Supplementary Information

New cyclometalated Ir(III) complexes with bulky ligands with potential applications in LEC devices. Experimental and theoretical studies of their photophysical properties

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^{1}H NMR Characterizations

$[Ir(F_2ppy)_2L1](PF_6)$ complex.

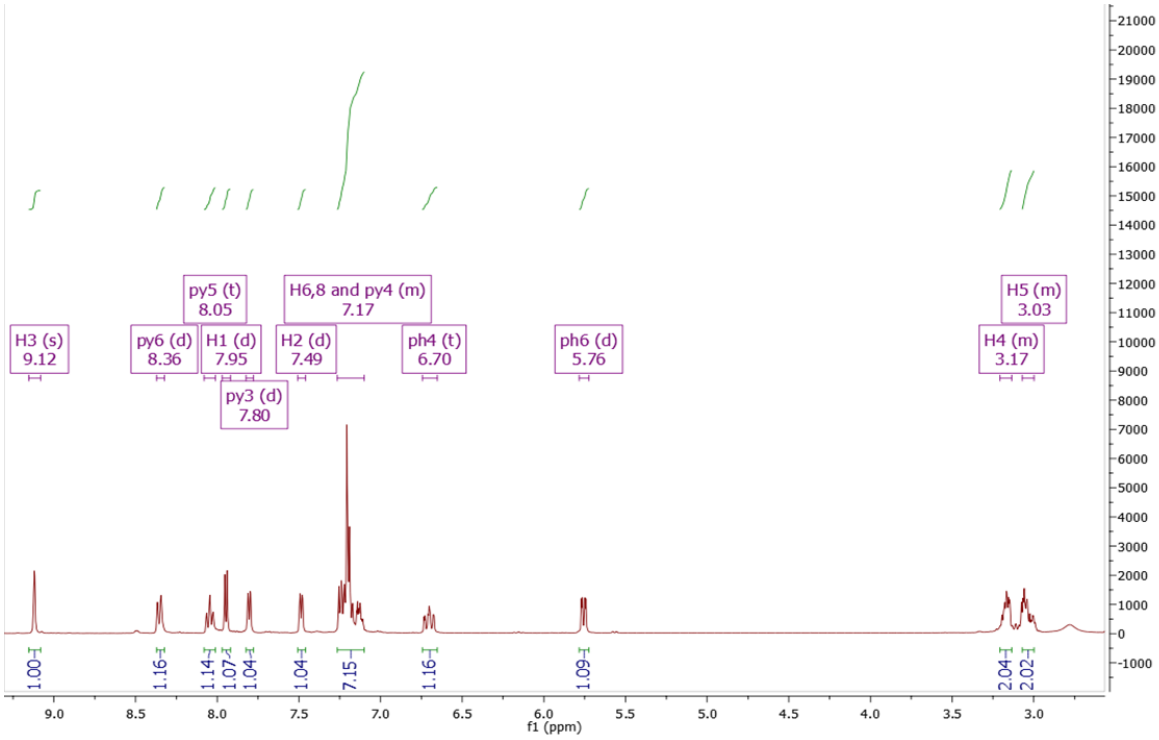


