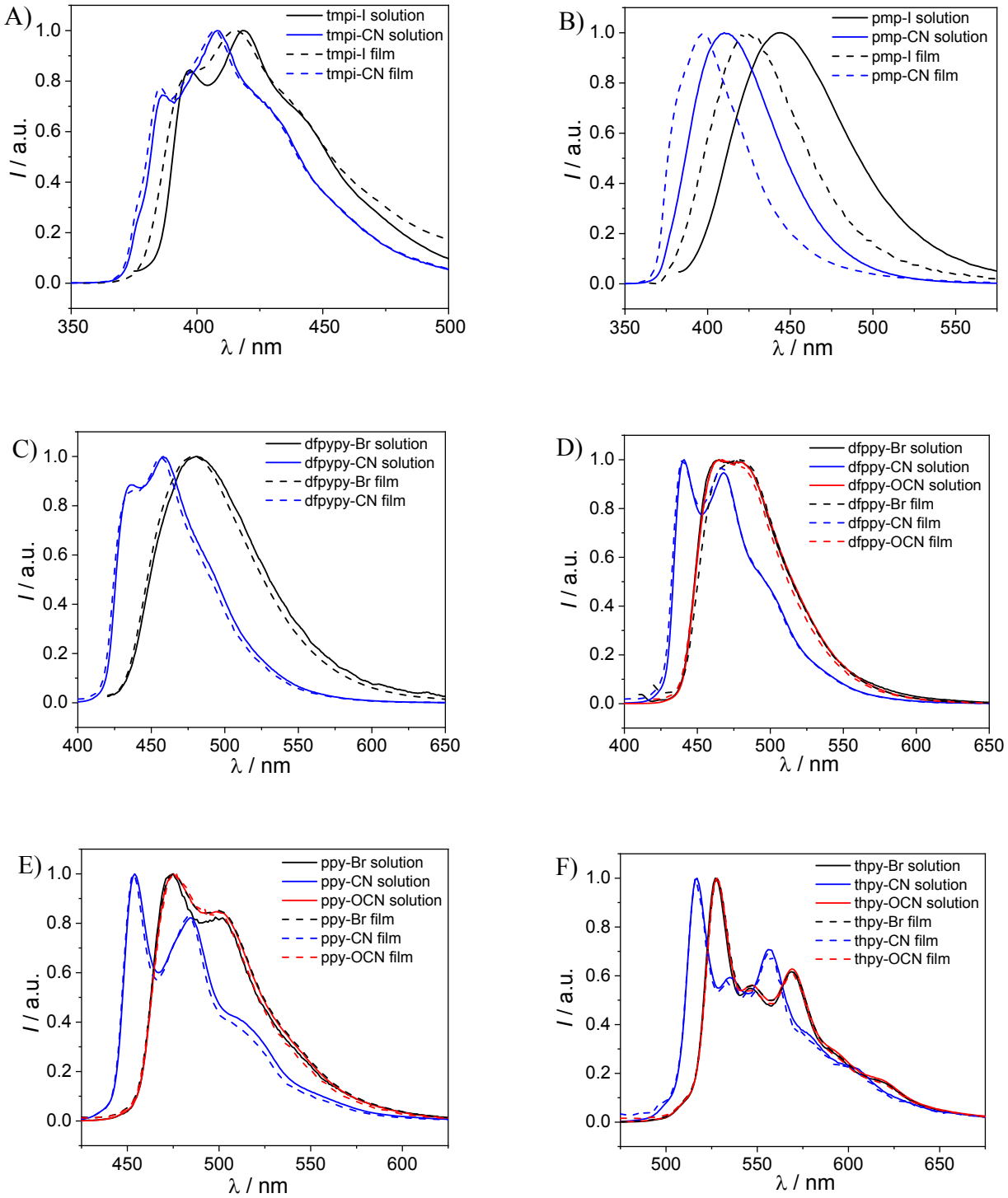


Fig. S1. Emission spectra (normalized) of solutions (concentration of 2.0×10^{-5} M in degassed CH_2Cl_2; solid lines) and thin-films (2 wt% in PMMA; dash lines) of Ir(III)-Br (black lines), Ir(III)-CN (blue lines) and Ir(III)-OCN (red lines) complexes at R.T.

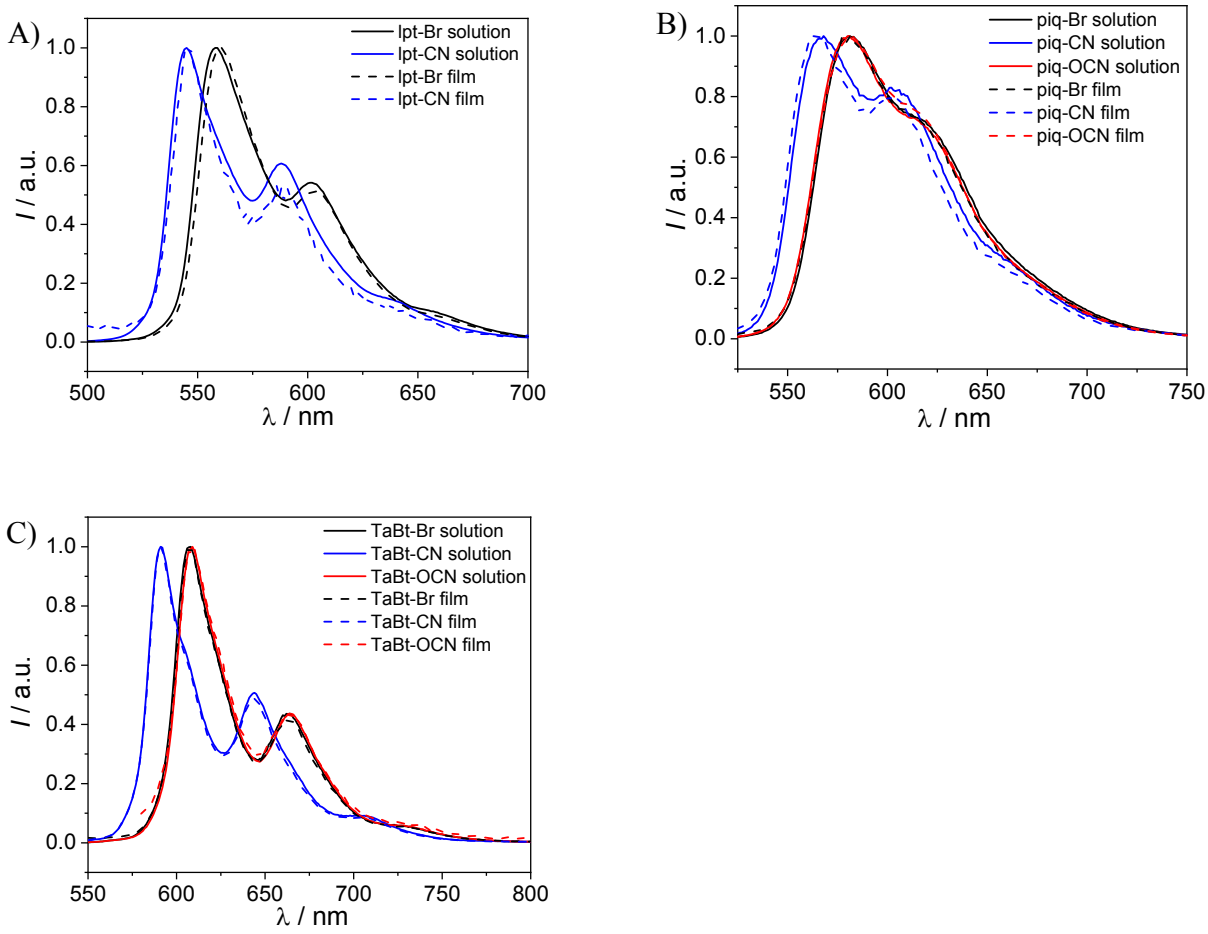


Fig. S2. Emission spectra (normalized) of solutions (concentration of 2.0×10^{-5} M in degassed CH_2Cl_2; solid lines) and thin-films (2 wt% in PMMA; dash lines) of Ir(III)-Br (black lines), Ir(III)-CN (blue lines) and Ir(III)-OCN (red lines) complexes at R.T..

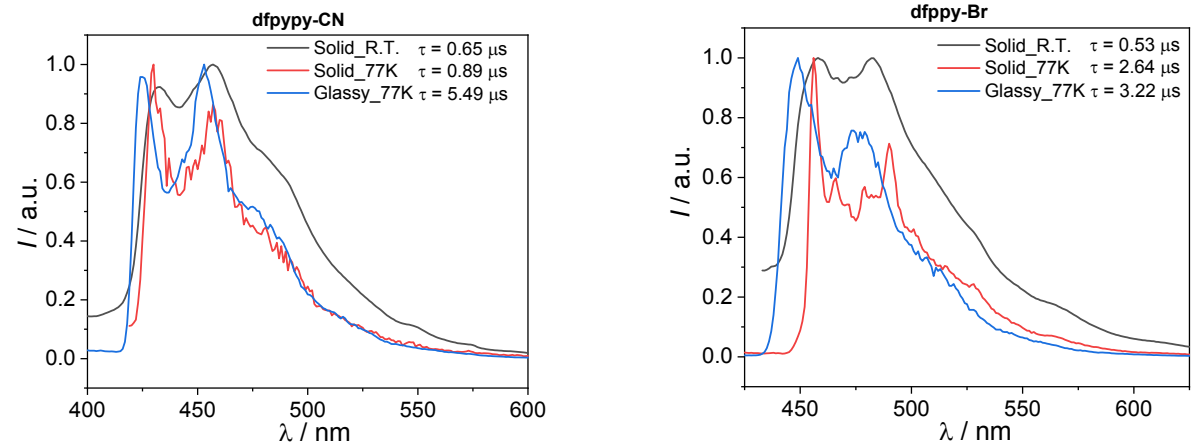


Fig. S3. Emission spectra (normalized) of iridium complexes at solid-state (77K and R.T.) and in 77K glassy solutions, with showing their lifetimes.

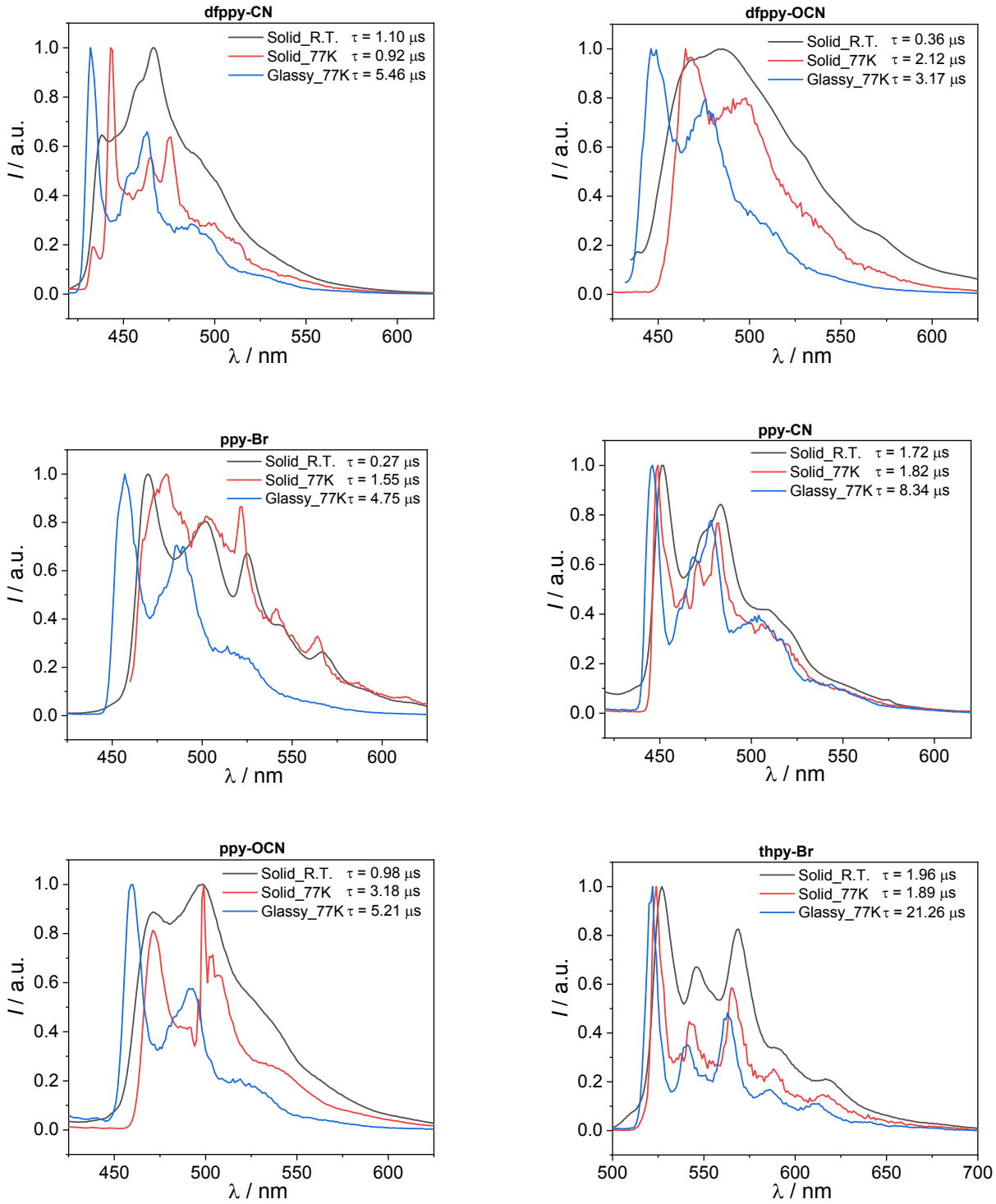


Fig. S4. Emission spectra (normalized) of iridium complexes at solid-state (77K and R.T.) and in 77K glassy solutions, with showing their lifetimes.

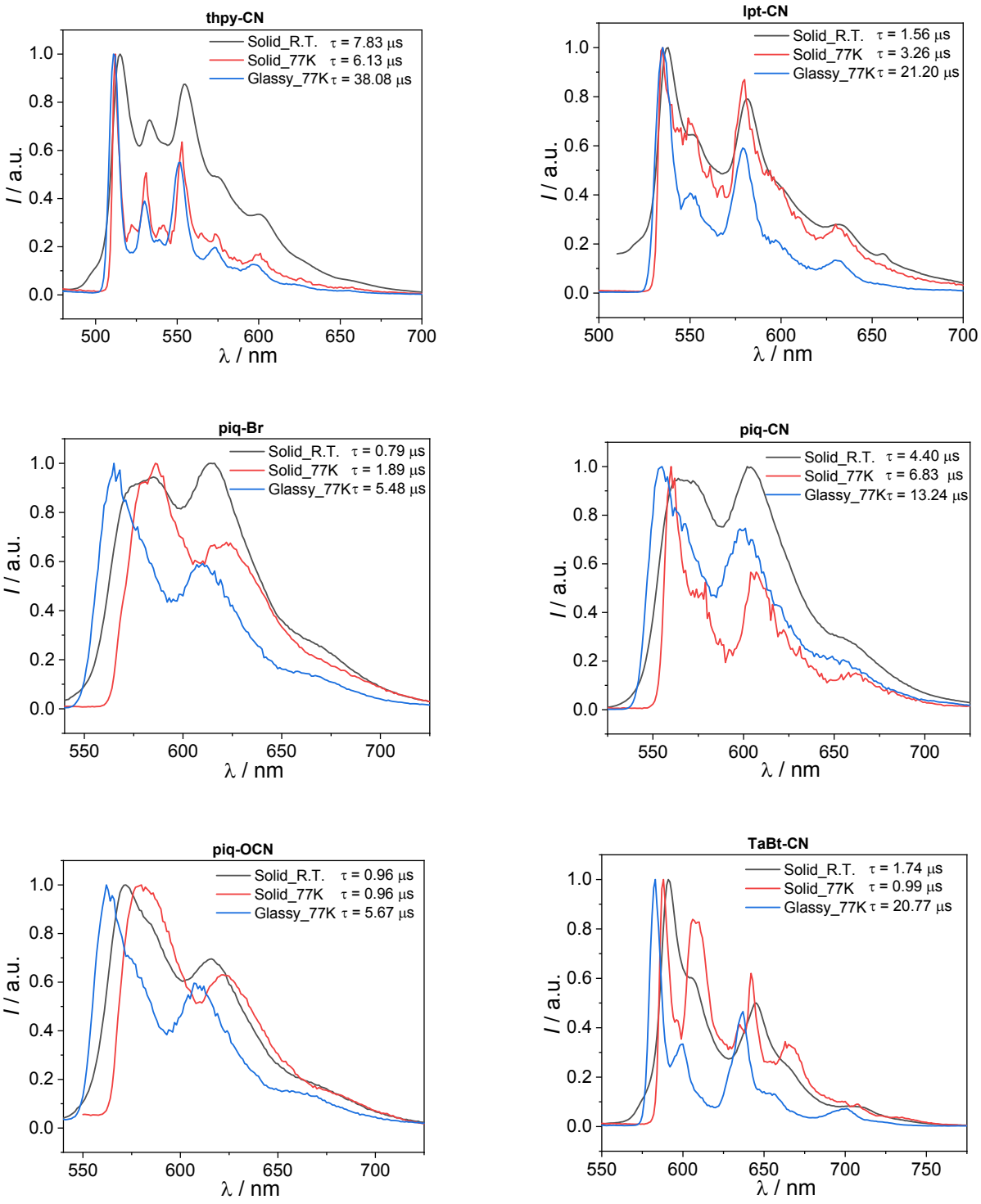


Fig. S5. Emission spectra (normalized) of iridium complexes at solid-state (77K and R.T.) and in 77K glassy solutions, with showing their lifetimes.

3. Cyclic voltammetry

Cyclic voltammetry measurements were performed on a PalmSens-EmStat3 potentiostat. The glassy-carbon electrode as working electrode was polished with 0.05 μm alumina on a microcloth, sonicated for 5 min in deionized water, and rinsed with CH_2Cl_2 before use. A standard calomel electrode (SCE) was used as reference electrode and a platinum wire as counter electrode. All solutions of samples were prepared in CH_2Cl_2 containing 0.1 mol·dm^{-3} tetra(*n*-butyl)ammonium hexafluorophosphate ($^nBu_4NPF_6$) as supporting electrolyte. The solutions were purged and maintained under N_2 atmosphere. Scan rates were 0.1 V·s^{-1} and the potentials were reported with respect to the potential of SCE. Ferrocene was used as internal reference and recorded with the potential at the range of 0.05 – 0.07 V for ferrocenium/ferrocene ($Fc^{+/0}$) vs SCE.

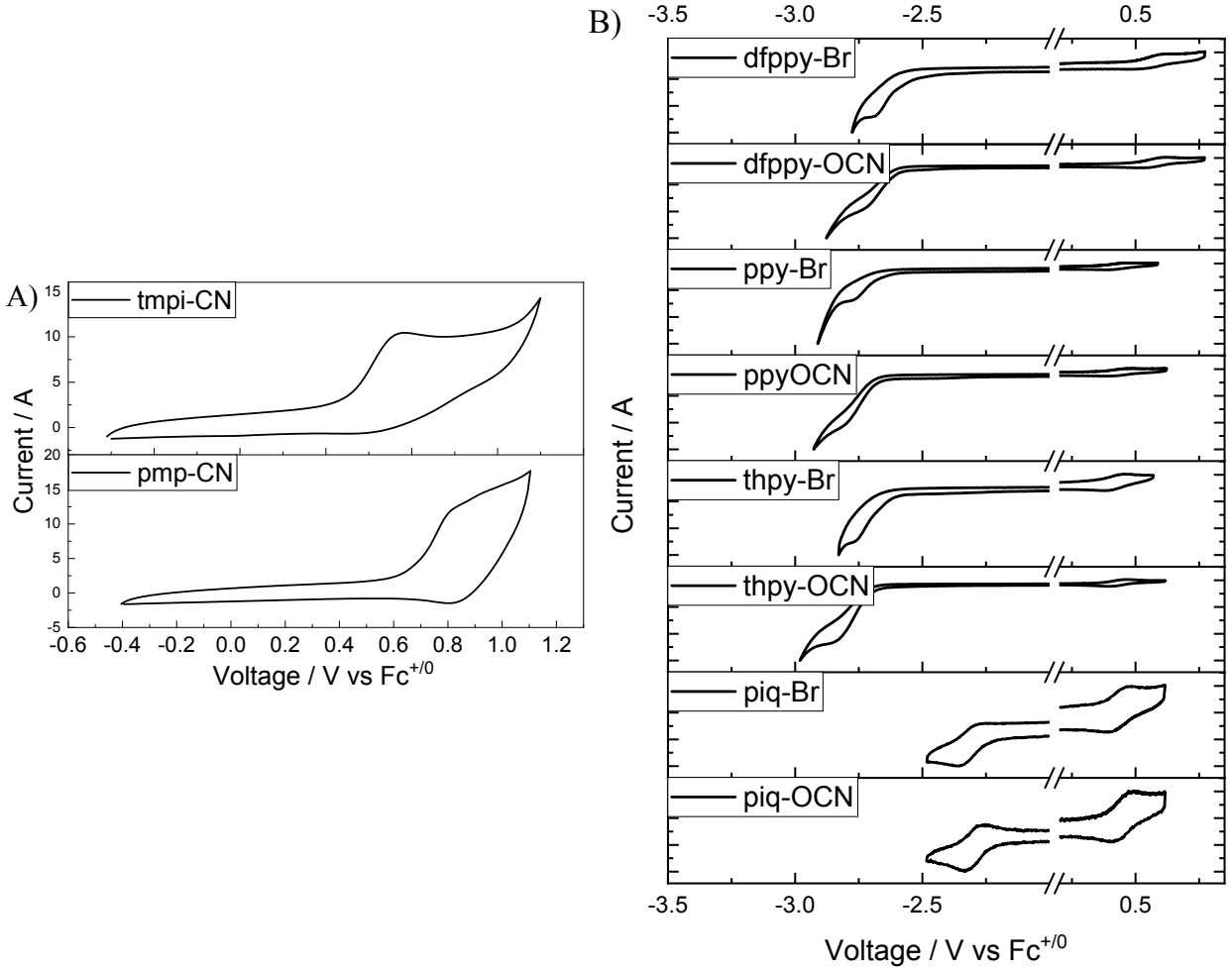


Fig. S6. Cyclic voltammograms of solution of Iridium complexes in CH_2Cl_2.

