Electronic Supplementary Material

For

Fluoro-benzenesulfonyl-functionalized 2-phenylthiazole-type iridinum(III) complexes for efficient solution-processed organic light-emitting diodes†

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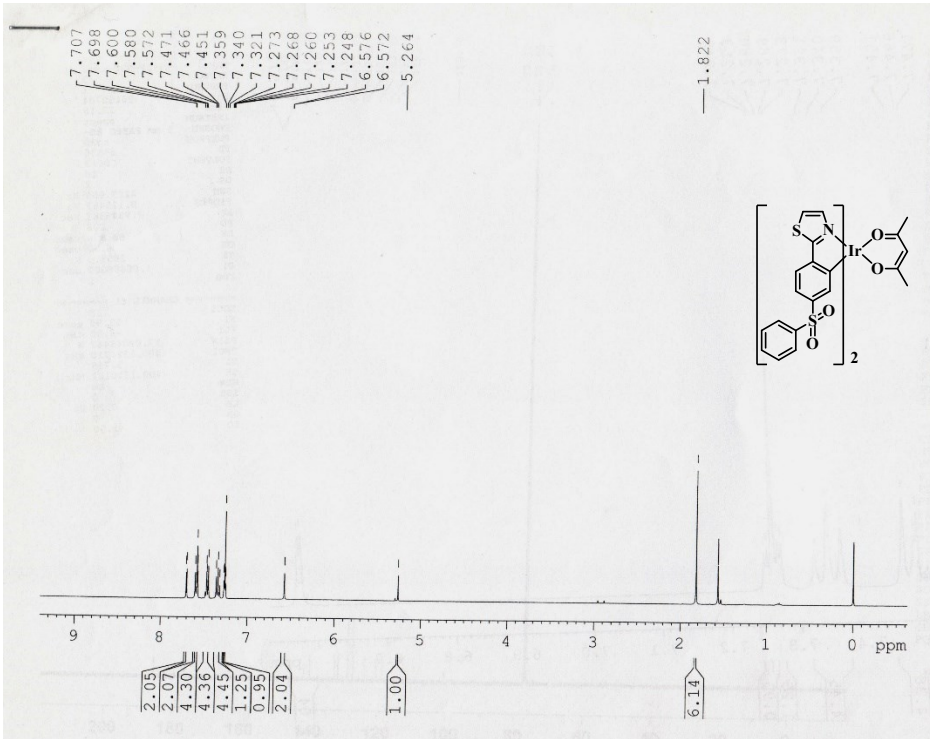
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7.260
7.253
7.248
6.576
6.572
5.264
1.822
S
N
Ir
O
O
O
S
O
2
9
8
7
6
5
4
3
2
1
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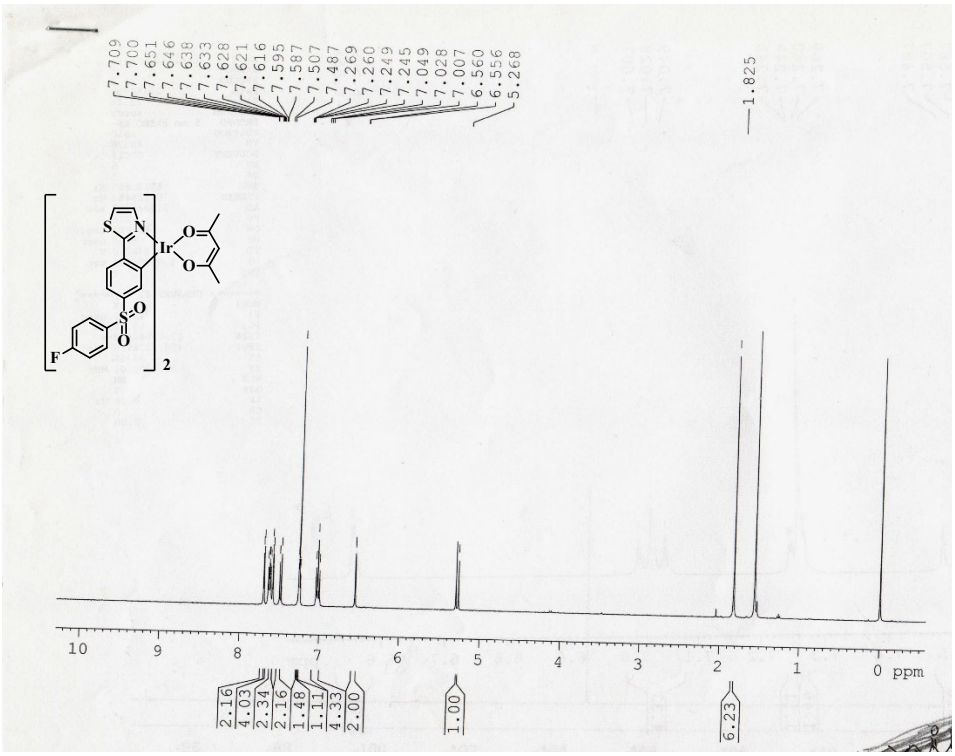
2.05
2.07
4.30
4.36
4.45
1.25
0.95
2.04
1.00
6.14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7.651
7.646
7.638
7.633
7.628
7.621
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7.595
7.587
7.507