***Figure S1.**^{1}H-NMR spectrum of $[Ir(F_2ppy)_2L1](PF_6)$ complex (400 MHz, $CO(CD_3)_2$).*

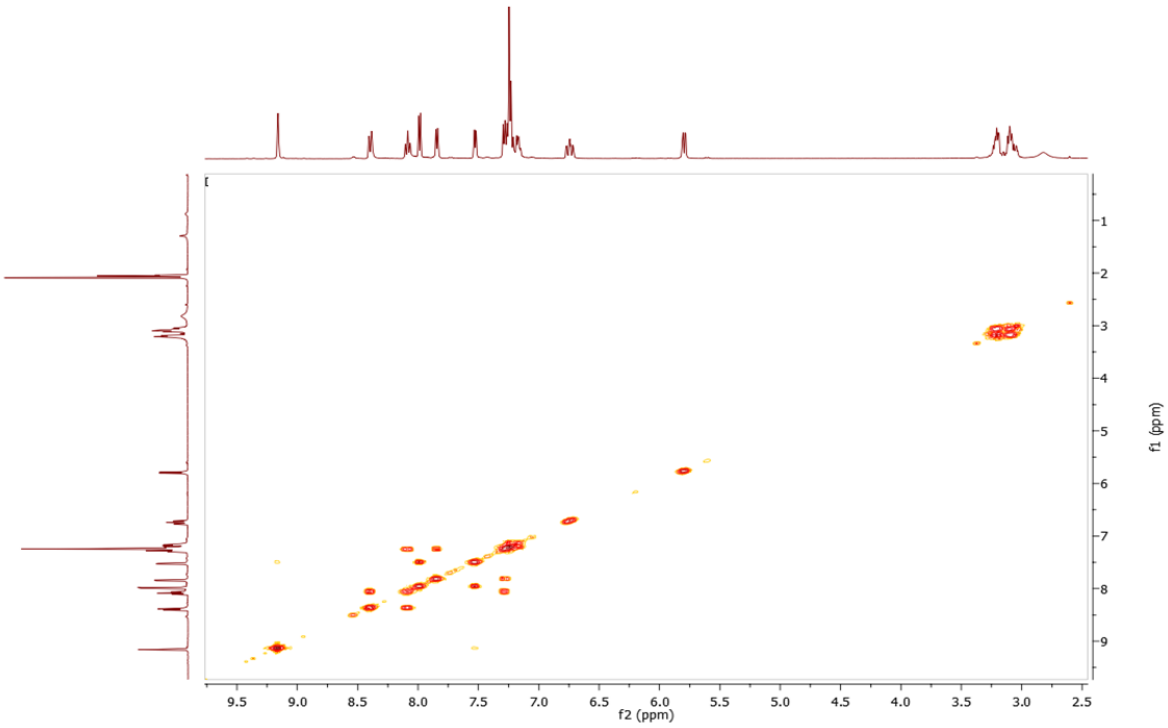


Figure S2. *2D-NMR spectrum of [Ir(F_2ppy)$_2$L1](PF_6) complex (400 MHz, $CO(CD_3)_2$).*

[Ir(F_2ppy)$_2$L2](PF_6) complex.

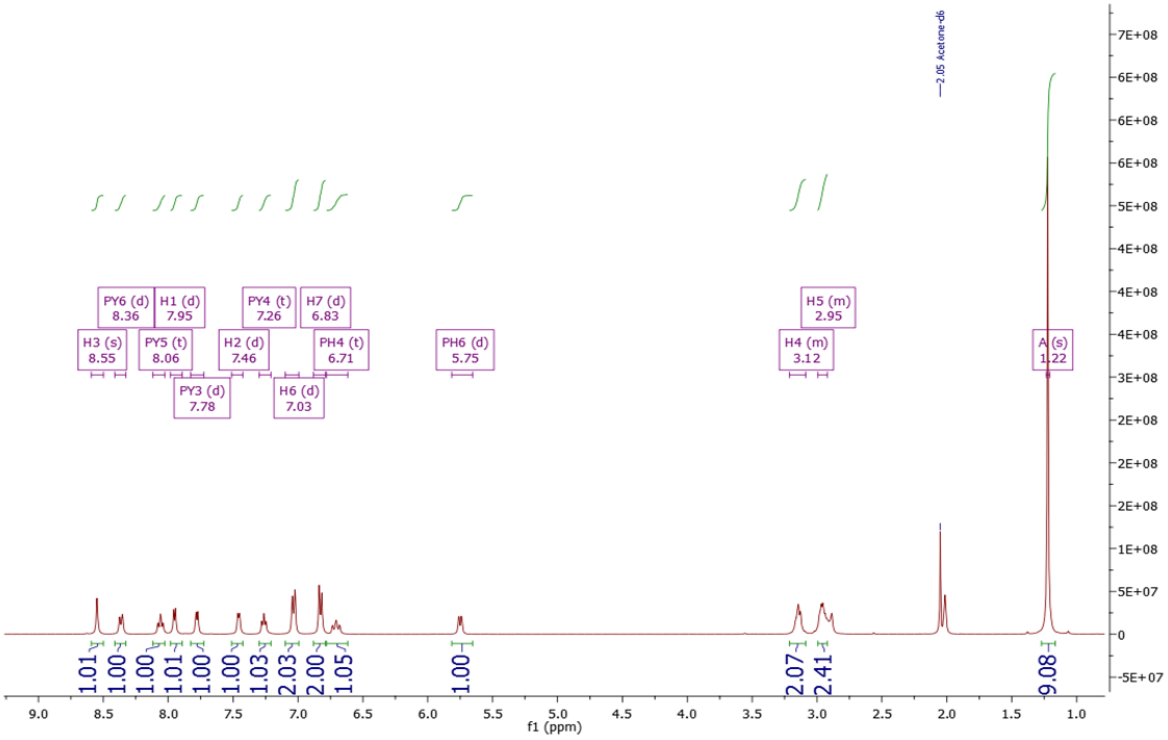


Figure S3. *^{1}H-NMR spectrum of [Ir(F_2ppy)$_2$L2](PF_6) complex (400 MHz, $CO(CD_3)_2$).*