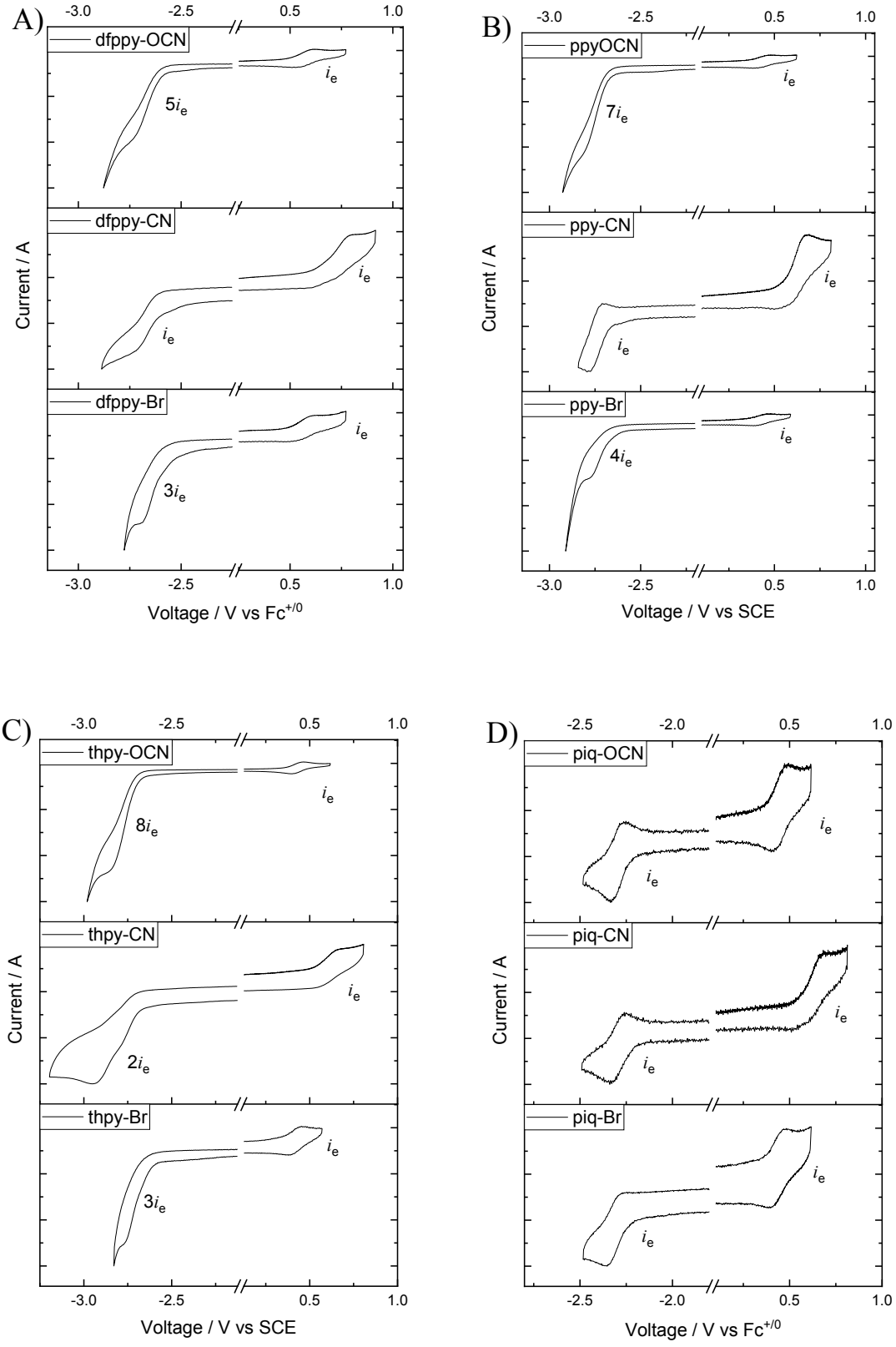


Fig. S7. Cyclic voltammograms of solution of Ir(III)-Br, Ir(III)-CN and Ir(III)-OCN complexes in CH_2Cl_2 with showing the currents for the reversible reduction (i_e).

4. TGA analysis

Thermogravimetric analysis (TGA) were performed with a Mettler TGA2 thermal gravimetric analyzer under a nitrogen gas flow rate of 40 mL·min^{-1} with a heating rate of 10 °C/min in the region from room temperature to 800 °C. Differential scanning calorimetry (DSC) experiments was performed at a heating rate of 10 °C min^{-1} under a nitrogen gas flow rate of 40 mL·min^{-1} with a Mettler DSC3 differential scanning calorimeter.

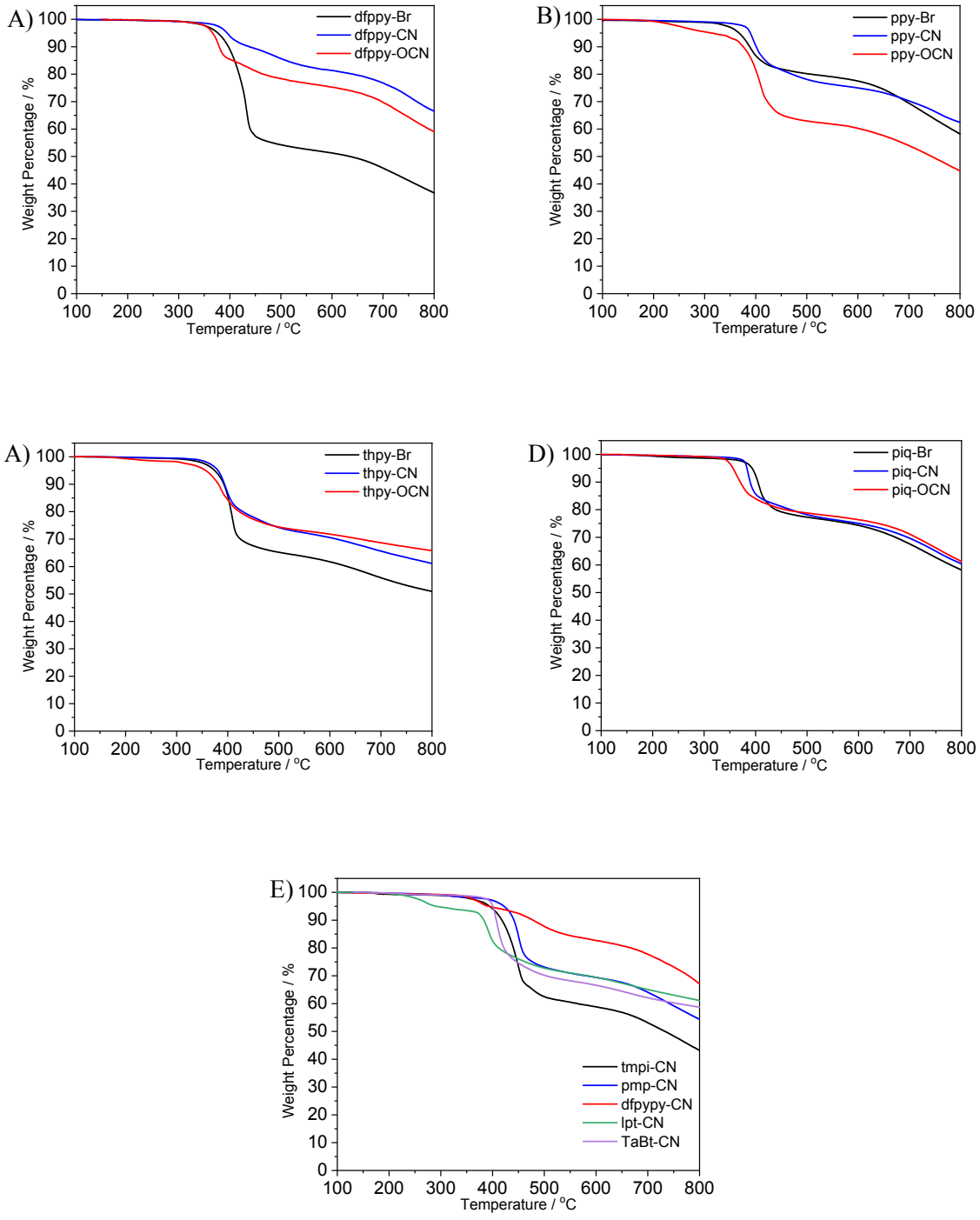


Fig. S8. TGA curves of iridium complexes.

5. DFT calculation

Density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations were performed to understand the geometries and the electronic structures of **thpy-Br**, **TaBt-CN**, **dfppy-CN**, **dfppy-OCN**, **ppy-Br**, **ppy-CN** and **ppy-OCN** using the Gaussian 09 package.[4] The vibrational frequency calculations at the same level were carried out to verify that every optimized structure is an energy minimum (no imaginary frequency). PBE0[5]/6-31G*(IANI2DZ)[6, 7] was used for both the geometry optimization and TDDFT calculations. The solvent effects were examined using the self-consistent reaction field (SCRF) method based on PCM models.[8, 9] The choice of solvents (DCM, a dielectric constant ε = 8.93) was based on the solvent media for experiments.

Table S3. Calculated first 10 singlet excited state energies (λ / nm), the associated oscillator strengths (*f*) and the nature of the transitions at the optimized *ground* state (S_0) geometries of **thpy-Br**, **TaBt-CN**, **dfppy-CN**, **dfppy-OCN**, **ppy-Br**, **ppy-CN** and **ppy-OCN** in the dichloromethane (DCM) by TD-PBE0. The values in the parentheses are the % contributions of that particular configuration state function (CSF).

thpy-Br	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	26551.76	376.62	0.0727	HOMO->LUMO (95%)	
2	27623.67	362.01	0.0001	H-1->LUMO (98%)	
3	30505.49	327.81	0.0008	HOMO->L+1 (71%)	
				H-2->LUMO (25%)	
4	31495.93	317.50	0.0182	HOMO->L+3 (93%)	
5	31636.27	316.09	0.1825	H-2->LUMO (65%)	HOMO->LUMO (3%)
				HOMO->L+1 (25%)	H-3->LUMO (2%)
6	32731.57	305.51	0.0005	H-1->L+1 (97%)	
7	32890.47	304.04	0.0037	H-1->L+3 (79%)	
				HOMO->L+2 (14%)	
8	33809.94	295.77	0.1183	H-3->LUMO (85%)	H-2->L+1 (5%)
					HOMO->L+2 (3%)
9	34533.42	289.58	0.0673	HOMO->L+2 (76%)	H-3->LUMO (4%)
				H-1->L+3 (12%)	H-2->L+1 (2%)
10	34572.13	289.25	0.1037	H-1->L+2 (93%)	
TaBt-CN	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	24809.6	403.07	0.2544	HOMO->LUMO (96%)	
2	26298.5	380.24	0.0000	H-1->LUMO (98%)	
3	29419.06	339.92	0.1354	H-3->LUMO (74%)	
				H-2->LUMO (21%)	
4	29767.49	335.94	0.2409	H-2->LUMO (77%)	HOMO->LUMO (2%)
				H-3->LUMO (19%)	
5	32033.1	312.18	0.2060	H-4->LUMO (93%)	
6	34084.17	293.39	0.0001	H-5->LUMO (97%)	
7	34814.1	287.24	0.0270	HOMO->L+1 (94%)	
8	35459.34	282.01	0.0180	HOMO->L+3 (42%)	
				H-1->L+2 (32%)	
				HOMO->L+4 (19%)	
9	35573.87	281.11	0.0334	H-6->LUMO (76%)	
				H-7->LUMO (10%)	
				HOMO->L+2 (10%)	
10	35662.59	280.41	0.0575	H-1->L+1 (52%)	HOMO->L+3 (5%)
				HOMO->L+4 (37%)	
dfppy-CN	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	28939.96	345.54	0.0263	H-1->LUMO (96%)	
2	29021.43	344.57	0.0000	HOMO->LUMO (98%)	
3	32602.53	306.72	0.1278	H-2->LUMO (93%)	
4	33931.73	294.71	0.0173	H-1->L+1 (93%)	
5	34166.43	292.69	0.0012	HOMO->L+1 (98%)	
6	34814.9	287.24	0.1197	H-3->LUMO (77%)	H-1->L+1 (3%)
				H-2->L+1 (14%)	
7	35466.6	281.95	0.1089	HOMO->L+2 (93%)	
8	36387.68	274.82	0.0000	H-4->LUMO (96%)	
9	36464.31	274.24	0.0485	H-1->L+2 (77%)	H-2->L+1 (2%)
				HOMO->L+3 (16%)	
10	36695.79	272.51	0.0125	H-5->LUMO (68%)	H-2->L+1 (8%)
					H-3->LUMO (6%)
					H-6->LUMO (5%)
					H-3->L+1 (2%)

dfppy-OCN	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	27650.28	361.66	0.0134	HOMO->LUMO (97%)	
2	28574.6	349.96	0.0186	H-1->LUMO (96%)	
3	31082.17	321.73	0.0318	HOMO->L+2 (92%)	
4	32108.11	311.45	0.0498	H-1->L+2 (83%)	
				H-2->LUMO (10%)	
5	32217.8	310.39	0.0802	H-2->LUMO (78%)	H-1->L+2 (9%)
					HOMO->L+1 (3%)
6	32717.06	305.65	0.0243	HOMO->L+1 (92%)	H-2->LUMO (4%)
7	33668.79	297.01	0.0084	H-1->L+1 (95%)	
8	34631.01	288.76	0.0058	H-2->L+2 (91%)	
				HOMO->L+3 (2%)	
9	34832.65	287.09	0.0878	HOMO->L+3 (67%)	
				H-1->L+3 (20%)	
10	34947.99	286.14	0.0861	H-3->LUMO (61%)	H-4->LUMO (9%)
				H-2->L+1 (19%)	
ppy-Br	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	26745.33	373.90	0.0347	HOMO->LUMO (97%)	
2	27513.98	363.45	0.0000	H-1->LUMO (97%)	
3	30974.09	322.85	0.0299	H-2->LUMO (51%)	
				HOMO->L+1 (45%)	
4	31215.25	320.36	0.0991	HOMO->L+1 (52%)	
				H-2->LUMO (43%)	
5	32001.64	312.48	0.0167	HOMO->L+3 (67%)	
				H-1->L+1 (28%)	
6	32082.3	311.70	0.0033	H-1->L+1 (69%)	
				HOMO->L+3 (27%)	
7	33008.22	302.95	0.0032	H-1->L+3 (82%)	
				HOMO->L+2 (11%)	
8	34367.27	290.97	0.0244	H-2->L+1 (45%)	HOMO->L+2 (7%)
				H-3->LUMO (39%)	H-5->LUMO (5%)
9	34510.03	289.77	0.1077	H-1->L+2 (92%)	
10	34961.7	286.03	0.1101	HOMO->L+2 (62%)	H-1->L+3 (8%)
				H-3->LUMO (24%)	
ppy-CN	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	28360.05	352.61	0.0467	HOMO->LUMO (96%)	
2	28630.25	349.28	0.0000	H-1->LUMO (98%)	
3	32267.81	309.91	0.0733	H-2->LUMO (75%)	
				HOMO->L+1 (18%)	
4	32521.06	307.49	0.0542	HOMO->L+1 (79%)	
				H-2->LUMO (18%)	
5	32996.12	303.07	0.0007	H-1->L+1 (98%)	
6	34526.16	289.63	0.0733	H-3->LUMO (76%)	H-3->L+1 (2%)
				H-2->L+1 (15%)	
7	35106.88	284.84	0.1073	H-1->L+2 (93%)	
8	35772.28	279.55	0.0000	H-4->LUMO (93%)	H-7-> LUMO (3%)
9	35807.77	279.27	0.0748	HOMO->L+2 (73%)	H-2->L+1 (9%)
					H-1->L+3 (8%)
					H-3->LUMO (5%)
					H-5->LUMO (2%)
10	36121.52	276.84	0.0226	H-2->L+1 (40%)	H-3->L+1 (6%)
				H-5->LUMO (19%)	H-1->L+3 (5%)
				HOMO->L+2 (12%)	H-6->LUMO (3%)
				H-3->LUMO (10%)	H-2->LUMO (3%)
ppy-OCN	Energy (cm^{-1})	λ (nm)	*f*	Major contribs	Minor contribs
1	27099.41	369.01	0.0309	HOMO->LUMO (97%)	H-2->LUMO (3%)
2	27960	357.65	0.0197	H-1->LUMO (97%)	H-2->LUMO (3%)
3	30610.34	326.69	0.0340	HOMO->L+2 (94%)	HOMO->L+1 (3%)
					H-1->L+2 (2%)
4	31318.49	319.30	0.0009	HOMO->L+1 (93%)	
5	31606.43	316.39	0.0350	H-1->L+2 (90%)	
6	31853.24	313.94	0.0999	H-2->LUMO (84%)	H-2->L+1 (2%)
7	32350.07	309.12	0.0047	H-1->L+1 (95%)	H-4->LUMO (6%)
					H-1->L+3 (5%)
8	34261.61	291.87	0.0066	H-2->L+2 (90%)	H-2->LUMO (3%)
9	34449.53	290.28	0.0897	HOMO->L+3 (57%)	H-2->LUMO (3%)
				H-1->L+3 (30%)	
10	34671.34	288.43	0.0483	H-3->LUMO (54%)	HOMO->L+1 (3%)
				H-2->L+1 (24%)	H-1->L+2 (2%)

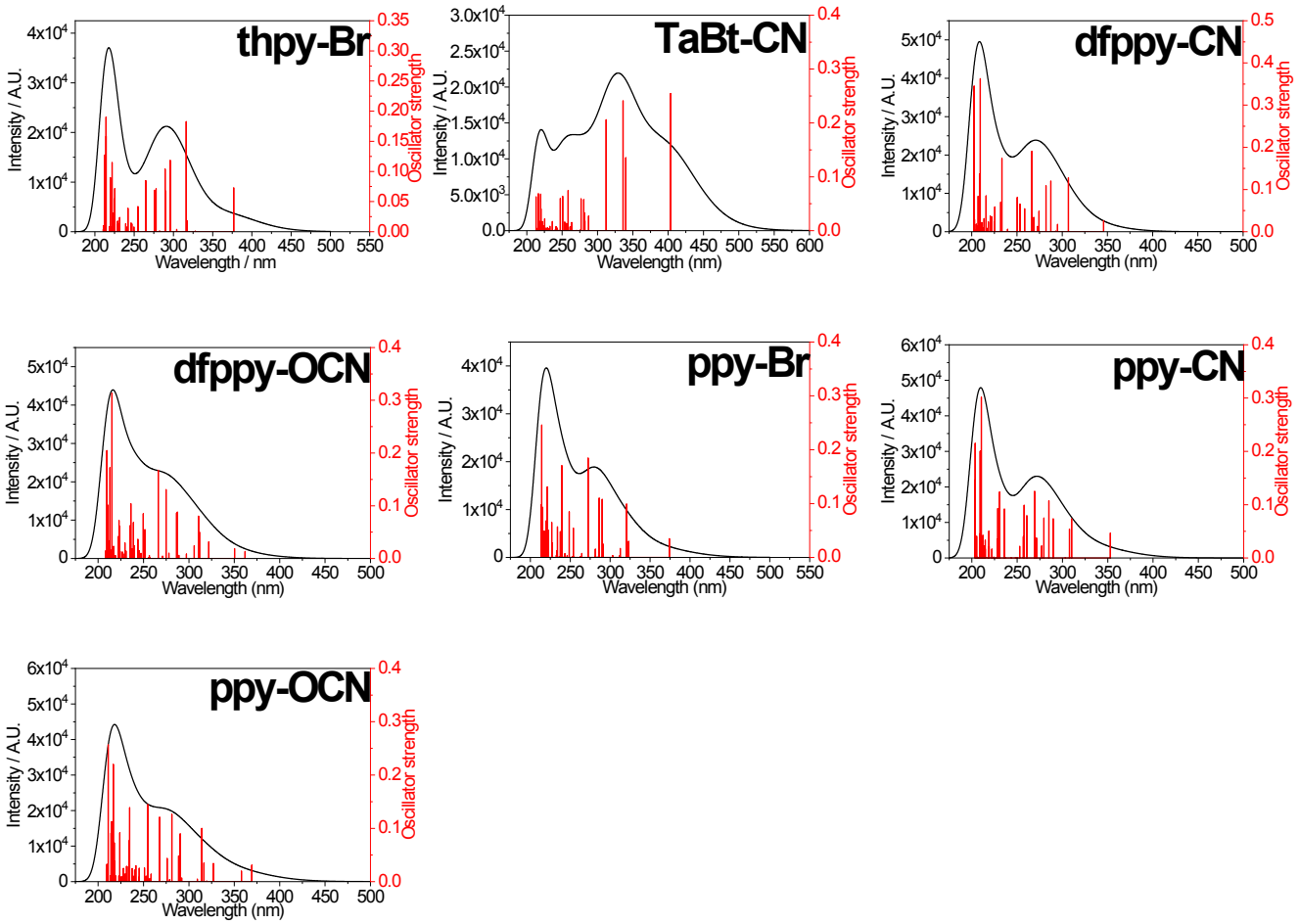


Fig. S9. Simulated absorption of **thpy-Br**, **TaBt-CN**, **dfppy-CN**, **dfppy-OCN**, **ppy-Br**, **ppy-CN** and **ppy-OCN**.

Table S4. Cartesian coordinates for optimized structures of **thpy-Br**, **TaBt-CN**, **dfppy-CN**, **dfppy-OCN**, **ppy-Br**, **ppy-CN** and **ppy-OCN**.