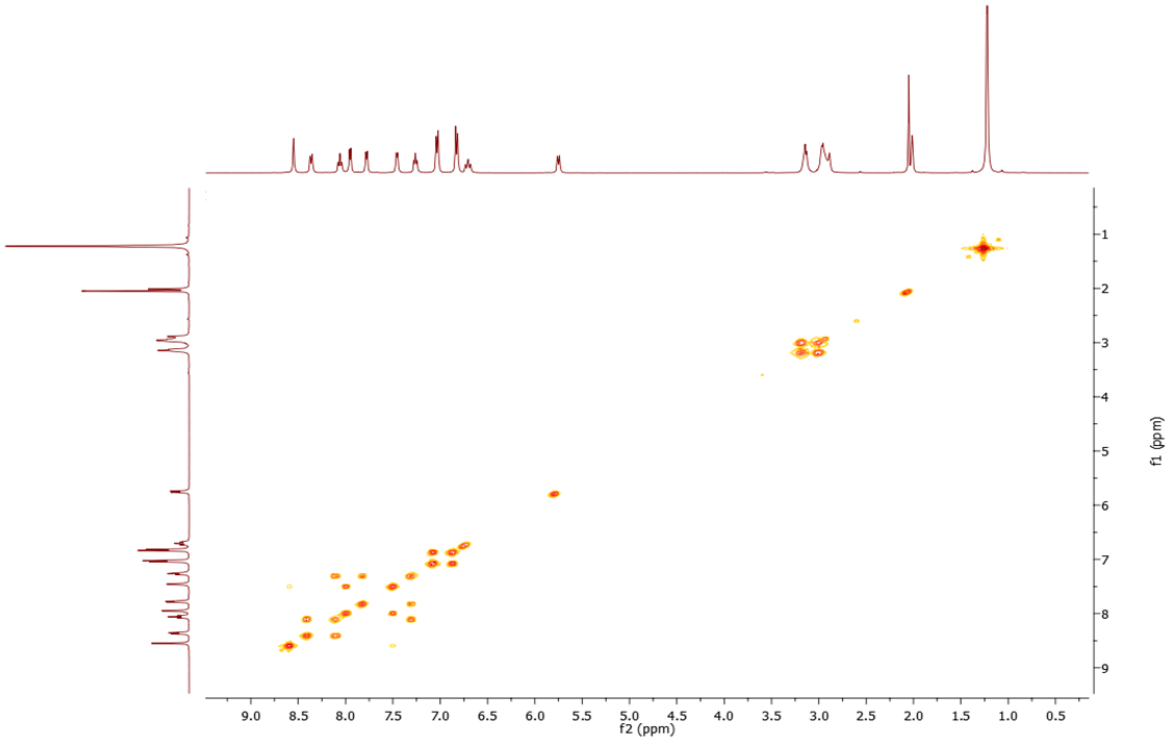


Figure S4. *2D-NMR spectrum of [Ir(F_2ppy)$_2$L2](PF_6) complex (400 MHz, $CO(CD_3)_2$).*

Mass Spectroscopy Characterizations

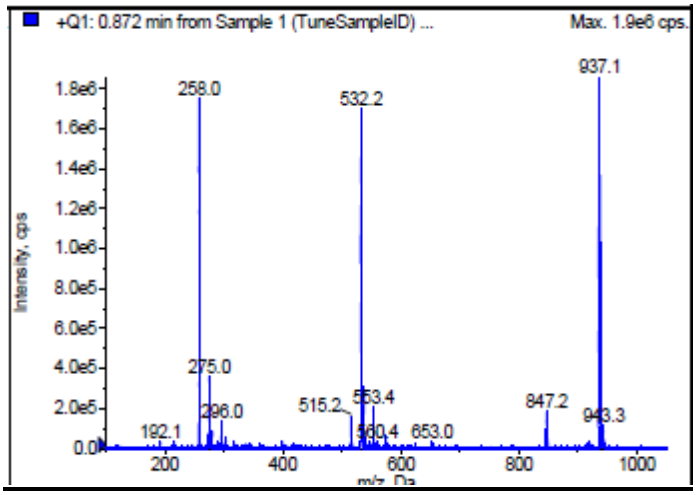


Figure S5. *Mass spectrum of* $[Ir(F_2ppy)_2L1](PF_6)$ *complex from acetonitrile solution.*