Ground state of **thpy-Br** (S_0)				Excited state of **thpy-Br** (T_1)			
Ir	0.60864100	-0.00022800	-0.24574000	Ir	0.61796900	-0.00007000	-0.24012500
Br	1.53985700	0.00000400	-2.70462500	Br	1.65433400	-0.00018900	-2.65434900
S	-2.51312500	0.00074800	2.97510800	S	-2.70594700	0.00033200	2.79118000
N	-1.47761400	0.00149800	-0.89643900	N	-1.42566100	0.00030400	-1.01446100
N	2.23786700	-2.29458300	0.44650200	N	2.23229000	-2.29479000	0.48380300
C	2.40795700	-0.00179900	0.53310500	C	2.39879100	-0.00043500	0.58091500
N	0.48122700	3.20590200	-0.37678400	N	0.47802500	3.21302900	-0.34643700
C	1.01035600	-2.00017400	-0.10228000	C	1.01290600	-2.00658100	-0.08422700
N	2.24138400	2.29129300	0.44751800	N	2.23327200	2.29398600	0.48372700
N	0.47609100	-3.20608300	-0.37779800	N	0.47668200	-3.21312300	-0.34638200
C	2.45233100	3.65242200	0.50901200	C	2.43663400	3.65457200	0.56799600
H	3.35977400	4.08852900	0.89552600	H	3.33720400	4.08921600	0.97186800
C	-3.27724200	0.00298300	-2.47255200	C	-3.17041300	0.00062300	-2.65693500
H	-3.59019000	0.00355100	-3.51074800	H	-3.43195600	0.00070200	-3.70879500

C	-3.31552000	-3.62087500	-0.30313700	C	-3.31392600	-3.60838700	-0.22506100
H	-3.41283000	-4.54847400	-0.88383100	H	-3.43478400	-4.52914900	-0.81206300
H	-3.51147600	-2.79611300	-1.00096600	H	-3.50678300	-2.77406100	-0.91217800
C	-3.30991000	3.62473800	-0.30159300	C	-3.31244500	3.60940800	-0.22463000
H	-3.50668900	2.80066900	-1.00001200	H	-3.50565100	2.77516000	-0.91174300
H	-3.40635400	4.55284500	-0.88162100	H	-3.43311000	4.53022400	-0.81158900
C	1.33131100	-4.23123400	-0.00692800	C	1.32361900	-4.23518400	0.04917400
H	1.07376600	-5.26934400	-0.15040900	H	1.06422700	-5.27464400	-0.08056500
C	4.32178500	1.22117300	1.38715700	C	4.30494200	1.22404300	1.44449700
H	4.83266400	2.15280700	1.61274000	H	4.81478900	2.15563600	1.67230200
C	1.33825500	4.22954600	-0.00592000	C	1.32541700	4.23474700	0.04903100
H	1.08244100	5.26809900	-0.14926200	H	1.06647300	5.27431100	-0.08076500
C	2.44633900	-3.65607900	0.50813500	C	2.43506600	-3.65545900	0.56815000
H	3.35304000	-4.09379500	0.89456600	H	3.33542900	-4.09046400	0.97209000
C	-1.88789400	3.49867100	0.22982300	C	-1.88092800	3.51211600	0.28614800
H	-1.79923300	2.59902700	0.85160600	H	-1.77401400	2.62399100	0.92184000
H	-1.64686900	4.35581800	0.87313200	H	-1.64040500	4.38211700	0.91193000
C	-1.89341900	-3.49656100	0.22846200	C	-1.88244900	-3.51153600	0.28591900
H	-1.65323600	-4.35446400	0.87107900	H	-1.64224300	-4.38167000	0.91163800
H	-1.80394000	-2.59750100	0.85097900	H	-1.77538300	-2.62350800	0.92172000
C	-2.37304500	0.00153000	0.13089600	C	-2.38522600	0.00040200	-0.00447900
C	-0.86903400	-3.39945500	-0.89242900	C	-0.87374100	-3.40521200	-0.84862800
H	-0.86528100	-4.30379500	-1.50922900	H	-0.87740200	-4.30378200	-1.47364400
H	-1.09192000	-2.54999000	-1.54166400	H	-1.10419600	-2.54852100	-1.48542400
C	-0.86364100	3.40158800	-0.89120700	C	-0.87238200	3.40563900	-0.84852900
H	-1.08763500	2.55322600	-1.54152500	H	-1.10318800	2.54911900	-1.48543000
H	-0.85871500	4.30670100	-1.50686100	H	-0.87581400	4.30431100	-1.47339900
C	-0.35232900	-0.00008200	1.50163900	C	-0.36860400	0.00007900	1.46741500
C	-1.73864300	0.00074400	1.41773800	C	-1.84114100	0.00027800	1.27520200
C	-3.75194400	0.00223600	-0.12072900	C	-3.77064400	0.00061000	-0.33224100
H	-4.44862500	0.00216100	0.71158000	H	-4.50432900	0.00067700	0.46803800
C	-1.92717900	0.00222000	-2.15812900	C	-1.82491900	0.00041200	-2.27894100
H	-1.14984200	0.00211300	-2.91737200	H	-1.02295200	0.00031700	-3.01307000
C	3.05250500	1.19633400	0.81736400	C	3.03968200	1.19837600	0.86592400
C	1.01339200	1.99906700	-0.10132700	C	1.01374300	2.00627100	-0.08424000
C	3.05069500	-1.20104600	0.81683900	C	3.03916500	-1.19951200	0.86597200
C	-0.97349200	-0.00043500	3.75547100	C	-1.15838500	0.00012700	3.67562000
H	-0.92969500	-0.00077800	4.83766500	H	-1.17738200	0.00010900	4.75709300
C	0.06770700	-0.00073500	2.86670100	C	-0.05804600	0.00001000	2.81952400
H	1.10751300	-0.00142200	3.17689100	H	0.95955200	-0.00013300	3.19742900
C	4.31995300	-1.22806500	1.38659400	C	4.30441700	-1.22570200	1.44454200
H	4.82944000	-2.16057100	1.61172800	H	4.81386600	-2.15750700	1.67237500
C	-4.20565400	0.00295600	-1.42884600	C	-4.15713200	0.00072000	-1.65177400
H	-5.27146300	0.00349500	-1.63671900	H	-5.21061800	0.00087800	-1.91462700
C	-4.34568100	3.60007200	0.81411300	C	-4.33046000	3.57564000	0.90727100
H	-5.36361000	3.68093500	0.41778900	H	-5.35546900	3.63382100	0.52546100
H	-4.19162400	4.42764900	1.51673300	H	-4.18171700	4.41224600	1.60034000

H	-4.27959500	2.66537500	1.38387500	H	-4.23722400	2.64752000	1.48419300
C	4.93831600	-0.00397200	1.66635700	C	4.91917200	-0.00095600	1.72920500
H	5.92906600	-0.00481200	2.11058400	H	5.90645400	-0.00115900	2.18099300
C	-4.35131200	-3.59596800	0.81254500	C	-4.33209900	-3.57434300	0.90668800
H	-5.36928800	-3.67589800	0.41614900	H	-5.35706700	-3.63221700	0.52472100
H	-4.28453500	-2.66158600	1.38274000	H	-4.23868500	-2.64626000	1.48363900
H	-4.19788200	-4.42399200	1.51478100	H	-4.18371100	-4.41100400	1.59976800
Ground state of **TaBt-CN** (S_0)				Excited state of **TaBt-CN** (T_1)			
Ir	0.58859400	-0.02591100	-0.83300500	Ir	0.59695400	-0.03510100	-0.83414200
S	-0.90165500	0.10480500	3.50043700	S	-1.02159000	0.13912700	3.43062400
S	-3.55304600	0.07048900	1.23733100	S	-3.63749600	0.11410100	1.12551600
N	-1.58453800	0.01041200	-0.45414400	N	-1.58801500	0.02977000	-0.53271500
N	0.44283600	-0.12302000	-4.02483500	N	0.54530400	-0.16542000	-4.03476000
N	2.32417000	-2.34527700	-0.87810300	N	2.29757300	-2.37994400	-0.82553200
N	2.38432300	2.24056300	-1.02523500	N	2.42505000	2.20434600	-1.02983500
N	0.45092600	3.17715500	-0.97044000	N	0.51027400	3.17778000	-0.97466900
C	0.51076900	0.03309100	1.23488400	C	0.50938500	0.04622600	1.21001100
C	-0.77323200	0.05770400	1.75242800	C	-0.87856900	0.08621700	1.70585900
C	0.83879600	0.09242000	3.60766200	C	0.74742100	0.11666100	3.59021500
C	1.57585000	0.11712300	4.79154500	C	1.42865500	0.14228400	4.78361800
H	1.07838300	0.14754300	5.75646700	H	0.89899800	0.18033100	5.73117700
C	2.96070900	0.10179200	4.70598400	C	2.83672000	0.11735000	4.75413500
H	3.55273300	0.12051900	5.61669200	H	3.39233400	0.13714600	5.68655400
C	3.59948300	0.06218200	3.45755100	C	3.50664000	0.06687100	3.53081900
H	4.68468900	0.05019600	3.40996700	H	4.59299200	0.04702100	3.51445000
C	2.86358100	0.03803300	2.28475000	C	2.81049800	0.04104800	2.32797800
H	3.36764200	0.00656200	1.32664900	H	3.34961800	0.00004100	1.38944400
C	1.45653200	0.05295600	2.32764000	C	1.39252300	0.06607800	2.31303800
C	-1.85939500	0.04489600	0.84164200	C	-1.91179500	0.07725700	0.79963600
C	-2.73600000	0.00205800	-1.22296300	C	-2.70068800	0.02186500	-1.31520100
C	-2.80772800	-0.03302200	-2.61940200	C	-2.73556400	-0.02420900	-2.72272100
H	-1.89450000	-0.05685000	-3.20381900	H	-1.80457300	-0.05731600	-3.27726500
C	-4.05899600	-0.03764300	-3.22030500	C	-3.96374300	-0.02869200	-3.36217300
H	-4.12477100	-0.06511100	-4.30395400	H	-3.99463500	-0.06468700	-4.44720200
C	-5.23508400	-0.00810900	-2.45933200	C	-5.16594600	0.01134800	-2.63996800
H	-6.20060500	-0.01279600	-2.95594200	H	-6.11480300	0.00613100	-3.16744300
C	-5.18181800	0.02717800	-1.07092300	C	-5.15646300	0.05767000	-1.24690100
H	-6.08931700	0.05016300	-0.47594800	H	-6.08444400	0.08839200	-0.68465700
C	-3.92820100	0.03202100	-0.46602200	C	-3.93076500	0.06295200	-0.59658100
C	0.47287600	-0.08660000	-2.85460300	C	0.53479600	-0.11721100	-2.86470700
C	2.54582700	-0.05553000	-0.97490800	C	2.55471800	-0.09389700	-0.94771900
C	3.25968400	1.13415200	-1.04985600	C	3.28460700	1.08453500	-1.03433300
C	4.65018600	1.13886300	-1.10180500	C	4.67530500	1.06876500	-1.07791200
H	5.21962500	2.06232000	-1.14904500	H	5.25854200	1.98311000	-1.13381300
C	5.31044700	-0.09507600	-1.08490800	C	5.31718800	-0.17440500	-1.04023600
H	6.39524300	-0.11061200	-1.12359000	H	6.40186400	-0.20612200	-1.07174600
C	4.61808400	-1.30984700	-1.02133300	C	4.60715700	-1.37833400	-0.96522300

H	5.16356600	-2.24868400	-1.00861400	H	5.13958400	-2.32429000	-0.93734200
C	3.22832000	-1.26576700	-0.97076600	C	3.21788700	-1.31381100	-0.92368300
C	2.51749600	-3.71145200	-0.87735100	C	2.47779500	-3.74712300	-0.79187700
H	3.49434400	-4.16537500	-0.92885500	H	3.45061600	-4.21128700	-0.82603200
C	1.28169700	-4.26606800	-0.81585400	C	1.23643000	-4.28888200	-0.72512500
H	0.97188100	-5.29955800	-0.79831200	H	0.91690100	-5.31884900	-0.68628500
N	0.36579700	-3.22580900	-0.78865000	N	0.33079000	-3.23968800	-0.72748000
C	-1.07500300	-3.39085100	-0.68887100	C	-1.11043600	-3.38940200	-0.61021400
H	-1.34917700	-4.28003000	-1.26545400	H	-1.40206900	-4.27797800	-1.17919500
H	-1.52834300	-2.52306300	-1.17398700	H	-1.55992800	-2.51781500	-1.09174700
C	-1.54120300	-3.50709600	0.75451200	C	-1.55642600	-3.49392700	0.84046300
H	-1.21511900	-2.61163300	1.29836000	H	-1.21669400	-2.59708200	1.37329400
H	-1.04648000	-4.36426300	1.23104400	H	-1.06207000	-4.35220800	1.31528200
C	-3.05380100	-3.65982600	0.85382500	C	-3.06872000	-3.62977000	0.96424800
H	-3.36354200	-4.57666800	0.33372900	H	-3.39420100	-4.55742600	0.47387300
H	-3.53849700	-2.82845200	0.32421800	H	-3.55197700	-2.80702900	0.42060500
C	-3.53576700	-3.69586800	2.29760200	C	-3.52987900	-3.61860200	2.41509900
H	-3.08932100	-4.53684100	2.84139300	H	-3.07845500	-4.44310900	2.97973700
H	-4.62468500	-3.79950000	2.35340400	H	-4.61825200	-3.71579900	2.48989900
H	-3.25865300	-2.77469600	2.82399900	H	-3.24176000	-2.68123200	2.90592500
C	0.98685400	-2.03319600	-0.81458300	C	0.96234300	-2.05393300	-0.77850200
C	2.61385500	3.59890700	-1.10171900	C	2.68065100	3.55788300	-1.10156400
H	3.60182900	4.02267900	-1.18630600	H	3.67680300	3.96272800	-1.18288600
C	1.39379700	4.18922300	-1.06141100	C	1.47205700	4.17182800	-1.06109100
H	1.11160800	5.23011200	-1.09719800	H	1.21006100	5.21807500	-1.09413400
C	-0.98243700	3.38642500	-0.84793500	C	-0.91587300	3.41368100	-0.82018400
H	-1.47072500	2.51396900	-1.28873300	H	-1.42966700	2.54845700	-1.24556600
H	-1.24514300	4.26060900	-1.45202000	H	-1.17843800	4.29171400	-1.41862200
C	-1.40859500	3.56807500	0.60109800	C	-1.29886100	3.60205700	0.64002200
H	-0.88110700	4.43002500	1.03175700	H	-0.75443200	4.46179200	1.05354400
H	-1.08839000	2.68535500	1.16874300	H	-0.96772800	2.71740600	1.19821900
C	-2.91392200	3.75896500	0.73625200	C	-2.79885200	3.79626200	0.81995300
H	-3.21789000	4.66871500	0.20063300	H	-3.11500200	4.71327500	0.30414600
H	-3.43139800	2.92518200	0.24269300	H	-3.33098300	2.96845700	0.33271000
C	-3.35386300	3.84237500	2.19143100	C	-3.19837600	3.86014700	2.28763100
H	-3.08147900	2.92857000	2.73310000	H	-2.91909900	2.93514600	2.80644900
H	-4.43824100	3.97157600	2.27521400	H	-4.27912200	3.99581200	2.40239400
H	-2.87371400	4.68629900	2.70081800	H	-2.69817900	4.69183800	2.79796500
C	1.03993600	1.96851500	-0.93564800	C	1.07506100	1.95797300	-0.94448700

Ground state of **dfppy-CN** (S_0)				Excited state of **dfppy-CN** (T_1)			
Ir	-0.74839600	0.00002400	-0.64158500	Ir	-0.77881300	0.00002700	-0.64520500
N	-2.39071200	-2.29273800	0.04248500	N	-2.39676100	-2.29373800	0.09304500
N	-2.39074200	2.29271100	0.04266100	N	-2.39701000	2.29351500	0.09336500
C	-1.14639100	2.00448300	-0.46762900	C	-1.16138400	2.00755600	-0.43941800
N	1.31483900	0.00006700	-1.24421700	N	1.22276000	0.00019200	-1.36793400
C	0.20674600	-0.00005100	1.16851500	C	0.23215900	-0.00005500	1.11568600
N	-0.58881600	-3.21199900	-0.68110500	N	-0.59165200	-3.21303000	-0.62510100

N	-0.58887500	3.21205000	-0.68090300	N	-0.59202900	3.21309700	-0.62473000
C	-1.14636400	-2.00445500	-0.46778000	C	-1.16115700	-2.00757600	-0.43968600
C	-3.22040200	-1.19847900	0.36851900	C	-3.22354100	-1.19904700	0.43030000
C	-2.57614400	-0.00001700	0.08822800	C	-2.58539900	-0.00012500	0.14212000
C	-1.44729200	4.23354100	-0.30564600	C	-1.43554500	4.23300700	-0.21508300
H	-1.17325100	5.27280700	-0.40201700	H	-1.15296900	5.27190200	-0.28821400
C	0.78260300	3.40955300	-1.11983800	C	0.78295100	3.40122500	-1.05760100
H	0.81642300	4.32578100	-1.71776000	H	0.82384000	4.30035300	-1.68061400
H	1.03483500	2.57210300	-1.77408000	H	1.03806700	2.54354100	-1.68325100
C	2.22475300	0.00002800	-0.23426100	C	2.21388700	0.00013000	-0.34239100
C	-3.22041700	1.19841600	0.36861400	C	-3.22366900	1.19868800	0.43047300
C	0.78267700	-3.40945000	-1.12001800	C	0.78336900	-3.40096400	-1.05792100
H	1.03491800	-2.57193800	-1.77417600	H	1.03846000	-2.54313200	-1.68337700
H	0.81652400	-4.32562400	-1.71802100	H	0.82436800	-4.29995900	-1.68111800
C	-0.40111400	-0.00011400	2.42850500	C	-0.30011300	-0.00016300	2.39130400
H	-1.48258000	-0.00012400	2.52549600	H	-1.37598500	-0.00020200	2.54056900
C	-1.44721800	-4.23352900	-0.30592800	C	-1.43507000	-4.23308500	-0.21561300
H	-1.17315600	-5.27278400	-0.40235700	H	-1.15237200	-5.27194000	-0.28885300
C	-2.58666600	-3.65412600	0.14544100	C	-2.57621100	-3.65354000	0.23337400
H	-3.50250100	-4.08779800	0.51427300	H	-3.48266900	-4.08739500	0.62454300
C	3.59478000	0.00006100	-0.53397500	C	3.60523400	0.00022200	-0.73315300
H	4.31773000	0.00003300	0.26765200	H	4.36090200	0.00017400	0.03909600
C	1.74341000	3.47908200	0.05897500	C	1.73497700	3.49953600	0.12650800
H	1.60641000	2.57500100	0.66453400	H	1.58050600	2.61899200	0.76227900
H	1.47600900	4.33069900	0.69895900	H	1.47919200	4.37794700	0.73424200
C	-4.49981500	1.22444000	0.91529900	C	-4.49513100	1.22470700	0.99560800
H	-5.01075100	2.15649600	1.13865500	H	-5.00334500	2.15622200	1.22719000
C	1.62972500	-0.00004200	1.10216300	C	1.70410200	-0.00000800	0.95186300
C	-2.58672000	3.65408900	0.14570500	C	-2.57660600	3.65327900	0.23387000
H	-3.50255900	4.08771900	0.51457600	H	-3.48310400	4.08698500	0.62511300
C	0.37227200	-0.00016300	3.57628500	C	0.52948000	-0.00023300	3.51349100
C	1.72863200	0.00013300	-2.52044900	C	1.60587300	0.00033700	-2.63421200
H	0.93893300	0.00016100	-3.26405900	H	0.80111800	0.00037900	-3.36375700
C	-5.12381800	-0.00007600	1.17912400	C	-5.11471700	-0.00034000	1.26791000
H	-6.12271400	-0.00009800	1.60453300	H	-6.10723500	-0.00042500	1.70792800
C	2.35489100	-0.00009700	2.29949300	C	2.48656300	-0.00009800	2.16775100
C	-4.49980200	-1.22456300	0.91519900	C	-4.49500100	-1.22528200	0.99542900
H	-5.01072700	-2.15664300	1.13848200	H	-5.00311500	-2.15688500	1.22687600
C	1.74344800	-3.47907500	0.05881800	C	1.73532300	-3.49944800	0.12623200
H	1.47603300	-4.33074700	0.69872300	H	1.47954200	-4.37798200	0.73379000
H	1.60642500	-2.57504500	0.66444900	H	1.58077200	-2.61902800	0.76215600
C	1.76044800	-0.00015700	3.54602200	C	1.93364800	-0.00020400	3.41201300
H	2.35568500	-0.00019700	4.45093200	H	2.55967200	-0.00026400	4.29694800
C	3.19728200	3.59193900	-0.38201900	C	3.19190900	3.56956100	-0.31298000
H	3.41643100	2.79856800	-1.10881900	H	3.39649000	2.74920000	-1.01377500
H	3.35072700	4.54416600	-0.90762000	H	3.36360400	4.50197500	-0.86778400
C	4.01639300	0.00013100	-1.85437600	C	3.96230900	0.00037000	-2.04804800

H	5.07768500	0.00015700	-2.08352700	H	5.00932400	0.00043700	-2.33353000
C	3.19733400	-3.59188800	-0.38214100	C	3.19228600	-3.56932600	-0.31317500
H	3.41649900	-2.79845600	-1.10886900	H	3.39686400	-2.74884900	-1.01383500
H	3.35080200	-4.54407100	-0.90781600	H	3.36407000	-4.50164800	-0.86810800
C	3.06733300	0.00016700	-2.87336100	C	2.94310400	0.00043300	-3.04331200
H	3.35034900	0.00022200	-3.92007200	H	3.17839500	0.00055100	-4.10104300
C	4.16332500	-3.48275200	0.79063000	C	4.15693300	-3.47603100	0.86186000
H	4.05788300	-2.51555800	1.29602700	H	4.05237700	-2.51415700	1.37662900
H	5.20371500	-3.57680000	0.46118400	H	5.19720100	-3.56532600	0.53059000
H	3.97453500	-4.26713500	1.53323000	H	3.96909800	-4.26965000	1.59488100
C	4.16331100	3.48271600	0.79071200	C	4.15663700	3.47615200	0.86197900
H	3.97453300	4.26703300	1.53338500	H	3.96879700	4.26964900	1.59513200
H	5.20369000	3.57680500	0.46124200	H	5.19687800	3.56556600	0.53065600
H	4.05789800	2.51547800	1.29603000	H	4.05218000	2.51419400	1.37661200
C	-1.43410300	0.00009900	-2.55982500	C	-1.56343300	0.00012300	-2.53133900
N	-1.77733400	0.00015300	-3.68011700	N	-1.96836300	0.00018800	-3.63051400
F	3.70697000	-0.00009000	2.28255800	F	3.83614900	-0.00006900	2.08693400
F	-0.23108800	-0.00022300	4.77558200	F	-0.00765400	-0.00034000	4.74116100

Ground state of **dfppy-OCN** (S_0)				Excited state of **dfppy-OCN** (T_1)			
Ir	-0.69340800	-0.07263000	-0.49176700	Ir	-0.70909200	-0.08206400	-0.49364100
F	0.17324600	-0.44396600	4.80435500	F	0.41732200	-0.13033600	4.76732200
F	3.90428700	0.16257000	2.07424200	F	4.03795200	0.25126700	1.82925500
N	-2.08164300	-2.56499900	0.03623600	N	-2.02921400	-2.57794100	0.18096500
N	-2.51758100	1.98303300	0.44345600	N	-2.54144900	1.97807000	0.41067600
O	-1.52329100	-0.02955500	-2.55945300	O	-1.63286300	-0.10183700	-2.50394400
C	-1.28279200	1.86411700	-0.14902400	C	-1.31155100	1.85885800	-0.19222400
N	1.27261300	0.18374900	-1.26137400	N	1.17978600	0.16224800	-1.40200800
C	0.35387600	-0.11759700	1.19545400	C	0.39281300	-0.03414600	1.13554000
N	-0.24652400	-3.23755600	-0.85448500	N	-0.18042500	-3.25587100	-0.68051000
N	-3.11207600	1.71443300	-3.12941500	N	-3.69539500	1.12568500	-2.86399500
N	-0.86924800	3.13597600	-0.30677400	N	-0.89850000	3.12784900	-0.36309700
C	-0.89842100	-2.11257400	-0.49975200	C	-0.86200200	-2.13150700	-0.39316700
C	-2.99287400	-1.58828200	0.50064400	C	-2.95454600	-1.59777400	0.61629900
C	-2.47167500	-0.31441400	0.31901500	C	-2.45967300	-0.32320500	0.38360000
C	-1.80858400	4.03189100	0.17425900	C	-1.83392800	4.02531200	0.11846700
H	-1.65402200	5.09901900	0.13229500	H	-1.68297700	5.09250800	0.06573300
C	0.44310200	3.50900100	-0.80852100	C	0.41878700	3.48888500	-0.86444200
H	0.34357000	4.46713800	-1.32757100	H	0.32254800	4.42609500	-1.42082900
H	0.73101600	2.75699400	-1.54607500	H	0.71706300	2.70697900	-1.56548700
C	2.25883800	0.19990700	-0.32848200	C	2.24832300	0.21187300	-0.47222500
C	-3.21997500	0.78664900	0.71331500	C	-3.22170000	0.78089000	0.73546400
C	1.10765100	-3.26460700	-1.38385400	C	1.17454800	-3.27339500	-1.21077800
H	1.23957300	-2.35720800	-1.97655400	H	1.29819300	-2.35863500	-1.79349100
H	1.18552300	-4.12138300	-2.06051900	H	1.25901300	-4.12529600	-1.89284900
C	-0.16380100	-0.27893300	2.48538300	C	-0.05254200	-0.09993400	2.44931200
H	-1.22993700	-0.39697900	2.64741300	H	-1.11106200	-0.19456900	2.66756000
C	-0.98672500	-4.36554900	-0.54272200	C	-0.88721000	-4.38034600	-0.29463800

H	-0.62617500	-5.36080500	-0.75197900	H	-0.50274400	-5.37733600	-0.44508800
C	-2.14826900	-3.94080700	0.01461100	C	-2.05713300	-3.95223700	0.24624500
H	-3.00011200	-4.49311400	0.37834400	H	-2.88859500	-4.50442600	0.65457200
C	3.59059300	0.36359700	-0.73354000	C	3.58618500	0.36583700	-0.98105300
H	4.38113700	0.37681900	0.00233600	H	4.41054700	0.40447300	-0.28275500
C	1.47058800	3.58523600	0.31206200	C	1.43493900	3.60880800	0.26270600
H	1.46246800	2.62838500	0.84803700	H	1.41573500	2.67655500	0.84053000
H	1.16723200	4.35381400	1.03551400	H	1.13482700	4.41344200	0.94726600
C	-4.47543000	0.64202200	1.29493500	C	-4.47055600	0.63863000	1.33211300
H	-5.06730300	1.49756600	1.60650900	H	-5.07617300	1.49489000	1.61334800
C	1.76516800	0.03518600	1.03716100	C	1.84288400	0.10427200	0.85870500
C	-2.85286800	3.30347200	0.64245000	C	-2.87440300	3.29869100	0.60272600
H	-3.78944000	3.61120100	1.07947700	H	-3.80601300	3.61026900	1.04757500
C	0.68820000	-0.28777800	3.57583600	C	0.85301900	-0.05604100	3.50020900
C	1.55993900	0.32245200	-2.56229600	C	1.42695700	0.25834300	-2.70040300
H	0.70064100	0.29265600	-3.22566100	H	0.54901800	0.21253100	-3.33944200
C	-4.96867100	-0.65607700	1.46926100	C	-4.93904400	-0.65977100	1.56050700
H	-5.94714400	-0.79006100	1.92022000	H	-5.91210300	-0.79251400	2.02315200
C	2.56620400	0.01827500	2.18371500	C	2.70268700	0.13480600	2.01136300
C	-2.34152300	0.87118200	-2.83506300	C	-2.69636700	0.52952800	-2.67346600
C	-4.24343000	-1.78715400	1.07757300	C	-4.19796400	-1.79429100	1.20851500
H	-4.65891800	-2.77947800	1.22608500	H	-4.59779000	-2.78593300	1.39805200
C	2.14589700	-3.33621900	-0.27307200	C	2.21309100	-3.34242700	-0.10017400
H	2.00228300	-4.25933000	0.30428000	H	2.08400900	-4.27207800	0.47005200
H	1.96701500	-2.50265500	0.41681300	H	2.02682500	-2.51496500	0.59553100
C	2.06445700	-0.14038700	3.46033800	C	2.24324900	0.06013000	3.29111000
H	2.71803000	-0.14881000	4.32386300	H	2.93207800	0.09089100	4.12776100
C	2.87410000	3.87629900	-0.20442400	C	2.84316300	3.86021200	-0.26194500
H	3.11369600	3.17351300	-1.01341000	H	3.07763700	3.11592300	-1.03470200
H	2.90369200	4.88076200	-0.64772800	H	2.88189800	4.84192200	-0.75328700
C	3.88725100	0.50795100	-2.08091700	C	3.81094800	0.46256200	-2.32371300
H	4.91865200	0.63508200	-2.39528200	H	4.82178000	0.57973100	-2.70146500
C	3.57159500	-3.26730400	-0.80671700	C	3.63439600	-3.24912300	-0.64172100
H	3.66238500	-2.40645600	-1.48248600	H	3.70632900	-2.38564300	-1.31642000
H	3.78348000	-4.15938700	-1.41139000	H	3.85501300	-4.13774500	-1.24858600
C	2.85682100	0.48814800	-3.01900500	C	2.70872200	0.41104500	-3.22610100
H	3.04887200	0.59760900	-4.08045700	H	2.84619400	0.48938500	-4.29806400
C	4.59769400	-3.13966900	0.31172200	C	4.66731200	-3.10367800	0.46795900
H	4.43348700	-2.22303100	0.89022500	H	4.50908500	-2.17425900	1.02657000
H	5.61814100	-3.10709600	-0.08490700	H	5.68484500	-3.08067000	0.06310000
H	4.53456900	-3.98608400	1.00589600	H	4.60802400	-3.93652800	1.17880400
C	3.92496400	3.75876800	0.89192500	C	3.89350100	3.78552500	0.83843200
H	3.71430900	4.44800600	1.71829200	H	3.67639400	4.49560400	1.64535900
H	4.92605900	3.98838500	0.51135700	H	4.89186400	4.01483600	0.45042200
H	3.94802100	2.74315800	1.30427900	H	3.92897600	2.78159000	1.27624500
Ground state of **ppy-Br** (S_0)				Excited state of **ppy-Br** (T_1)			
Ir	-0.56251800	-0.00006600	-0.24540200	Ir	-0.57064500	0.00005100	-0.25363800

N	-2.20695900	-2.29261700	0.42026600	N	-2.18979800	-2.29425400	0.46871700
N	-2.20830700	2.29166600	0.41972500	N	-2.18916000	2.29476300	0.46886900
C	-0.96912200	1.99936700	-0.10412900	C	-0.96330000	2.00892500	-0.08620500
N	1.49487600	0.00035400	-0.89605600	N	1.41505600	-0.00014700	-1.07908000
C	0.39658600	0.00025700	1.51465900	C	0.45897200	-0.00016800	1.42751700
N	-0.43054700	-3.20771200	-0.36712500	N	-0.41663600	-3.21436700	-0.32466000
N	-0.43233000	3.20763800	-0.36764400	N	-0.41575100	3.21443500	-0.32446700
C	-0.96799700	-1.99971900	-0.10374600	C	-0.96385600	-2.00872200	-0.08633400
C	-3.02920900	-1.19871000	0.76815900	C	-3.00280400	-1.19829600	0.83911200
C	-2.37881100	-0.00051100	0.49941000	C	-2.35819300	0.00027500	0.56580100
C	-1.29716600	4.23066600	-0.01371600	C	-1.26251800	4.23486800	0.07106000
H	-1.03884200	5.26949400	-0.15046100	H	-0.99647100	5.27471100	-0.04091300
C	0.92260900	3.40571600	-0.85340300	C	0.94908000	3.40101200	-0.79112000
H	0.93069100	4.31361900	-1.46491400	H	0.97244700	4.29430300	-1.42314900
H	1.16068100	2.56109100	-1.50387500	H	1.19363900	2.53668100	-1.41210600
C	2.40116500	0.00055400	0.11358700	C	2.40437500	-0.00028600	-0.08494500
C	-3.02991500	1.19736500	0.76788300	C	-3.00246900	1.19900700	0.83919700
C	0.92435900	-3.40512800	-0.85322100	C	0.94816500	-3.40127800	-0.79126700
H	1.16190300	-2.56030700	-1.50361600	H	1.19292700	-2.53705300	-1.41232100
H	0.93270100	-4.31293200	-1.46487500	H	0.97135200	-4.29463300	-1.42321200
C	-0.18495100	0.00017800	2.79149400	C	-0.03576600	-0.00021700	2.73281200
H	-1.26811600	0.00002000	2.88058000	H	-1.11256800	-0.00012200	2.88124400
C	-1.29474400	-4.23117800	-0.01288800	C	-1.26368500	-4.23459000	0.07080900
H	-1.03581300	-5.26988900	-0.14937900	H	-0.99791800	-5.27449900	-0.04120600
C	-2.41899500	-3.65354400	0.47850900	C	-2.38636500	-3.65376400	0.56665700
H	-3.33409500	-4.08920400	0.84705500	H	-3.28959500	-4.08885900	0.96401000
C	3.77151500	0.00081600	-0.17221100	C	3.78107200	-0.00036400	-0.47650300
H	4.49248300	0.00100700	0.63704200	H	4.54969800	-0.00045900	0.28883800
C	1.92300800	3.49801600	0.28939300	C	1.92214500	3.51280100	0.37391200
H	1.81570100	2.60074100	0.91121600	H	1.78346900	2.63637100	1.01935300
H	1.67273300	4.35673500	0.92694200	H	1.67409200	4.39652200	0.97747800
C	-4.31218300	1.22362800	1.30766900	C	-4.27554600	1.22566300	1.40032600
H	-4.82746100	2.15570100	1.52142600	H	-4.78851400	2.15712800	1.62146300
C	1.81488800	0.00049200	1.45158800	C	1.92948500	-0.00031500	1.22953100
C	-2.42115800	3.65248000	0.47761800	C	-2.38533400	3.65432100	0.56692800
H	-3.33659200	4.08767600	0.84587800	H	-3.28843000	4.08964100	0.96434200
C	0.59111400	0.00028900	3.94637100	C	0.80779100	-0.00037800	3.84127200
C	1.91442900	0.00039000	-2.16953400	C	1.77450900	-0.00009300	-2.35653500
H	1.12033300	0.00017900	-2.91083000	H	0.95121600	0.00003400	-3.06625900
C	-4.93582600	-0.00114400	1.57284100	C	-4.89345300	0.00059000	1.67708800
H	-5.93683400	-0.00139100	1.99352800	H	-5.88656900	0.00071300	2.11573200
C	2.59216100	0.00060300	2.61935000	C	2.77263100	-0.00045900	2.39257400
C	-4.31146700	-1.22560900	1.30794300	C	-4.27588800	-1.22463500	1.40024000
H	-4.82620600	-2.15793700	1.52189000	H	-4.78911400	-2.15597200	1.62131700
C	1.92508500	-3.49716500	0.28931700	C	1.92116400	-3.51316500	0.37381000
H	1.67535300	-4.35609900	0.92678100	H	1.67290300	-4.39676900	0.97746300
H	1.81755900	-2.60002300	0.91130600	H	1.78265000	-2.63663500	1.01915300

C	1.98588100	0.00049500	3.86655400	C	2.21963700	-0.00049300	3.64534300
H	2.59129500	0.00058500	4.76833200	H	2.87394100	-0.00061100	4.51411000
C	3.35778000	3.61437200	-0.20865600	C	3.37099400	3.58008800	-0.09014400
H	3.56087700	2.79705200	-0.91318300	H	3.57187300	2.73354100	-0.75960400
H	3.47899400	4.54845900	-0.77400200	H	3.52902100	4.49211800	-0.68201800
C	4.20380000	0.00084700	-1.48872100	C	4.12681700	-0.00030900	-1.80120300
H	5.26578300	0.00104400	-1.71499300	H	5.17179200	-0.00036700	-2.09681800
C	3.35977800	-3.61284300	-0.20914400	C	3.37001600	-3.58081500	-0.09017300
H	3.56228900	-2.79542800	-0.91374500	H	3.57110500	-2.73439600	-0.75972900
H	3.48125900	-4.54687300	-0.77452100	H	3.52787900	-4.49295200	-0.68192600
C	3.25661500	0.00063200	-2.51229900	C	3.10262800	-0.00017900	-2.78209900
H	3.54742800	0.00065500	-3.55705600	H	3.32826300	-0.00012800	-3.84219000
C	4.36842000	-3.55889100	0.93036900	C	4.34642300	-3.53985300	1.07786300
H	4.27158600	-2.61948500	1.48783200	H	4.21180500	-2.61977700	1.65932400
H	5.39693200	-3.62689400	0.55990400	H	5.38553600	-3.57284300	0.73285100
H	4.21088200	-4.38082500	1.63876100	H	4.19036100	-4.38674200	1.75677300
C	4.36610100	3.56088000	0.93117100	C	4.34745900	3.53907600	1.07784300
H	4.20814400	4.38290400	1.63936500	H	4.19159500	4.38606900	1.75666800
H	5.39470800	3.62906000	0.56100400	H	5.38656000	3.57183000	0.73277200
H	4.26932700	2.62154000	1.48876100	H	4.21270100	2.61909400	1.65941700
H	0.10650000	0.00020500	4.92023200	H	0.40284900	-0.00041100	4.84851600
H	3.67767400	0.00077200	2.55897200	H	3.85275400	-0.00055000	2.28218500
Br	-1.52987400	-0.00065900	-2.70436700	Br	-1.69699100	0.00024600	-2.63103200

Ground state of **ppy-CN** (S_0)				Excited state of **ppy-CN** (T_1)			
Ir	-0.63697600	-0.00012800	-0.51392800	Ir	-0.65817200	-0.00049300	-0.50610600
N	-2.31898200	-2.29316100	0.05700500	N	-2.31811000	-2.29679100	0.11780900
N	-2.32129300	2.29123000	0.05691200	N	-2.32465100	2.29084200	0.11864000
C	-1.04691800	2.00113900	-0.37323900	C	-1.06086900	2.00691800	-0.34503600
N	1.48208500	0.00085800	-0.91076400	N	1.40365800	0.00266200	-1.11166000
C	0.13714500	-0.00008900	1.38843600	C	0.23118800	0.00014000	1.30626400
N	-0.47859500	-3.20881000	-0.56730100	N	-0.48380800	-3.21448600	-0.52453500
N	-0.48173000	3.20871200	-0.56713600	N	-0.49305100	3.21400200	-0.52359200
C	-1.04498800	-2.00181200	-0.37337500	C	-1.05518700	-2.00909100	-0.34595100
C	-3.16935800	-1.19990100	0.32684800	C	-3.16062700	-1.20325800	0.41693300
C	-2.51225000	-0.00104100	0.07686700	C	-2.50665800	-0.00325400	0.17030900
C	-1.36352700	4.23154400	-0.25472700	C	-1.36341400	4.23312800	-0.17325700
H	-1.08736100	5.27076900	-0.34524300	H	-1.08506400	5.27307100	-0.24744500
C	0.90422000	3.40408400	-0.95667600	C	0.90185000	3.40448000	-0.88643300
H	0.95580400	4.30500900	-1.57649200	H	0.97085800	4.29698500	-1.51646000
H	1.18338900	2.55194300	-1.58030100	H	1.19313300	2.54057500	-1.48740300
C	2.27230700	0.00096100	0.19316700	C	2.30259100	0.00297300	-0.02883300
C	-3.17057700	1.19715500	0.32679800	C	-3.16404400	1.19479700	0.41733800
C	0.90737500	-3.40294900	-0.95731500	C	0.91147100	-3.40075000	-0.88802500
H	1.18566800	-2.55026700	-1.58058400	H	1.20032900	-2.53468000	-1.48702400
H	0.95947700	-4.30350800	-1.57760600	H	0.98262500	-4.29157200	-1.52020000
C	-0.56099300	-0.00068100	2.60437800	C	-0.35188300	-0.00061600	2.56873900
H	-1.64852800	-0.00115800	2.58987800	H	-1.43729600	-0.00152600	2.64050300

C	-1.35921800	-4.23251200	-0.25441200	C	-1.35107600	-4.23620800	-0.17407400
H	-1.08198800	-5.27146800	-0.34478400	H	-1.06966800	-5.27533200	-0.24827900
C	-2.52255800	-3.65525900	0.13451200	C	-2.51088800	-3.65760100	0.22612000
H	-3.45937100	-4.09085600	0.44358500	H	-3.43813200	-4.09288100	0.56328000
C	3.66600000	0.00157000	0.05511100	C	3.71254700	0.00470700	-0.29858900
H	4.29555600	0.00163600	0.93710200	H	4.40841000	0.00498000	0.53310800
C	1.82423200	3.51069300	0.25066900	C	1.78623200	3.52189500	0.34663400
H	1.67727100	2.62258400	0.87747200	H	1.60342600	2.64742900	0.98352600
H	1.53175200	4.37783400	0.85829500	H	1.49133200	4.40634500	0.92777600
C	-4.47698700	1.22243600	0.80542000	C	-4.46566400	1.21880400	0.90905000
H	-4.99815700	2.15445400	1.00438200	H	-4.98859400	2.14970700	1.10834900
C	1.55319300	0.00040600	1.46680900	C	1.72003400	0.00150000	1.23667200
C	-2.52632300	3.65312600	0.13408900	C	-2.52154900	3.65107900	0.22680900
H	-3.46364700	4.08779500	0.44291900	H	-3.45013100	4.08358800	0.56385200
C	0.09686200	-0.00073400	3.83119300	C	0.40403200	-0.00050800	3.74385800
C	2.04053400	0.00138400	-2.13157900	C	1.87828000	0.00389700	-2.34744300
H	1.34151000	0.00120500	-2.96154200	H	1.13043200	0.00342800	-3.13499100
C	-5.11441300	-0.00234000	1.03454300	C	-5.09750700	-0.00711700	1.14773900
H	-6.13459300	-0.00287200	1.40615000	H	-6.11335400	-0.00862700	1.53089300
C	2.21717600	0.00033100	2.70326900	C	2.47876800	0.00133100	2.46558100
C	-4.47574100	-1.22647900	0.80545300	C	-4.46217700	-1.23115600	0.90861100
H	-4.99600400	-2.15901100	1.00438700	H	-4.98246800	-2.16361800	1.10752500
C	1.82784400	-3.50943500	0.24969300	C	1.79646900	-3.51883600	0.34454700
H	1.53608500	-4.37699000	0.85707300	H	1.50396500	-4.40537300	0.92372000
H	1.68051600	-2.62166100	0.87689800	H	1.61170400	-2.64634600	0.98360100
C	1.49251700	-0.00022900	3.88580700	C	1.83101900	0.00041700	3.66673900
H	2.00835900	-0.00030800	4.84186600	H	2.41051000	0.00039300	4.58681900
C	3.28939000	3.62396200	-0.15100800	C	3.26568200	3.59464400	-0.00753600
H	3.54297300	2.79528000	-0.82519200	H	3.52195300	2.74478500	-0.65357300
H	3.44550600	4.54848700	-0.72346500	H	3.46231600	4.50291200	-0.59354900
C	4.24053100	0.00211400	-1.20522700	C	4.17616100	0.00601800	-1.58631700
H	5.32089600	0.00262300	-1.31321000	H	5.24293300	0.00734900	-1.78810200
C	3.29295000	-3.62165000	-0.15248300	C	3.27598100	-3.58714100	-0.01028500
H	3.54570300	-2.79285600	-0.82685100	H	3.52992000	-2.73516800	-0.65444900
H	3.44959000	-4.54611900	-0.72487800	H	3.47462800	-4.49356800	-0.59846400
C	3.41145100	0.00202900	-2.32665400	C	3.24352800	0.00562200	-2.65265100
H	3.81365500	0.00249400	-3.33359100	H	3.56099200	0.00657300	-3.68878300
C	4.22134200	-3.59297700	1.05423600	C	4.16211300	-3.56379200	1.22796200
H	4.09383000	-2.66083700	1.61767500	H	3.99023600	-2.64875500	1.80762700
H	5.27231100	-3.66452000	0.75418100	H	5.22396500	-3.60072500	0.96173200
H	4.00862600	-4.42399100	1.73705200	H	3.94968800	-4.41622700	1.88409700
C	4.21741400	3.59614600	1.05600400	C	4.15138100	3.57062200	1.23100700
H	4.00405300	4.42727200	1.73848800	H	3.93674200	4.42115000	1.88889600
H	5.26843700	3.66814500	0.75624500	H	5.21325500	3.61054400	0.96530300
H	4.09022100	2.66411800	1.61968400	H	3.98132700	2.65395700	1.80863600
H	-0.47862700	-0.00114900	4.75441100	H	-0.07909700	-0.00130900	4.71627000
H	3.30320100	0.00061300	2.75188700	H	3.56395900	0.00203600	2.43950500

C	-1.11052600	-0.00017800	-2.49775500	C	-1.30671900	-0.00014000	-2.45353700
N	-1.31971600	-0.00022400	-3.65107800	N	-1.63289600	0.00046600	-3.57863700
Ground state of **ppy-OCN** (S_0)				Excited state of **ppy-OCN** (T_1)			
Ir	-0.57657600	-0.09857000	-0.35970100	Ir	-0.57704900	-0.09397800	-0.35533100
N	-1.89019800	-2.64947300	0.06415300	N	-1.85724900	-2.63824000	0.19459300
N	-2.55522500	1.87388400	0.42936900	N	-2.54409600	1.89579000	0.41392300
O	-1.22278100	-0.08474300	-2.50525300	O	-1.35029400	-0.14409200	-2.44156700
C	-1.27806800	1.80778200	-0.07651700	C	-1.27824400	1.82342500	-0.11714800
N	1.44251200	0.23659800	-0.95964800	N	1.37468000	0.22200800	-1.14657000
C	0.32898700	-0.10350600	1.41654700	C	0.40177800	-0.01524600	1.33820900
N	0.02691800	-3.23782500	-0.70458200	N	0.05292000	-3.24679300	-0.57999000
N	-2.75825700	1.65301800	-3.22026500	N	-3.39464100	1.04525400	-2.98370200
N	-0.91859500	3.09650200	-0.23053200	N	-0.91255200	3.10645200	-0.28713800
C	-0.69102000	-2.14345600	-0.38258000	C	-0.67253200	-2.14829100	-0.30308500
C	-2.87379700	-1.71470400	0.46177700	C	-2.83691900	-1.69368600	0.58783100
C	-2.39719200	-0.41859400	0.31427900	C	-2.36954500	-0.40064200	0.40355500
C	-1.93025400	3.95162100	0.17103800	C	-1.91010600	3.96826700	0.12964100
H	-1.82582500	5.02433500	0.11904600	H	-1.80182100	5.04024700	0.07038400
C	0.39456300	3.52351200	-0.68283000	C	0.41608700	3.51444600	-0.71741800
H	0.27294600	4.47012900	-1.21813400	H	0.31609600	4.44308600	-1.28739600
H	0.74557500	2.77709300	-1.39859100	H	0.78254000	2.73830800	-1.39214700
C	2.33372400	0.27293100	0.06128900	C	2.35169900	0.29248100	-0.14676300
C	-3.22027200	0.64744000	0.65408000	C	-3.19551300	0.67333500	0.70243600
C	1.40994300	-3.20458400	-1.15065600	C	1.43806800	-3.21317100	-1.02460600
H	1.54676500	-2.27429500	-1.70577700	H	1.57127900	-2.28037500	-1.57604600
H	1.55725100	-4.03598100	-1.84715600	H	1.59031600	-4.04528200	-1.71911800
C	-0.26342200	-0.27301000	2.67583100	C	-0.10526800	-0.10024700	2.63571300
H	-1.33779900	-0.42237000	2.73901700	H	-1.17661900	-0.22618300	2.76720300
C	-0.68804700	-4.39820200	-0.45892700	C	-0.64235400	-4.39834200	-0.25863800
H	-0.27584200	-5.37573800	-0.65678200	H	-0.22259300	-5.38117100	-0.40836400
C	-1.90084400	-4.02642100	0.02177100	C	-1.85156700	-4.01388900	0.22603900
H	-2.75328800	-4.61599200	0.31962000	H	-2.68931800	-4.59678800	0.57448800
C	3.69265600	0.47270600	-0.20742200	C	3.71549000	0.48505700	-0.53271200
H	4.40860100	0.49995400	0.60599400	H	4.48131800	0.54451700	0.23322600
C	1.37511300	3.66043800	0.47232600	C	1.35932700	3.68105000	0.46531900
H	1.38912100	2.71310100	1.02502400	H	1.33698700	2.75580200	1.05456800
H	1.01491800	4.42857800	1.16988500	H	0.99332400	4.48493200	1.11835300
C	-4.50571600	0.44641200	1.14668100	C	-4.47654600	0.48235900	1.21062600
H	-5.15513000	1.27450700	1.41498400	H	-5.13190000	1.31444900	1.44978300
C	1.73723700	0.09108900	1.38275500	C	1.86936500	0.16519400	1.16047400
C	-2.96683100	3.17911100	0.58248800	C	-2.94389100	3.20298700	0.56684300
H	-3.94436000	3.44676100	0.95091100	H	-3.91194500	3.47942600	0.95338900
C	0.49319600	-0.25417200	3.84383900	C	0.72189500	-0.04136900	3.75410600
C	1.85363400	0.39474400	-2.22559200	C	1.71789500	0.33398600	-2.42240700
H	1.06631900	0.34786100	-2.97212200	H	0.89441400	0.26686100	-3.12891900
C	-4.95258000	-0.87248600	1.28762500	C	-4.91271800	-0.83350200	1.40105600
H	-5.95365500	-1.05028300	1.66849700	H	-5.90996700	-1.00384300	1.79477000