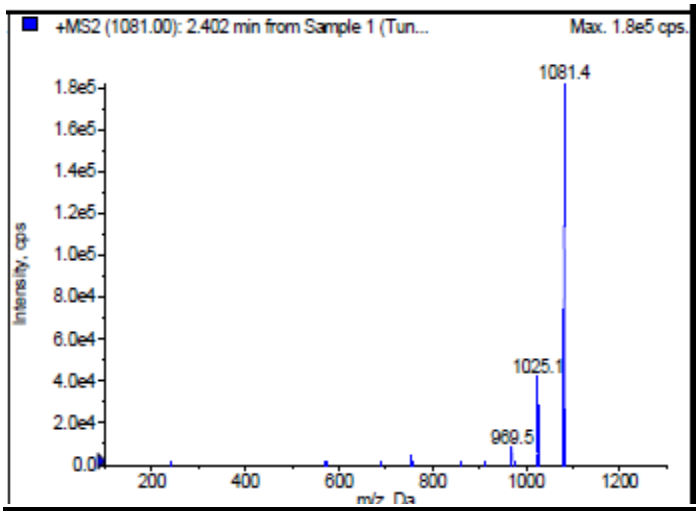
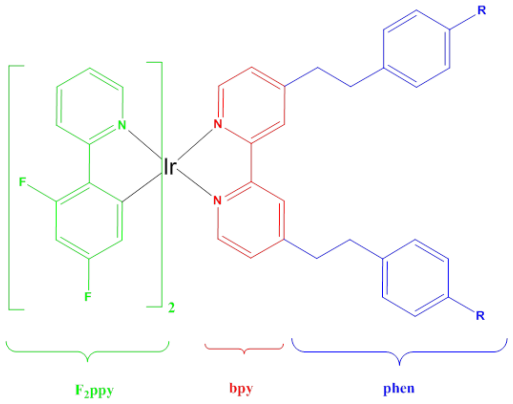


Figure S6. *Mass spectrum of* $[Ir(F_2ppy)_2L2](PF_6)$ *complex from acetonitrile solution.*

Theoretical Calculations - Frontier molecular orbitals

Table S1. Orbital compositions of selected frontier molecular orbitals in complexes $[Ir(F_2ppy)_2L1]^+$ and $[Ir(F_2ppy)_2L2]^+$.



				L1	
[Ir(F2ppy)2L1]+	*E* (eV)	Ir	$(F_2ppy)_2$	bpy	phen
LUMO+2	-1.76	6	91	3	0
LUMO+1	-1.84	5	92	3	0
LUMO	-2.40	3	2	90	5
HOMO	-5.94	46	51	3	0
HOMO-1	-6.41	11	87	1	1
HOMO-2	-6.52	22	74	2	2
HOMO-3	-6.66	21	11	6	62

				L2	
[Ir(F2ppy)2L2]+	*E* (eV)	Ir	$(F_2ppy)_2$	bpy	phen
LUMO+2	-1.76	6	91	3	0
LUMO+1	-1.83	5	92	3	0
LUMO	-2.38	3	2	90	5
HOMO	-5.84	0	0	2	98
HOMO-1	-5.84	0	0	3	97
HOMO-2	-5.94	46	51	3	0
HOMO-3	-6.41	11	88	1	0

Theoretical Calculations – Optimized structures in triplet exited state

Table S2. Selected bond distances (Å) and angles (°) of complexes $[Ir(F_2ppy)_2L1]^+$ and $[Ir(F_2ppy)_2L2]^+$in triplet excited states (T_2 and T_3). T_3 state for the $[Ir(F_2ppy)_2L1]^+$ was not obtained due to convergence problems.

Parameter	$[Ir(F_2ppy)_2L1]^+$	$[Ir(F_2ppy)_2L2]^+$	
	T2	T2	T3
dIr-N_{bpy}	2.22	2.22	2.21
dIr-N_{F2ppy}	2.07	2.07	2.07
dIr-C_{F2ppy}	2.00	2.00	2.01
d(C5-C6)$_{bpy}$	1.48	1.48	1.48
d(N3-C5)$_{bpy}$	1.36	1.36	1.36
d(C3-C4)$_{F2ppy}$	1.43	1.43	1.43
∠C1-Ir-C2	90.77	90.76	89.39
∠C1-Ir-N1	80.91	80.91	80.74
∠C2-Ir-N1	95.38	95.40	95.49
∠N1-Ir-N2	174.75	174.78	174.74
∠C1-Ir-N3	97.50	97.50	97.86
∠C2-Ir-N3	171.60	171.59	172.52
∠N1-Ir-N3	87.47	87.52	87.53
∠N2-Ir-N3	96.73	96.65	96.66
∠N3-Ir-N4	74.28	74.30	74.96