C	2.49268200	0.10969500	2.56390500	C	2.69464800	0.21320200	2.33446300
C	-2.01517100	0.81168700	-2.85633500	C	-2.40532000	0.46768700	-2.70373700
C	-4.15186400	-1.96950100	0.94949900	C	-4.11062700	-1.93828000	1.09097500
H	-4.53256800	-2.97970900	1.06909300	H	-4.48889200	-2.94516300	1.24092600
C	2.38524700	-3.28076000	0.01512600	C	2.40318300	-3.28250400	0.15041300
H	2.23095800	-4.22095400	0.56156000	H	2.25865600	-4.22795000	0.69064000
H	2.15327200	-2.46745500	0.71381300	H	2.15320800	-2.47410000	0.84881200
C	1.87619300	-0.06300700	3.79418600	C	2.12952400	0.11462300	3.57757000
H	2.46473000	-0.04803100	4.70683900	H	2.76948900	0.15726100	4.45577500
C	2.78069800	4.00262700	-0.00465200	C	2.78834000	3.96897200	0.02416900
H	3.09495400	3.26560900	-0.75546700	H	3.10652900	3.19543100	-0.68701500
H	2.77258100	4.97735000	-0.51125100	H	2.82414600	4.92495100	-0.51610200
C	4.12068600	0.63593200	-1.51586100	C	4.05103800	0.59735600	-1.85660800
H	5.17383700	0.79168000	-1.72884300	H	5.08662800	0.74458200	-2.14827800
C	3.83455000	-3.17320000	-0.44222700	C	3.85455900	-3.14527700	-0.29067300
H	3.94944800	-2.27811200	-1.06782200	H	3.95919500	-2.23990400	-0.90281800
H	4.08566900	-4.03154900	-1.08001400	H	4.12702600	-3.99208200	-0.93532000
C	3.18460400	0.59790500	-2.55015700	C	3.03438900	0.52344700	-2.84240900
H	3.47709900	0.72181700	-3.58686300	H	3.25779500	0.61070400	-3.89916000
C	4.80136600	-3.09633000	0.73169600	C	4.80704000	-3.06389000	0.89471600
H	4.57731200	-2.22685600	1.36144100	H	4.56067100	-2.20390000	1.52925300
H	5.83884500	-3.00863700	0.39185100	H	5.84625700	-2.95467100	0.56639500
H	4.72887300	-3.98916300	1.36392600	H	4.74423500	-3.96396800	1.51787700
C	3.78604100	4.02048300	1.13889900	C	3.75483800	3.99850300	1.20071600
H	3.51429200	4.76841400	1.89308400	H	3.47675900	4.77475900	1.92354700
H	4.79501100	4.25390600	0.78234400	H	4.78027700	4.19795400	0.87135300
H	3.82210100	3.04512900	1.63908200	H	3.74999600	3.03699500	1.72829500
H	3.56843600	0.26170600	2.52630000	H	3.76955900	0.33350300	2.23955000
H	0.00180200	-0.38900900	4.80475300	H	0.30998200	-0.11890300	4.75533000

6. Device fabrication and characterization

OLEDs were fabricated in a Kurt J. Lesker SPECTROS vacuum deposition system with a base pressure of 10^{-8} mBar. In the vacuum chamber, organic materials were thermally deposited in sequence at a rate of ~0.1 nm s^{-1}. The doping process in the emitting layer was realized by co-deposition technology. LiF (1.2 nm) and Al (100 nm) were thermally deposited at rates of 0.03 and 0.2 nm s^{-1}, respectively. Film thicknesses were determined in situ using calibrated oscillating quartz crystal sensors. EL spectra, J-V-L charateristics, CIE coordinates, CRI, EQE, CE and PE were measured using a keithley 2400 source-meter and an absolute external quantum efficiency measurement system (C9920-12, Hamamatsu Photonics). EL distribution was measured with an angle-dependent device testing system (C9920-11, Hamamatsu Photonics). All devices were characterized at room temperature without encapsulation. TAPC, TCTA, TmPyPB, Liq, CzSi, TSPO1 and LiF were products from PURI Materials.

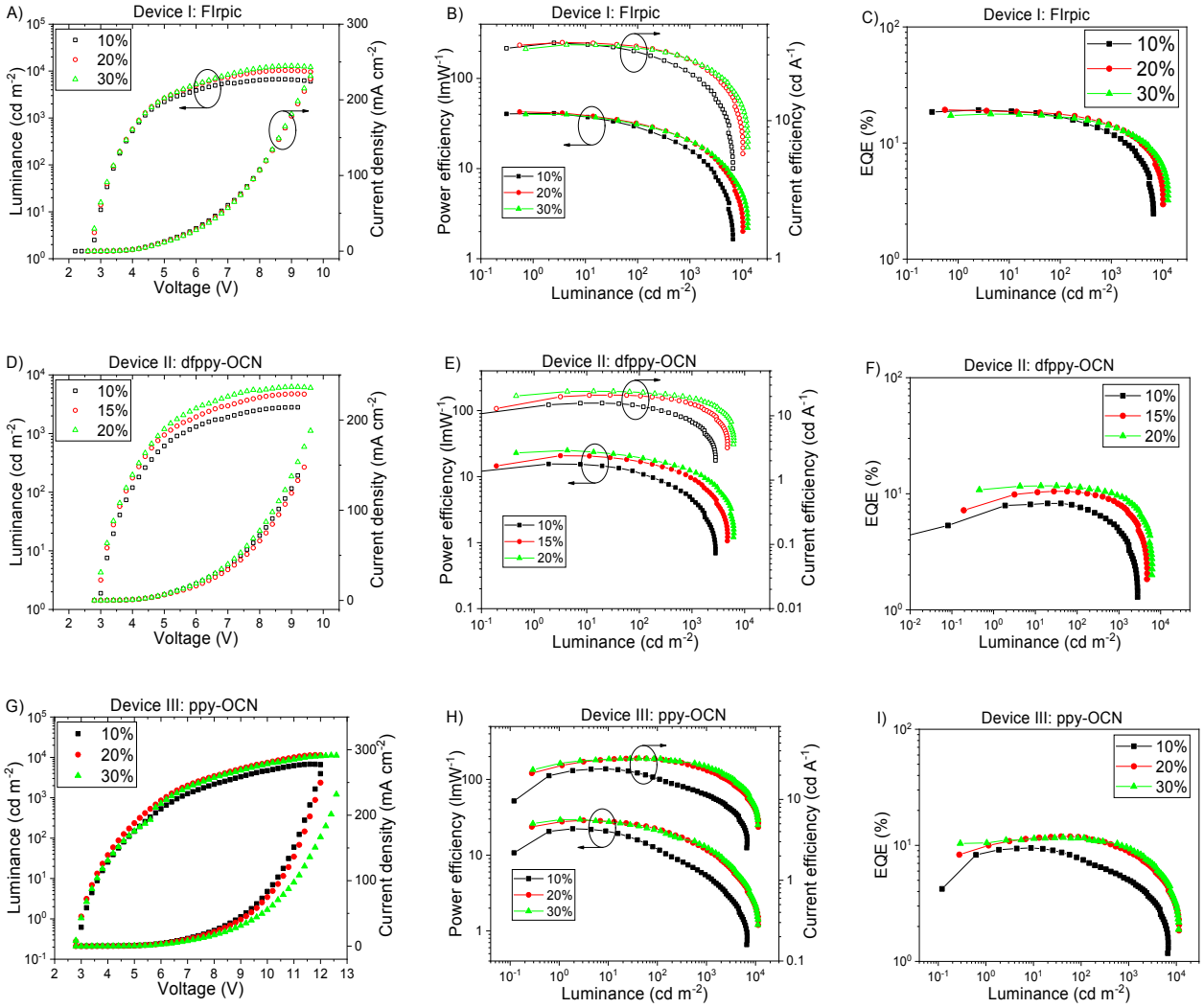


Fig. S10. *J-V-L* characteristics, η_{PE}-*L*-η_L characteristics and η_{Ext}-*L* characteristics of devices I-III with dopants at specified concentrations. Device configuration: ITO/HAT-CN (10 nm)/TAPC (50 nm)/ TCTA (Ir complexes: x wt%, 10 nm; x = 10, 15, 20, 30)/TmPyPB (50 nm)/ Liq (2 nm)/Al(120 nm).

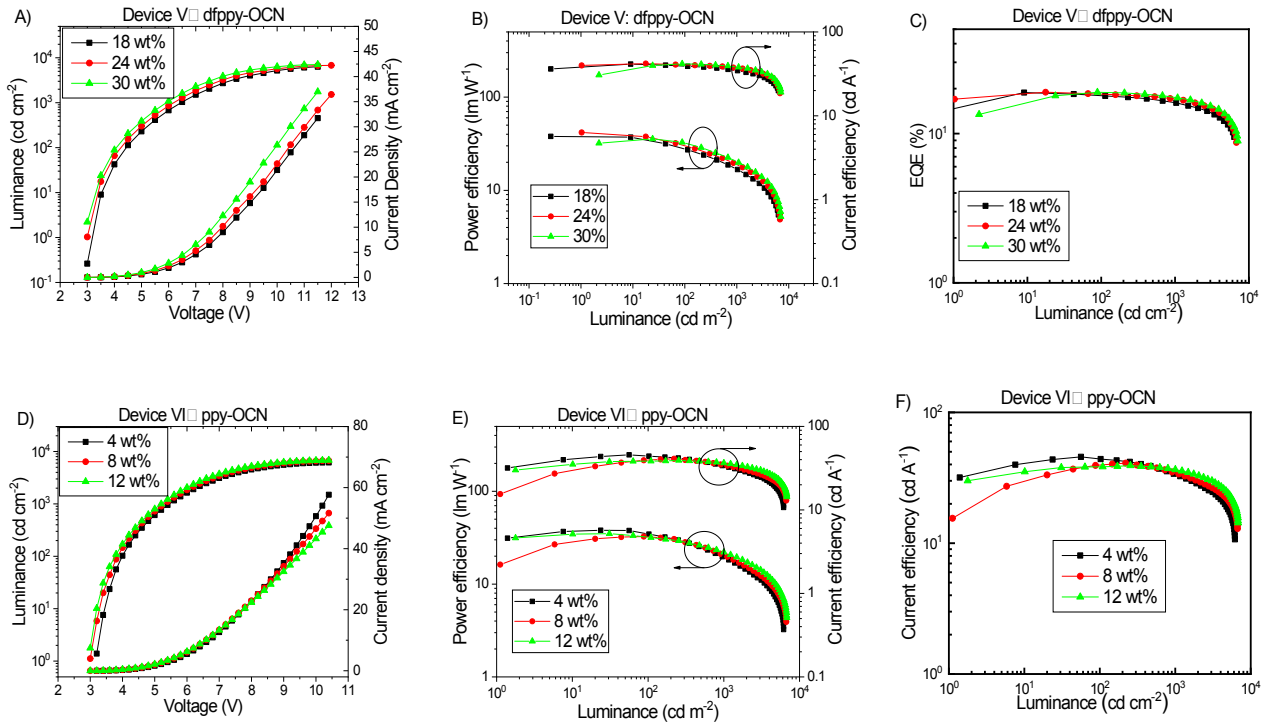


Fig. S11. *J*-*V*-*L* characteristics, η_{PE}-*L*-η_L characteristics and η_{Ext}-*L* characteristics of devices V-VI with dopants at specified concentrations. Device configuration: ITO/HAT-CN (5 nm)/TAPC (30 nm)/TCTA (10 nm)/CzSi (3 nm)/ CzSi (Ir complexes: x wt%, 17 nm; x = 4, 8, 12, 18, 24, 30)/TSPO1 (40 nm)/LiF (1.2 nm)/Al (100 nm).

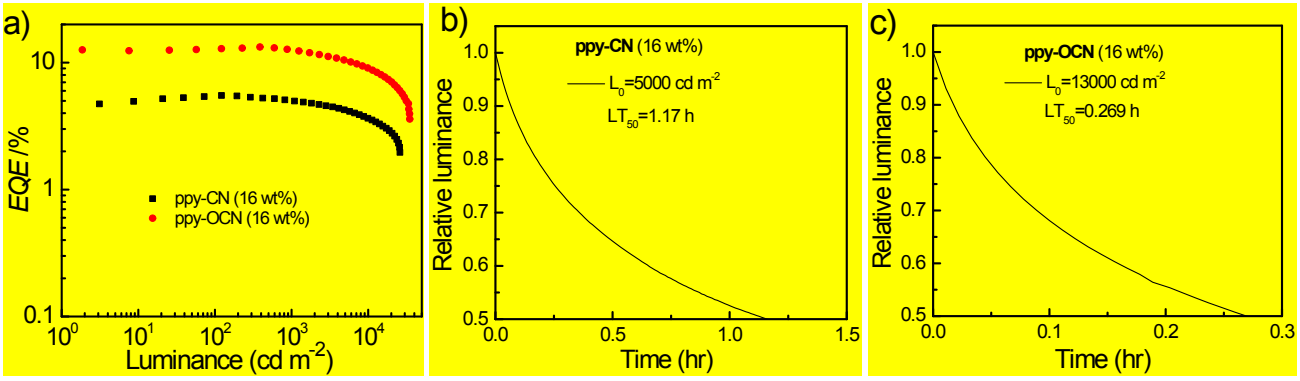


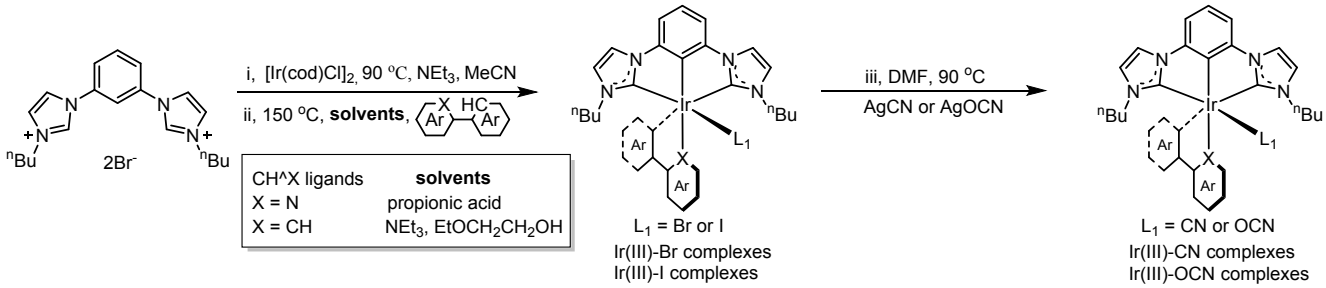
Fig. S12. The EQE–luminance and operational lifetime of devices based on complexes **ppy-CN** and **ppy-OCN**. Device configuration: ITO/HAT-CN (10 nm)/NPB (40 nm)/Tris-PCz (10 nm)/Ir-emitter: mCBP (20 nm)/mCBT (8 nm)/BPy-TP2 (40 nm)/Yb (2 nm)/Ag (100 nm).

7. Synthesis and characterization of iridium complexes

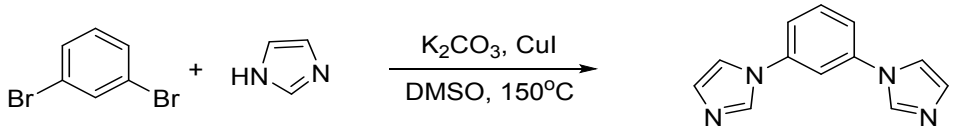
Unless otherwise specified, all starting chemicals including 2-phenylpyridine (**ppy**), 2-(2,4-difluorophenyl)pyridine (**dfppy**), 2-(thiophen-2-yl)pyridine (**thpy**) and 1-phenylisoquinoline (**piq**) ligands were used without further purification as received from commercial sources. 3-Methyl-1-(4-(trifluoromethyl)phenyl)-1*H*-3λ^4-imidazole iodide (**tmpi**),[10] *N*-phenyl,*N*-methyl-pyridoimidazol-2-yl iodide (**pmp**),[11] 2',6'-difluoro-2,3'-bipyridine (**dfpypy**),[12] 4-methyl-2-(thiophen-2-yl)quinolone (**lpt**)[13] and 2-(benzo[*b*]thiophen-2-yl)benzo[*d*]thiazole (**TaBt**)[14] ligands were synthesized following the literature

procedure. NMR spectra were recorded on a Bruker AV-400 spectrometer (solvent: $CDCl_3$ or DMSO-d_6; chemical shifts: δ, ppm; J, Hz). Mass spectra were obtained on a Thermo Scientific DFS High Resolution Magnetic Sector MS instrument by using the electron-impact ionization technique (40 eV).

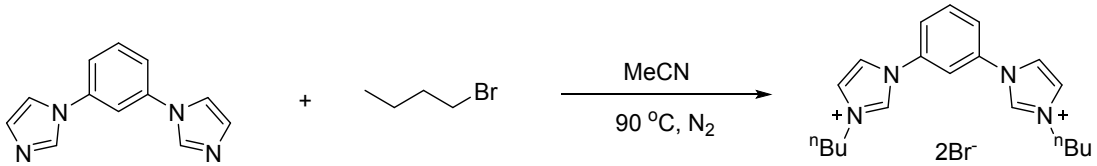
General procedure for preparation of Ir(III)-Br, Ir(III)-CN and Ir(III)-OCN complexes.



Under a nitrogen atmosphere, the tridentate C^C^C ligand was first metalation with an iridium reagent $[Ir(cod)Cl]_2$ (cod = 1,5-cyclooctadiene) in the presence of NEt_3 in CH_3CN at 90 °C. After that, the NEt_3 and MeCN were removed under vacuum without isolation of the intermediate species. Next, the intermediate species were treated with the bidentate ligands in propionic acid at 150 °C to give the Ir(III)-Br or Ir(III)-I complexes, except the **tmpi-I** and **pmp-I**, which were treated with the bidentate ligands in NEt_3 and $EtOCH_2CH_2OH$ at 150 °C. And the Ir(III)-CN or Ir(III)-OCN complexes were obtained by reacting the Ir(III)-Br or Ir(III)-I complexes with AgCN or AgOCN in DMF at 90 °C, respectively. The Ir(III) complexes were characterized by ^1H, ^{19}F NMR spectroscopy and mass spectrometry.

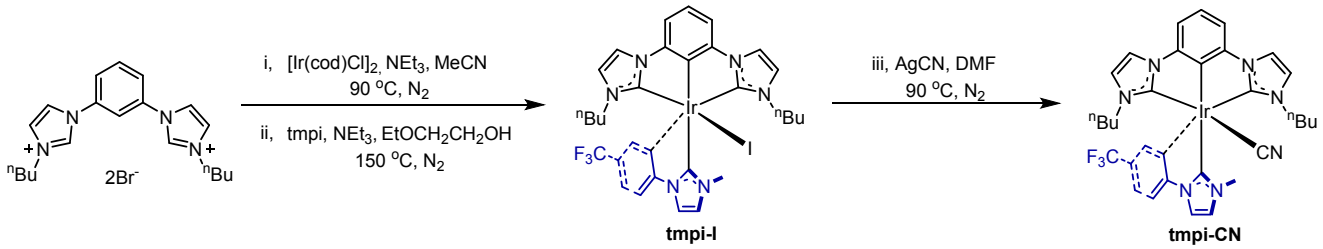


1,3-di(imidazol-1-yl)benzene: To a 100 mL round bottom flask with a stir bar was added 1,3-dibromobenzene (2.36 g, 10 mmol), imidazole (4.08 g, 60 mmol), CuI (95 mg, 0.5 mmol), potassium carbonate (25.3 g, 0.183 mol) and DMSO (60 mL). The suspension was heated at 150 °C for 2 days. The reaction cooled below 60 °C and filtered through the celite and the solid residue was washed by EA. After EA was removed from the mixture, DMSO was distilled under vacuum. The residue was extracted by CH_2Cl_2 and then washed by water. The organic layer was dried by $MgSO_4$, filtered, and evaporated. The resulting white solid 1,3-di(imidazol-1-yl)benzene (2.09 g, 10 mmol, yield: 99%) was used in the following procedure without further purification. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.93 (s, 2H), 7.63 (t, J = 8.0 Hz, 1H), 7.40–7.45 (m, 3H), 7.32 (s, 2H), 7.23 (s, 2H) ppm.



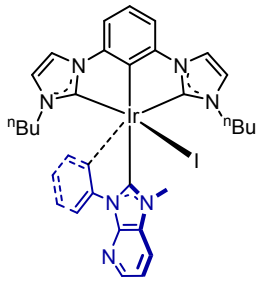
1,3-Bis(1-butylimidazolium-3-yl)benzene dibromide: To a 25 mL Schlenk tube with a stir bar was added 1,3-di(imidazol-1-yl)benzene (5.8 g, 27.6 mmol), *n*-butylbromide (18.9 g, 138 mmol) and MeCN (15 mL). The solution was heated at 90 °C for 12h under nitrogen protection. MeCN was removed under vacuum and the residue was dissolved in EtOH (~50 mL), concentrate to 5 mL, then add Et_2O (~20 mL). The resulting white precipitate was collected by filtered as a white solid (10.69 g, 22.1 mmol, yield: 80%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.51 (s, 2H), 9.13 (t, *J* = 1.9 Hz, 2H), 9.06 (d, *J* = 2.2 Hz, 1H), 8.38 (dd, *J* = 8.3, 2.1 Hz, 2H), 7.67 (t, *J* = 8.2 Hz, 1H), 7.52 (d, *J* = 1.8 Hz, 2H), 4.48 (t, *J* = 7.4 Hz, 4H), 2.05 (p, *J* = 7.4 Hz, 4H), 1.46 (dt, *J* = 14.8, 7.4 Hz, 4H), 1.03 (t, *J* = 7.4 Hz, 6H) ppm.

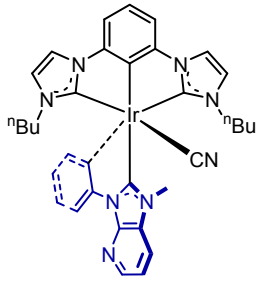


tmpi-I: To a 25 mL Schlenk tube with a stir bar was added 1,3-bis(1-butylimidazolium-3-yl)benzene dibromide (0.14 g, 0.30 mmol), $[Ir(cod)Cl]_2$ (0.10 g, 0.15 mmol) and MeCN (10 mL). The orange solution was degassed by N_2 for 5 mins, then NEt_3 (1 mL) was added. The reaction was heated at 90 °C for 4 h. After that, MeCN and NEt_3 were removed under vacuum and the mixture was transferred to a Schlenk tube, tmpi ligand (0.11 g, 0.30 mmol), NEt_3 (2 mL) and $EtOCH_2CH_2OH$ (20 mL) was then added. The orange solution was degassed by N_2 for 5 mins. And the Schlenk tube was placed into oil bath with temperature at 150 °C for overnight. Subsequently the reaction was cooled, and the precipitate was filtered. The solvent was then removed by rotary evaporation and the crude mixture was separated through SiO_2 column chromatography (with eluent CH_2Cl_2 to CH_2Cl_2/MeCN, v/v = 10/1) to obtain a white solid. **tmpi-I** (95.1 mg, 0.12 mmol, 40% yield) was obtained by recrystallized with CH_2Cl_2/Et_2O (2 mL/20 mL). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.59 (dd, *J* = 6.0, 2.0 Hz, 1H), 7.43 (t, *J* = 2.5 Hz, 2H), 7.22 – 7.17 (m, 4H), 7.01 (t, *J* = 7.0 Hz, 1H), 6.94 (d, *J* = 7.3 Hz, 1H), 6.70 (t, *J* = 2.4 Hz, 2H), 6.07 (d, *J* = 1.7 Hz, 1H), 4.57 (d, *J* = 13.1 Hz, 3H), 3.60 – 3.47 (m, 2H), 3.47 – 3.34 (m, 2H), 1.50 – 1.36 (m, 2H), 1.21 – 1.12 (m, 2H), 1.09 – 0.90 (m, 4H), 0.76 (t, *J* = 7.3 Hz, 6H) ppm.

tmpi-CN: To a 50 mL round bottom flask with a stir bar was added **tmpi-I** (55.9 mg, 0.068 mmol), AgCN (18.3 mg, 0.137 mmol) and DMF (10 mL) under N_2 gas protection. The reaction mixture was heated at 90 °C for 2 h. After that, DMF was removed under vacuum and the crude mixture was separated through SiO_2 column chromatography (with eluent CH_2Cl_2 to CH_2Cl_2/MeCN, v/v = 10/1) to obtain a white solid. **tmpi-CN** (10 mg, 0.013 mmol, 19% yield) was obtained by recrystallized with CH_2Cl_2/Et_2O (2 mL/20 mL). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.60 (d, *J* = 2.0 Hz, 1H), 7.47 (d, *J* = 2.0 Hz, 2H), 7.29 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.23 – 7.16 (m, 3H), 7.07 (d, *J* = 8.2 Hz, 1H), 7.00 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.75 (d, *J* = 2.0 Hz, 2H), 6.10 (d, *J* = 1.5 Hz, 1H), 4.42 (s, 3H), 3.45 – 3.30 (m, 4H), 1.50 – 1.37 (m, 2H), 1.07 – 0.91 (m, 2H), 0.93 – 0.81 (m, 4H), 0.77 (t, *J* = 7.3 Hz, 6H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -61.66 (s) ppm.

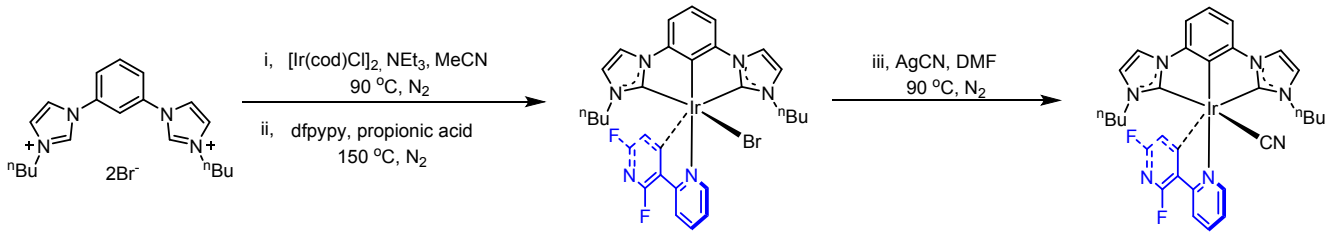


pmp-I: The synthetic method is similar to that of **tmpi-I**. White solid, yield: 49%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.72 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.52 – 8.46 (m, 1H), 7.83 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 2H), 7.37 (dd, *J* = 8.0, 5.1 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.25 – 7.18 (m, 2H), 6.96 – 6.76 (m, 1H), 6.69 (d, *J* = 2.0 Hz, 2H), 6.46 – 6.42 (m, 1H), 6.00 (dd, *J* = 7.8, 1.4 Hz, 1H), 4.82 (s, 3H), 3.54 – 3.34 (m, 4H), 1.41 – 1.28 (m, 2H), 1.08 – 0.96 (m, 2H), 0.82 – 0.71 (m, 2H), 0.78 – 0.43 (m, 8H) ppm.



pmp-CN

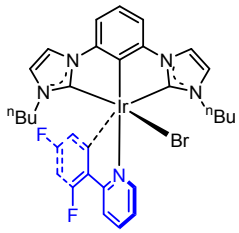
pmp-CN: The synthetic method is similar to that of **tmpi-CN**. White solid, yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.76 (d, *J* = 7.8 Hz, 1H), 8.49 (d, *J* = 4.8 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 2.2 Hz, 2H), 7.36 (dd, *J* = 7.9, 5.0 Hz, 1H), 7.31 (dd, *J* = 8.5, 7.0 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 2H), 6.94 – 6.84 (m, 1H), 6.71 (d, *J* = 2.1 Hz, 2H), 6.58 – 6.37 (m, 1H), 5.96 (d, *J* = 7.2 Hz, 1H), 4.67 (s, 3H), 3.42 – 3.23 (m, 4H), 1.34 – 1.17 (m, 2H), 0.99 – 0.83 (m, 2H), 0.83 – 0.67 (m, 2H), 0.63 – 0.27 (m, 8H) ppm.



dfpypy-Br **dfpypy-CN**

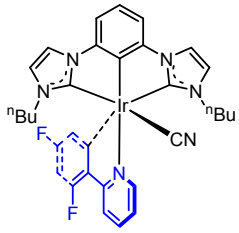
dfpypy-Br: To a 25 mL Schlenk tube with a stir bar was added 1,3-bis(1-butylimidazolium-3-yl)benzene dibromide (0.14 g, 0.30 mmol), $[Ir(cod)Cl]_2$ (0.10 g, 0.15 mmol) and MeCN (10 mL). The orange solution was degassed by N_2 for 5 mins, then NEt_3 (1 mL) was added. The reaction was heated at 90 °C for 4 h. After that, MeCN and NEt_3 were removed under vacuum and the mixture was transferred to a Schlenk tube, dfpypy ligand (57.7 mg, 0.30 mmol) and propionic acid (20 mL) was then added. The orange solution was degassed by N_2 for 5 mins. And the Schlenk tube was placed into oil bath with temperature at 150 °C for overnight. Subsequently the reaction was cooled, and the precipitate was filtered. The solvent was then removed by rotary evaporation and the crude mixture was separated through SiO_2 column chromatography (with eluent CH_2Cl_2 to CH_2Cl_2/EA, v/v = 10/1) to obtain a pale yellow solid. **dfpypy-Br** (82.1 mg, 0.10 mmol, 35% yield) was obtained by recrystallized with CH_2Cl_2/Et_2O (2 mL/20 mL). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.52 (d, *J* = 5.3 Hz, 1H), 8.38 (d, *J* = 8.3 Hz, 1H), 7.94 (t, *J* = 8.1 Hz, 1H), 7.49 – 7.38 (m, 3H), 7.23 – 7.19 (m, 1H), 7.19 – 7.13 (m, 2H), 6.75 (d, *J* = 2.4 Hz, 2H), 5.54 (d, *J* = 6.4 Hz, 1H), 3.32 – 3.11 (m, 4.7 Hz, 4H), 1.43 – 1.35 (m, 2H), 1.15 – 1.06 (m, 2H), 0.91 – 0.76 (m, 4H), 0.71 (t, *J* = 6.4 Hz, 6H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -70.13 (d, *J* = 10.0 Hz), -70.33 (d, *J* = 9.9 Hz), -74.03 (d, *J* = 9.8 Hz), -74.23 (d, *J* = 10.0 Hz) ppm.

dfpypy-CN: The synthetic method is similar to that of **tmpi-CN**. White solid, yield: 82%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.28 (d, *J* = 5.0 Hz, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.50 (d, *J* = 2.1 Hz, 2H), 7.40 – 7.37 (m, 1H), 7.29 (s, 1H), 7.16 (d, *J* = 7.5 Hz, 2H), 6.80 (d, *J* = 2.0 Hz, 2H), 5.50 (s, 1H), 3.38 – 3.22 (m, 2H), 3.22 – 3.09 (m, 2H), 1.49 – 1.38 (m, 2H), 1.35 – 1.31 (m, 2H), 1.18 – 1.12 (m, 2H), 0.85 – 0.78 (m, 2H), 0.73 (t, *J* = 6.9 Hz, 6H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -69.66 (d, *J* = 9.6 Hz), -74.02 (dd, *J* = 9.6, 1.7 Hz) ppm.



dfppy-Br

dfppy-Br: The synthetic method is similar to that of **dfpypy-Br**. White solid, yield: 49%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.54 (dt, *J* = 5.4, 1.5 Hz, 1H), 8.40 (d, *J* = 8.5 Hz, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 2.1 Hz, 2H), 7.37 – 7.32 (m, 1H), 7.24 – 7.18 (m, 1H), 7.18 – 7.14 (m, 2H), 6.74 (d, *J* = 2.1 Hz, 2H), 6.26 (ddd, *J* = 13.1, 9.0, 2.5 Hz, 1H), 5.56 (dd, *J* = 9.2, 2.5 Hz, 1H), 3.34 – 3.15 (m, 4H), 1.45 – 1.34 (m, 2H), 1.17 – 1.06 (m, 2H), 0.94 – 0.83 (m, 2H), 0.83 – 0.68 (m, 8H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -109.78 (q, *J* = 9.5 Hz), -111.31 (ddd, *J* = 12.8, 9.8, 2.7 Hz) ppm. ESI-MS: $[M\text{-}Br+MeCN]^+$: m/z: 745.2419; calculated: 745.2442.

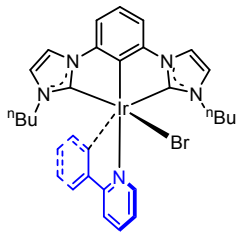


dfppy-CN

dfppy-CN: The synthetic method is similar to that of **tmpi-CN**. White solid, yield: 60%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.27 (d, *J* = 5.4 Hz, 1H), 8.39 (d, *J* = 9.8 Hz, 1H), 7.89 (t, *J* = 7.9 Hz, 1H), 7.47 (d, *J* = 2.0 Hz, 2H), 7.31 – 7.27 (m, 1H), 7.24 – 7.20 (m, 1H), 7.13 (d, *J* = 7.8 Hz, 2H), 6.76 (d, *J* = 2.0 Hz, 2H), 6.25 (ddd, *J* = 13.1, 8.9, 2.4 Hz, 1H), 5.48 (dd, *J* = 8.6, 2.4 Hz, 1H), 3.26 (ddd, *J* = 13.5, 10.0, 6.0 Hz, 2H), 3.17 (ddd, *J* = 13.4, 10.0, 5.8 Hz, 2H), 1.46 – 1.38 (m, 2H), 1.18 – 1.09 (m, 2H), 0.92 – 0.85 (m, 2H), 0.83 – 0.76 (m, 2H), 0.72 (t, *J* = 7.1 Hz, 6H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -109.84 (q, *J* = 8.4 Hz), -110.81 (t, *J* = 11.1 Hz) ppm.

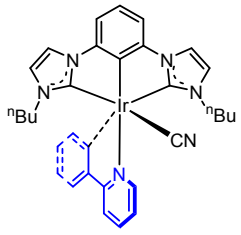
dfppy-Br **dfppy-OCN**

dfppy-OCN: To a 50 mL round bottom flask with a stir bar was added **dfppy-Br** (550 mg, 0.70 mmol), AgOCN (130 mg, 0.87 mmol) and DMF (10 mL) under N_2 gas protection. The reaction mixture was heated at 90 °C for 2 h. After that, DMF was removed under vacuum and the crude mixture was separated through SiO_2 column chromatography (with eluent CH_2Cl_2 to CH_2Cl_2/MeCN, v/v = 10/1) to obtain a white solid. **dfppy-OCN** (420 mg, 0.56 mmol, 80% yield) was obtained by recrystallized with CH_2Cl_2/Et_2O (2 mL/20 mL). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.93 – 9.86 (m, 1H), 8.43 – 8.36 (m, 1H), 7.93 – 7.86 (m, 1H), 7.48 (d, *J* = 2.0 Hz, 2H), 7.40 (ddd, *J* = 7.2, 5.6, 1.3 Hz, 1H), 7.24 (dd, *J* = 8.6, 6.8 Hz, 1H), 7.18 – 7.13 (m, 2H), 6.75 (d, *J* = 2.1 Hz, 2H), 6.22 (ddd, *J* = 13.1, 9.0, 2.5 Hz, 1H), 5.48 (dd, *J* = 9.4, 2.5 Hz, 1H), 3.30 – 3.12 (m, 4H), 1.41 – 1.30 (m, 2H), 1.19 – 1.06 (m, 2H), 0.94 – 0.84 (m, 2H), 0.84 – 0.69 (m, 8H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -109.96 (q, *J* = 9.4 Hz), -111.38 (t, *J* = 11.3 Hz) ppm. ESI-MS: $[M\text{-OCN+MeCN}]^+$: m/z: 745.2420; calculated: 745.2442.



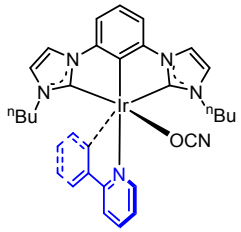
ppy-Br

ppy-Br: The synthetic method is similar to that of **dfpypy-Br**. Pale yellow solid, yield: 26%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.55 – 10.47 (m, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.88 – 7.82 (m, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.43 (d, *J* = 2.0 Hz, 2H), 7.34 (t, *J* = 6.5 Hz, 1H), 7.23 – 7.12 (m, 3H), 6.76 (t, *J* = 7.4 Hz, 1H), 6.70 (d, *J* = 2.1 Hz, 2H), 6.58 – 6.53 (m, 1H), 6.05 (d, *J* = 7.8 Hz, 1H), 3.30 (ddd, *J* = 13.3, 10.1, 5.9 Hz, 2H), 3.19 (ddd, *J* = 13.1, 10.0, 5.6 Hz, 2H), 1.48 – 1.35 (m, 2H), 1.18 – 1.06 (m, 2H), 0.84 (dq, *J* = 30.7, 9.5, 8.2 Hz, 4H), 0.71 (t, *J* = 6.8 Hz, 6H) ppm. ESI-MS: $[M\text{-Br+MeCN}]^+$: m/z: 709.2631; calculated: 709.2610.



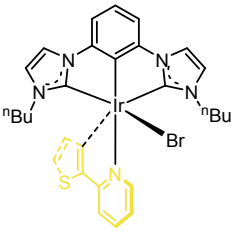
ppy-CN

ppy-CN: The synthetic method is similar to that of **tmpi-CN**. White solid, yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.22 (d, *J* = 5.5 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.44 (s, 2H), 7.33 – 7.20 (m, 2H), 7.12 (d, *J* = 7.7 Hz, 2H), 6.80 (t, *J* = 7.6 Hz, 1H), 6.72 (s, 2H), 6.59 (t, *J* = 7.3 Hz, 1H), 5.99 (d, *J* = 7.6 Hz, 1H), 3.30 – 3.12 (m, 4H), 1.48 – 1.38 (m, 2H), 1.08 – 1.18 (m, 2H), 0.95 – 0.77 (m, 4H), 0.75 – 0.68 (m, 6H) ppm.



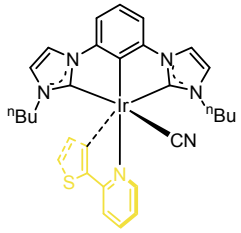
ppy-OCN

ppy-OCN: The synthetic method is similar to that of **dfppy-OCN**. Pale yellow solid, yield: 63%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.87 (d, *J* = 5.4 Hz, 1H), 8.07 – 7.97 (m, 1H), 7.87 (t, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 2H), 7.39 (t, *J* = 6.3 Hz, 1H), 7.27 – 7.19 (m, 1H), 7.15 (d, *J* = 7.7 Hz, 2H), 6.79 – 6.67 (m, 3H), 6.53 (q, *J* = 7.2 Hz, 1H), 5.97 (d, *J* = 7.7 Hz, 1H), 3.25 (ddd, *J* = 13.1, 9.7, 6.0 Hz, 2H), 3.17 (ddd, *J* = 13.2, 9.7, 5.8 Hz, 2H), 1.37 (ddp, *J* = 15.2, 10.2, 5.5 Hz, 2H), 1.20 – 1.07 (m, 2H), 0.93 – 0.85 (m, 2H), 0.84 – 0.77 (m, 2H), 0.73 (t, *J* = 7.2 Hz, 6H) ppm.



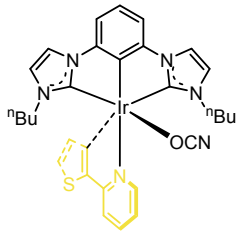
thpy-Br

thpy-Br: The synthetic method is similar to that of **dfpypy-Br**. Pale yellow solid, yield: 27%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.25 (d, *J* = 5.7 Hz, 1H), 7.73 (td, *J* = 7.6, 1.5 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 2.0 Hz, 2H), 7.15 (dt, *J* = 7.9, 3.4 Hz, 4H), 6.93 (d, *J* = 4.8 Hz, 1H), 6.74 (d, *J* = 2.0 Hz, 2H), 5.70 (d, *J* = 4.8 Hz, 1H), 3.41 (ddd, *J* = 13.3, 10.0, 5.9 Hz, 2H), 3.31 (ddd, *J* = 13.3, 9.9, 5.8 Hz, 2H), 1.40 (ddd, *J* = 15.3, 12.1, 6.6 Hz, 2H), 1.18 – 1.06 (m, 2H), 0.97 – 0.84 (m, 2H), 0.83 – 0.71 (m, 8H) ppm. ESI-MS: $[M\text{-}Br+MeCN]^+$: m/z: 715.2195; calculated: 715.2176.



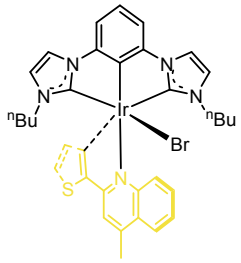
thpy-CN

thpy-CN: The synthetic method is similar to that of **tmpi-CN**. White solid, yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.92 (d, *J* = 5.6 Hz, 1H), 7.80 – 7.72 (m, 1H), 7.60 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.46 (d, *J* = 2.1 Hz, 2H), 7.22 – 7.18 (m, 1H), 7.13 – 7.09 (m, 3H), 6.92 (d, *J* = 4.6 Hz, 1H), 6.78 (d, *J* = 2.1 Hz, 2H), 5.67 (d, *J* = 4.6 Hz, 1H), 3.39 – 3.24 (m, 4H), 1.45 – 1.38 (m, 2H), 1.19 – 1.11 (m, 2H), 0.92 – 0.78 (m, 4H), 0.74 (t, *J* = 7.0 Hz, 6H) ppm.



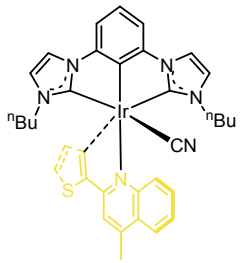
thpy-OCN

thpy-OCN: The synthetic method is similar to that of **dfppy-OCN**. Pale yellow solid, yield: 82%. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.44 (d, *J* = 5.7 Hz, 1H), 8.06 (d, *J* = 2.0 Hz, 2H), 7.95 – 7.89 (m, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.38 (m, 3H), 7.27 (d, *J* = 2.0 Hz, 2H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.03 (d, *J* = 4.8 Hz, 1H), 5.37 (d, *J* = 4.7 Hz, 1H), 3.33 – 3.27 (m, 2H), 3.21 (td, *J* = 12.5, 11.1, 5.5 Hz, 2H), 1.37 – 1.21 (m, 2H), 1.10 – 0.96 (m, 2H), 0.92 – 0.78 (m, 2H), 0.78 – 0.64 (m, 8H) ppm.



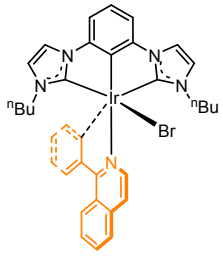
lpt-Br

lpt-Br: The synthetic method is similar to that of **dfpypy-Br**. Yellow solid, yield: 33%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.78 (d, *J* = 8.8 Hz, 1H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.60 – 7.53 (m, 2H), 7.41 (d, *J* = 2.0 Hz, 2H), 7.19 – 7.06 (m, 3H), 6.90 (d, *J* = 4.8 Hz, 1H), 6.72 (d, *J* = 2.0 Hz, 2H), 5.65 (d, *J* = 4.8 Hz, 1H), 3.44 – 3.35 (m, 2H), 3.30 – 3.20 (m, 2H), 2.86 (s, 3H), 1.30 – 1.36 (m, 2H), 1.02 – 0.94 (m, 2H), 0.53 – 0.24 (m, 10H) ppm.



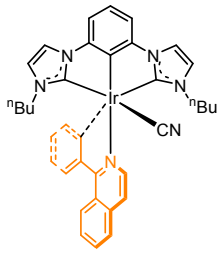
lpt-CN

lpt-CN: The synthetic method is similar to that of **tmpi-CN**. Yellow solid, yield: 45%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98 (d, *J* = 8.8 Hz, 1H), 7.89 (t, *J* = 7.4 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.45 (d, *J* = 1.9 Hz, 2H), 7.25 – 7.20 (m, 2H), 7.13 (d, *J* = 7.7 Hz, 2H), 6.93 (d, *J* = 4.7 Hz, 1H), 6.77 (d, *J* = 1.9 Hz, 2H), 5.65 (d, *J* = 4.7 Hz, 1H), 3.32 – 3.23 (m, 2H), 3.21 – 3.11 (m, 2H), 2.85 (s, 3H), 1.33 – 1.29 (m, 2H), 1.00 – 0.92 (m, 2H), 0.46 (t, *J* = 7.1 Hz, 6H), 0.39 – 0.29 (m, 4H) ppm.



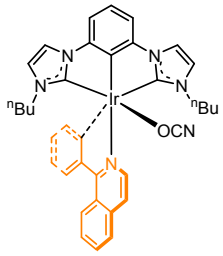
piq-Br

piq-Br: The synthetic method is similar to that of **dfpypy-Br**. Orange solid, yield: 56%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.45 (d, *J* = 6.2 Hz, 1H), 8.92 (d, *J* = 8.5 Hz, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 8.06 – 7.98 (m, 1H), 7.81 – 7.75 (m, 1H), 7.71 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.66 (d, *J* = 6.3 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 2H), 7.25 – 7.19 (m, 1H), 7.19 – 7.15 (m, 2H), 6.85 (td, *J* = 8.0, 7.5, 1.3 Hz, 1H), 6.69 (d, *J* = 2.1 Hz, 2H), 6.59 (td, *J* = 7.5, 7.1, 1.4 Hz, 1H), 6.24 (dd, *J* = 7.8, 1.3 Hz, 1H), 3.26 – 3.10 (m, 4H), 1.31 – 1.22 (m, 2H), 1.01 – 0.90 (m, 2H), 0.67 – 0.56 (m, 2H), 0.52 – 0.36 (m, 8H) ppm. ESI-MS: [M-Br+MeCN]$^+$: m/z: 759.2765; calculated: 759.2787.



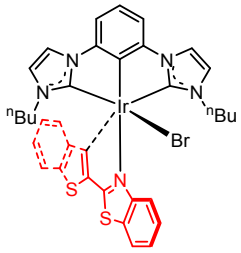
piq-CN

piq-CN: The synthetic method is similar to that of **tmpi-CN**. Orange solid, yield: 34%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.13 (d, *J* = 6.3 Hz, 1H), 8.90 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 7.9 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 6.3 Hz, 1H), 7.46 (d, *J* = 2.1 Hz, 2H), 7.21 (s, 1H), 7.16 – 7.13 (m, 2H), 6.88 (t, *J* = 7.2 Hz, 1H), 6.71 (d, *J* = 2.1 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.19 (d, *J* = 7.5 Hz, 1H), 3.14 (ddd, *J* = 15.7, 9.8, 5.9 Hz, 4H), 1.37 – 1.32 (m, 2H), 1.01 – 0.95 (m, 2H), 0.67 – 0.61 (m, 2H), 0.50 – 0.43 (m, 8H) ppm.



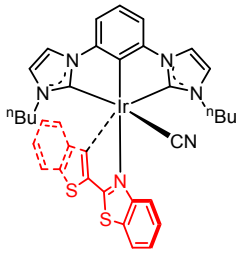
piq-OCN

piq-OCN: The synthetic method is similar to that of **dfppy-OCN**. Pale yellow solid, yield: 68%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (d, *J* = 6.2 Hz, 1H), 8.93 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.03 (d, *J* = 7.7 Hz, 1H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.47 (d, *J* = 2.0 Hz, 2H), 7.27 – 7.22 (m, 1H), 7.18 (d, *J* = 7.4 Hz, 2H), 6.83 (t, *J* = 7.5 Hz, 1H), 6.70 (d, *J* = 2.0 Hz, 2H), 6.56 (t, *J* = 7.3 Hz, 1H), 6.17 (d, *J* = 7.7 Hz, 1H), 3.21 – 3.08 (m, 4H), 1.39 – 1.15 (m, 2H), 1.03 – 0.88 (m, 2H), 0.71 – 0.55 (m, 2H), 0.52 – 0.40 (m, 8H) ppm. ESI-MS: [M-Br+MeCN]$^+$: m/z: 759.2772; calculated: 759.2787.



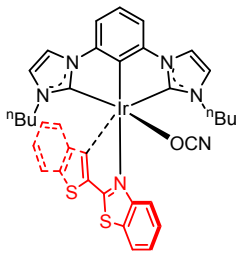
TaBt-Br

TaBt-Br: The synthetic method is similar to that of **dfpypy-Br**. Orange solid, yield: 33%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.08 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.43 – 7.39 (m, 3H), 7.29 – 7.26 (m, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 2.0 Hz, 2H), 6.08 (d, *J* = 8.2 Hz, 1H), 3.45 – 3.35 (m, 2H), 3.30 – 3.20 (m, 2H), 1.39 – 1.32 (m, 2H), 1.14 – 1.06 (m, 2H), 0.59 – 0.43 (m, 10H) ppm.



TaBt-CN

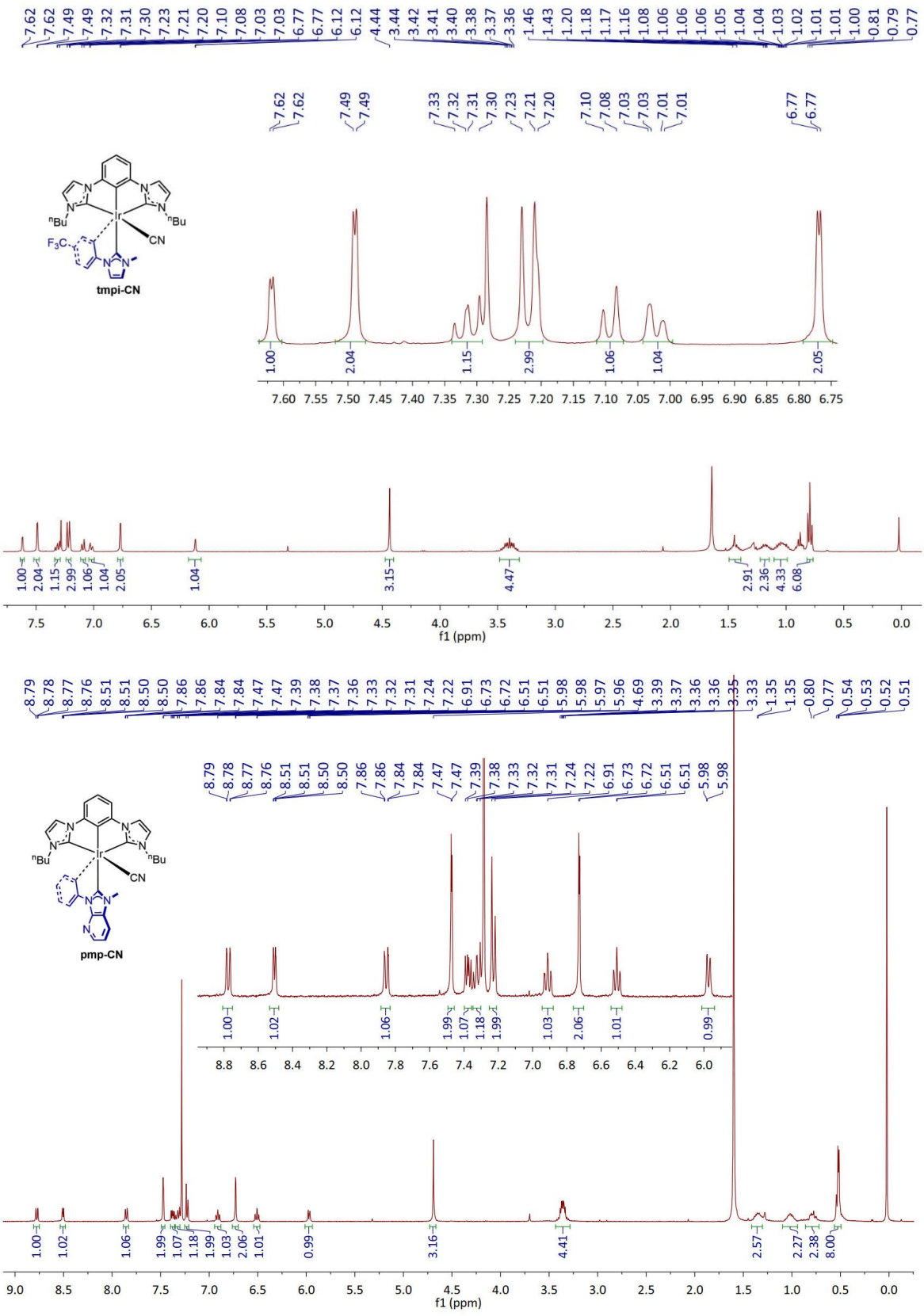
TaBt-CN: The synthetic method is similar to that of **tmpi-CN**. Orange solid, yield: 33%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.68 (d, *J* = 8.2 Hz, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.5 – 7.42 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.07 – 7.02 (m, 1H), 6.73 (d, *J* = 2.0 Hz, 3H), 5.86 (d, *J* = 8.1 Hz, 1H), 3.34 – 3.25 (m, 2H), 3.23 – 3.13 (m, 2H), 1.39 – 1.32 (m, 2H), 1.14 – 1.05 (m, 2H), 0.57 – 0.39 (m, 10H) ppm.

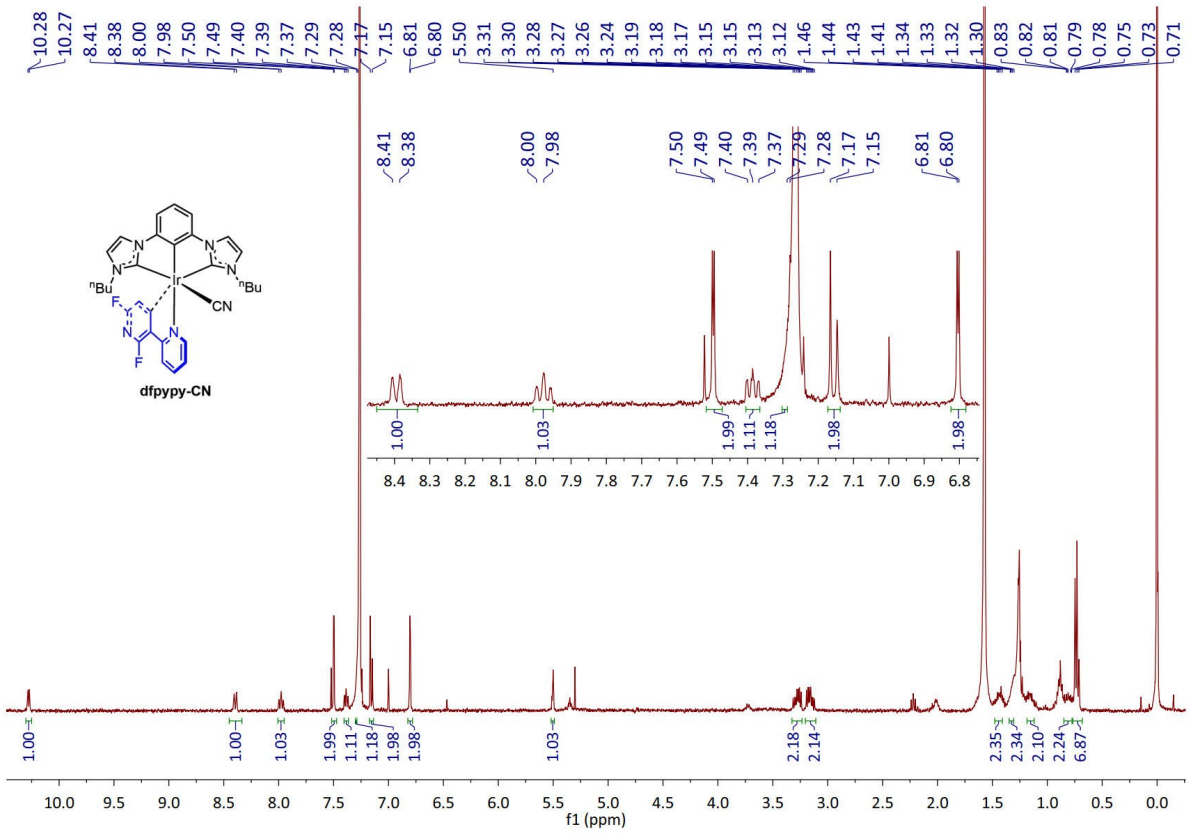


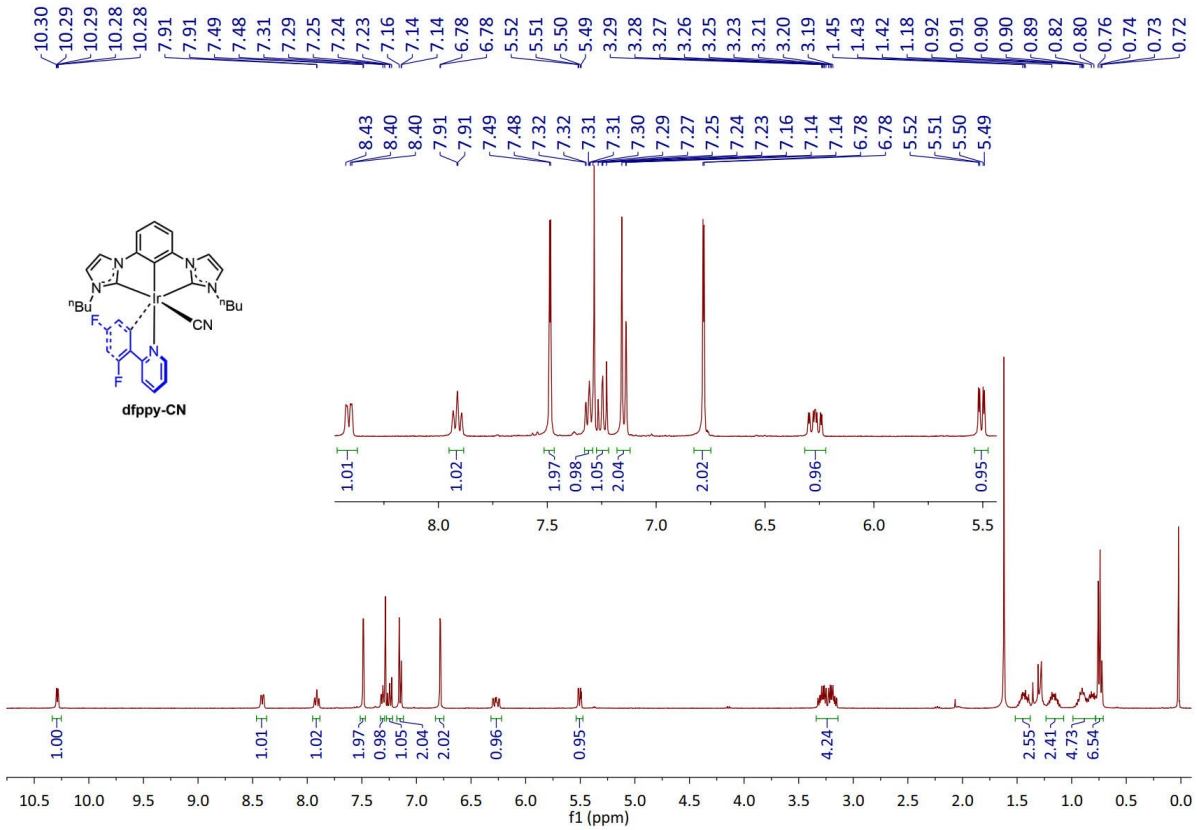
TaBt-OCN

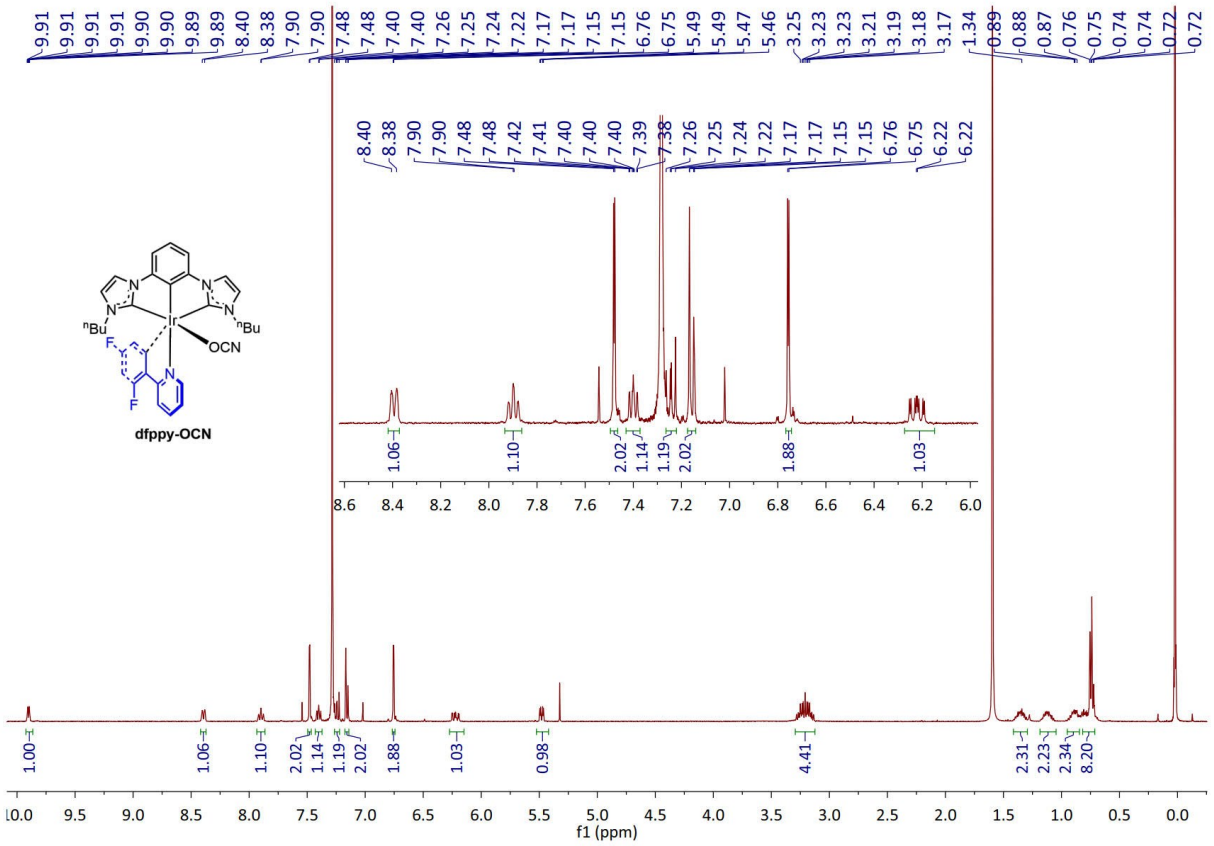
TaBt-OCN: The synthetic method is similar to that of **dfppy-OCN**. Orange solid, yield: 91%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.27 (d, *J* = 8.3 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 2H), 7.46 – 7.40 (m, *J* = 11.0, 4.9 Hz, 3H), 7.34 – 7.29 (m, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.75 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 1.9 Hz, 2H), 6.11 (d, *J* = 8.1 Hz, 1H), 3.34 – 3.26 (m, 2H), 3.22 – 3.14 (m, 2H), 1.34 – 1.21 (m, 2H), 1.13 – 1.00 (m, 2H), 0.62 – 0.43 (m, 10H) ppm.

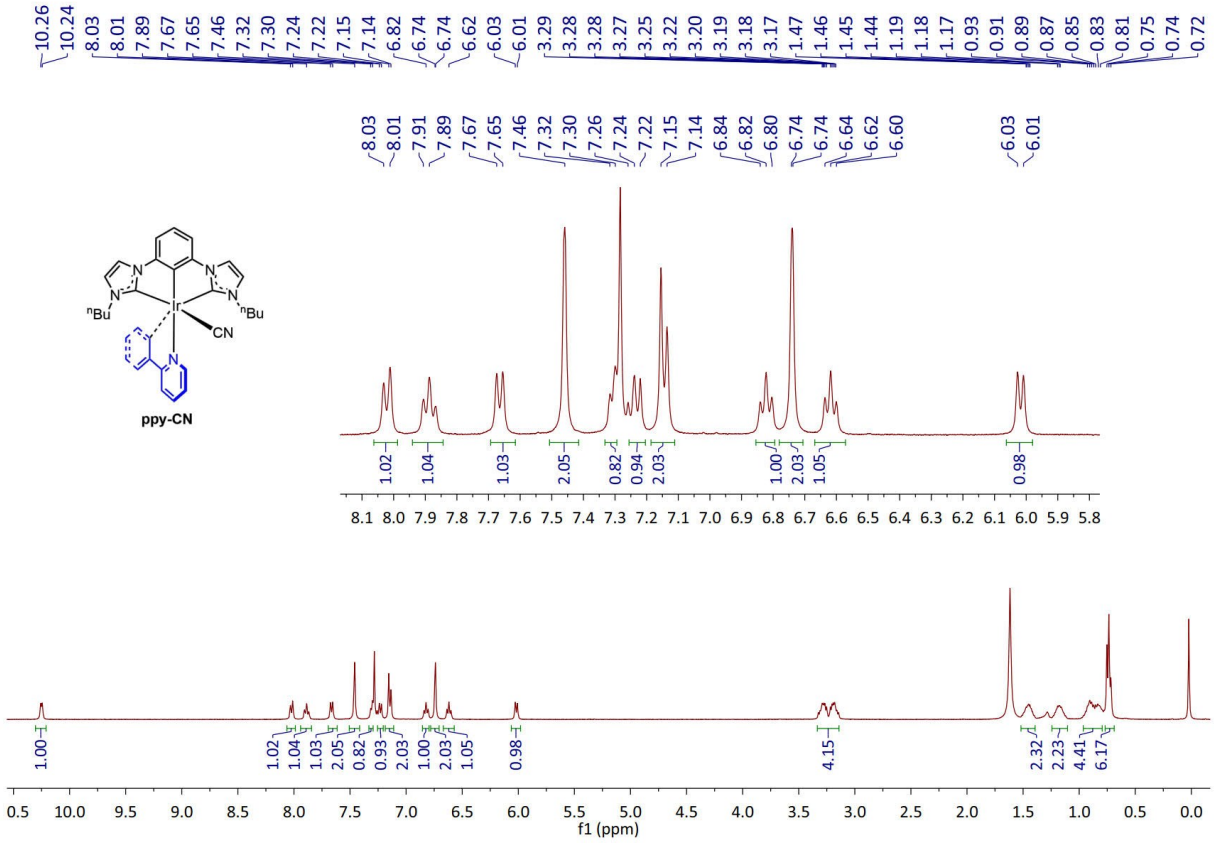
8. NMR spectra

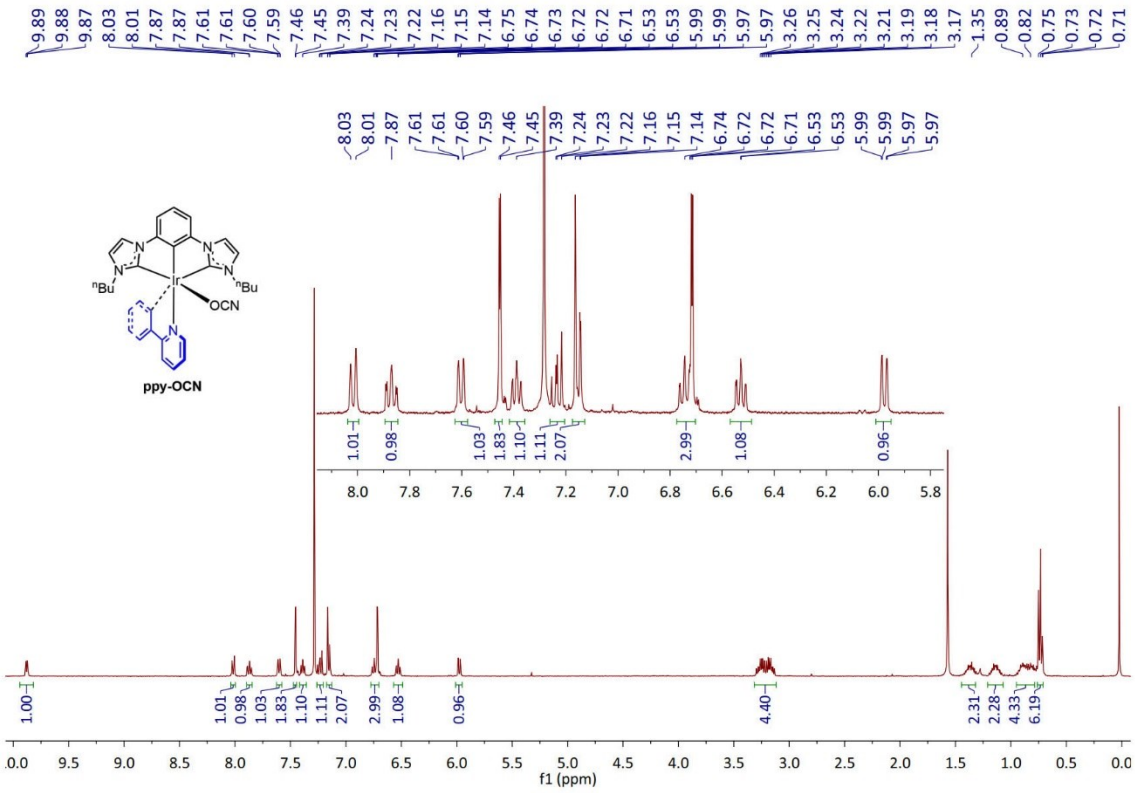


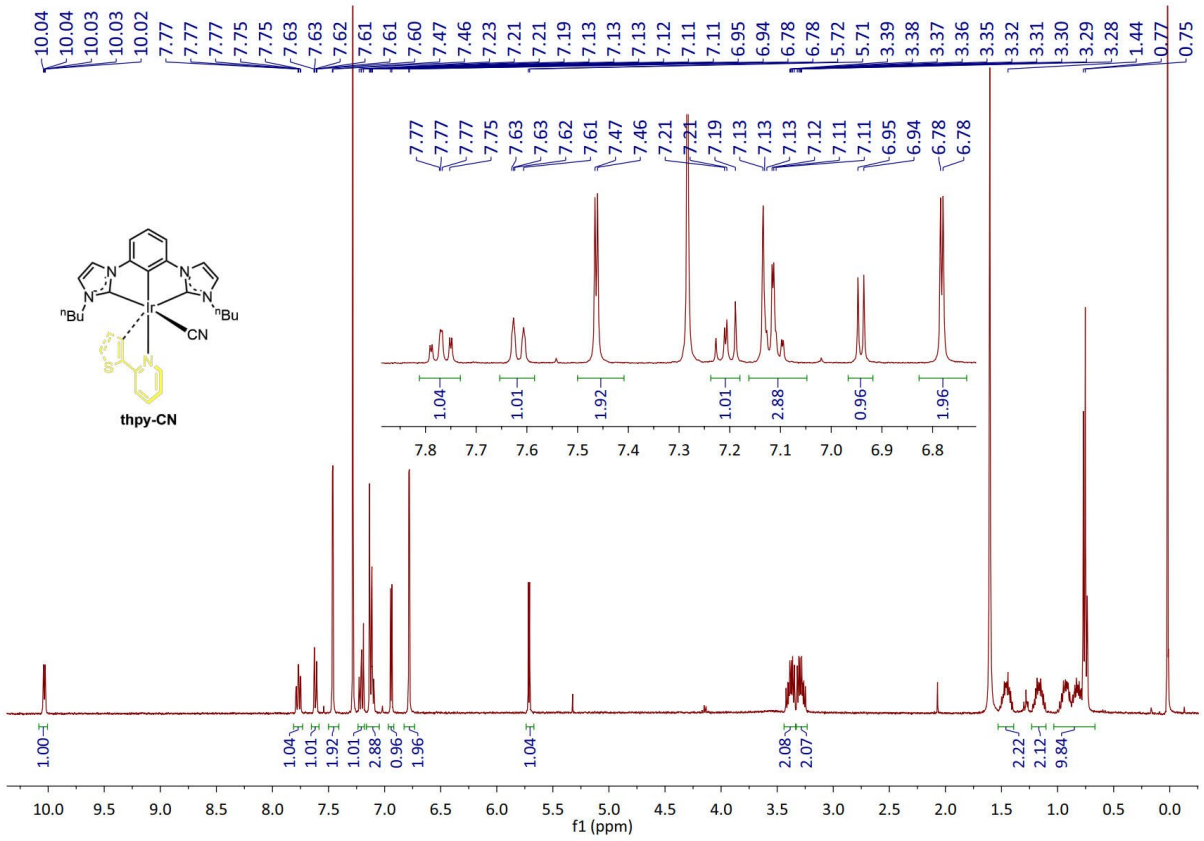

dfpypy-CN
f1 (ppm)

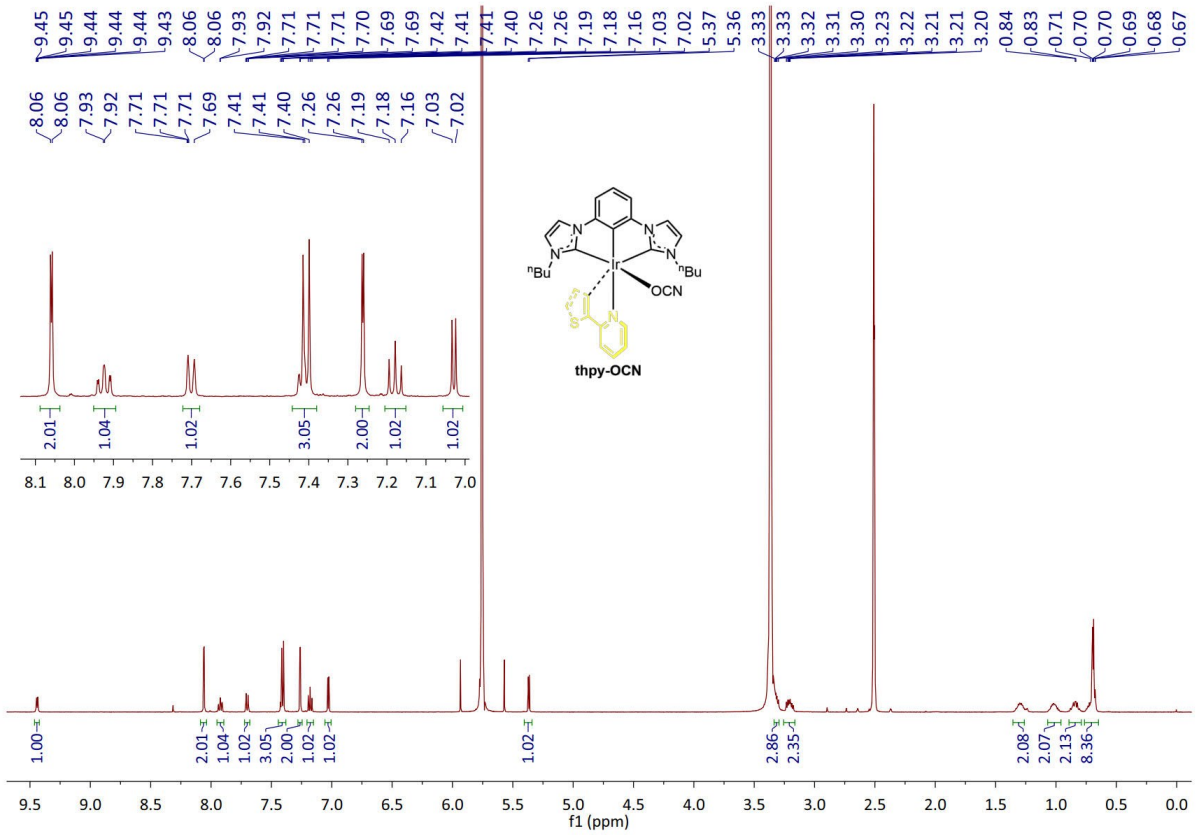

dfppy-CN
f1 (ppm)

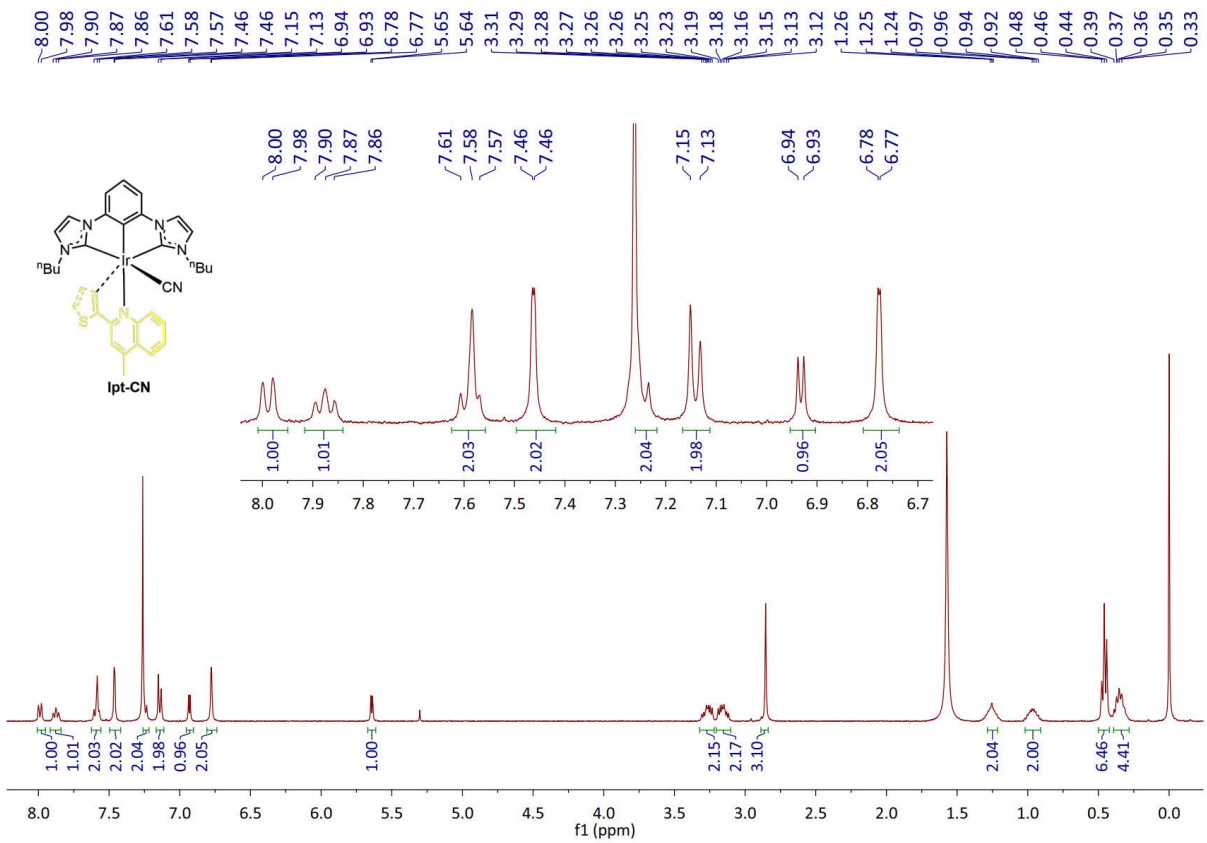

dfppy-OCN
f1 (ppm)

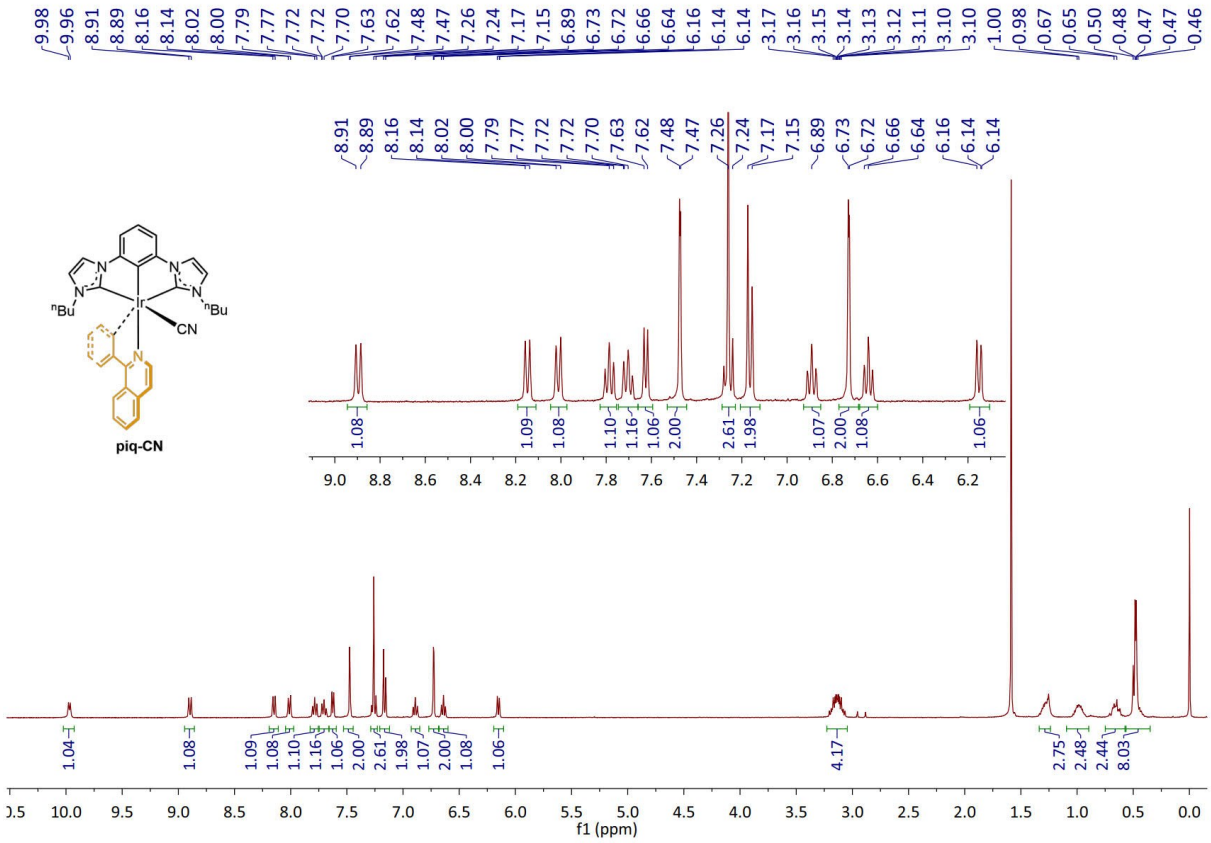

ppy-CN
f1 (ppm)

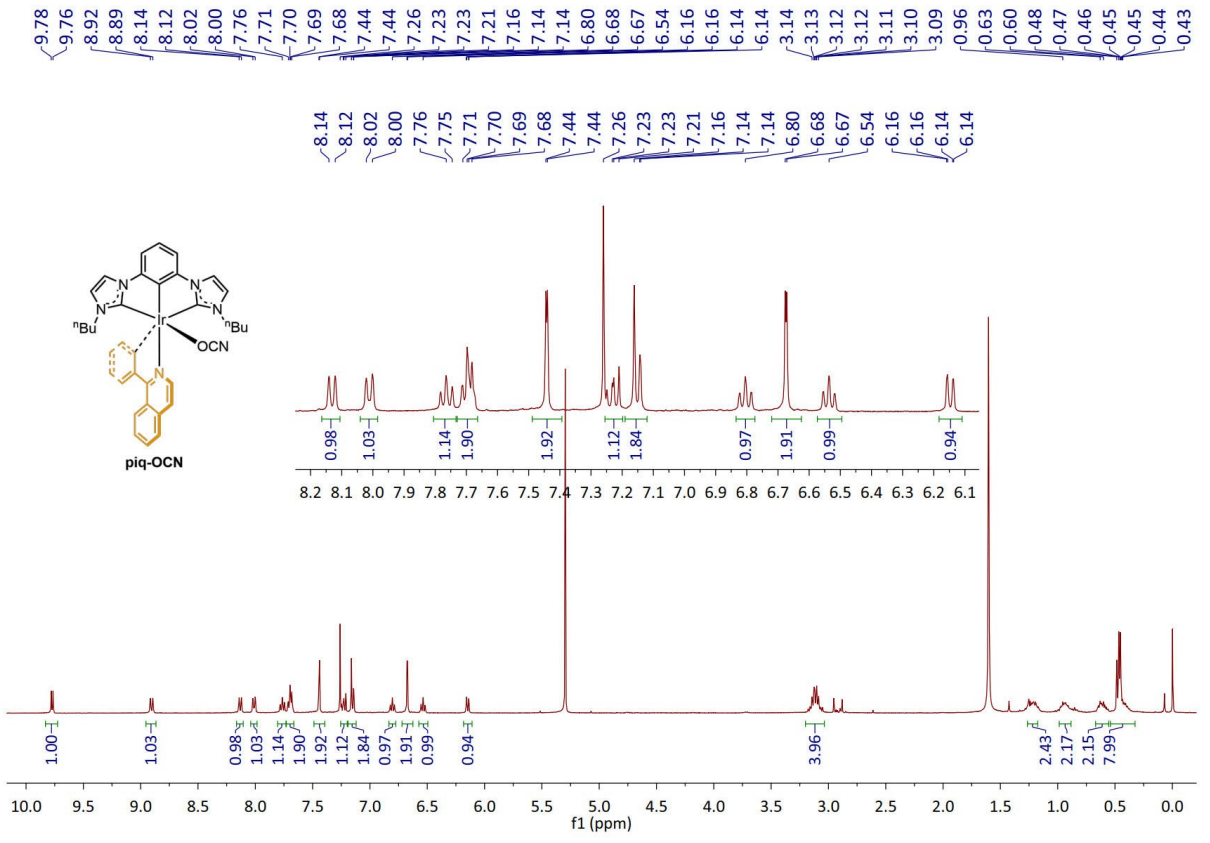

ppy-OCN
f1 (ppm)

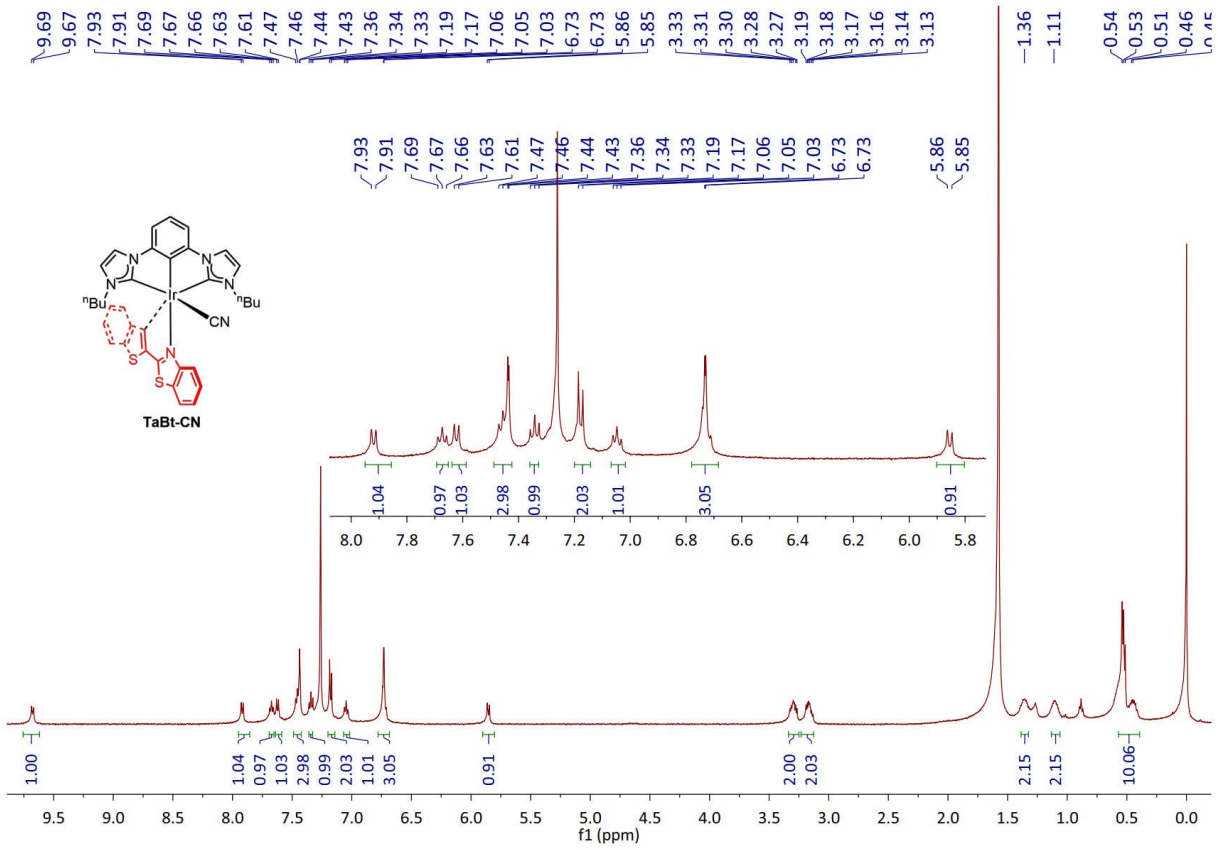

thpy-CN
f1 (ppm)

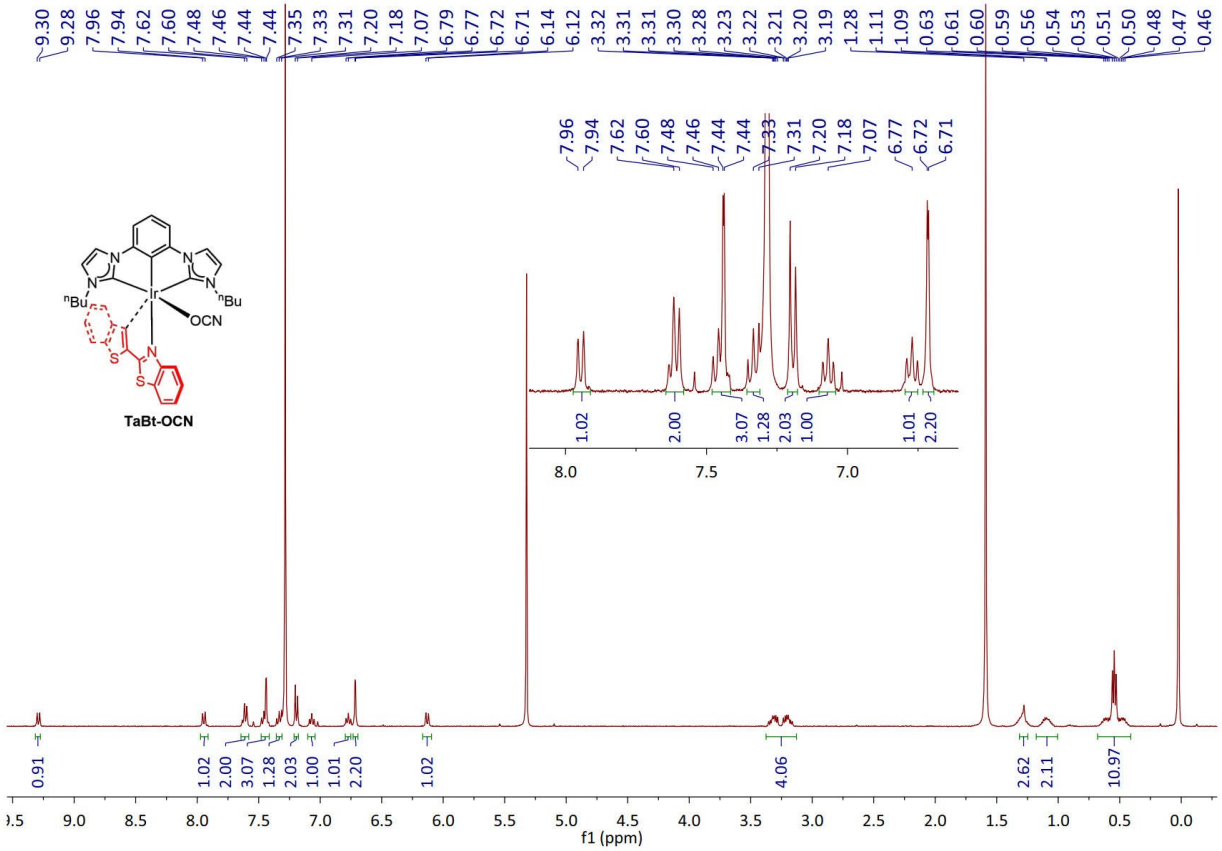

thpy-OCN


lpt-CN


piq-CN
f1 (ppm)


piq-OCN
f1 (ppm)


TaBt-CN
f1 (ppm)


TaBt-OCN
f1 (ppm)

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