7.487
7.269
7.260
7.249
7.245
7.049
7.028
7.007
6.560
6.556
5.268
1.825
S
N
Ir
O
O
O
S
O
F
2
10
9
8
7
6
5
4
3
2
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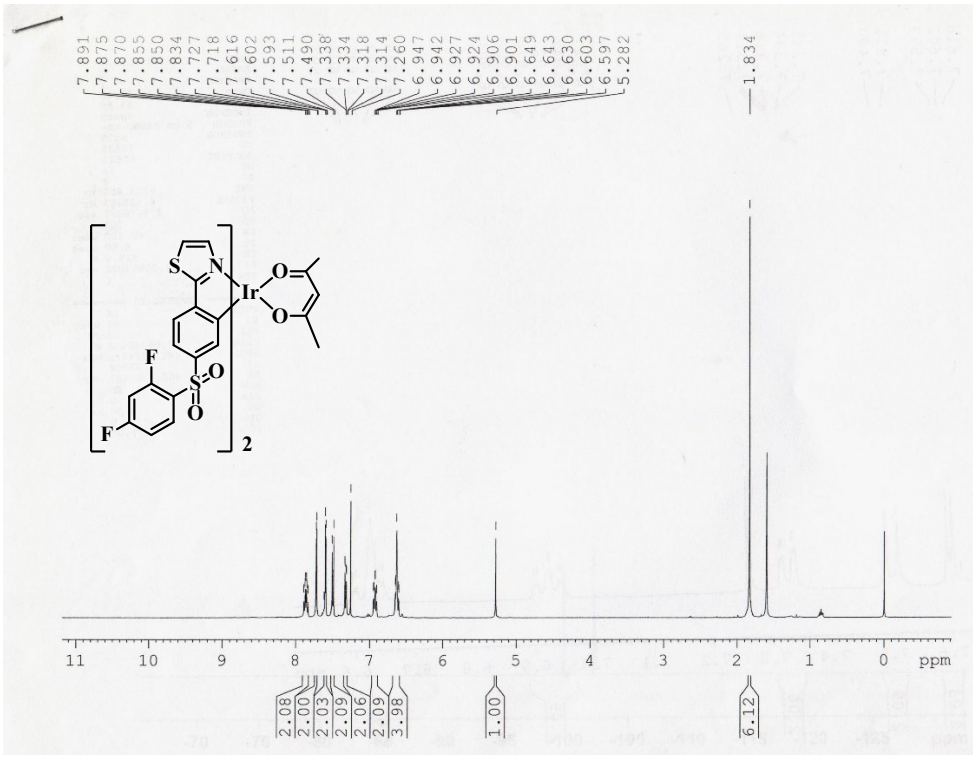
1.48
1.11
4.33
2.00
1.00
6.23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7.338
7.334
7.318
7.314
7.260
6.947
6.942
6.927
6.924
6.906
6.901
6.649
6.643
6.630
6.603
6.597
5.282
1.834
S
N
Ir
O
O
F
S
O
O
F
2
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.08
2.00
2.03
2.09
2.06
2.09
3.98
1.00
6.12


7.744
7.736
7.665
7.656
7.558
7.538
7.303
7.287
7.271
7.266
7.260
6.515
6.511
5.295
1.842
1.586
S
N
Ir
O
O
F
S
O
O
F
F
2
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2.05
2.07
6.01
2.03
1.00
6.09

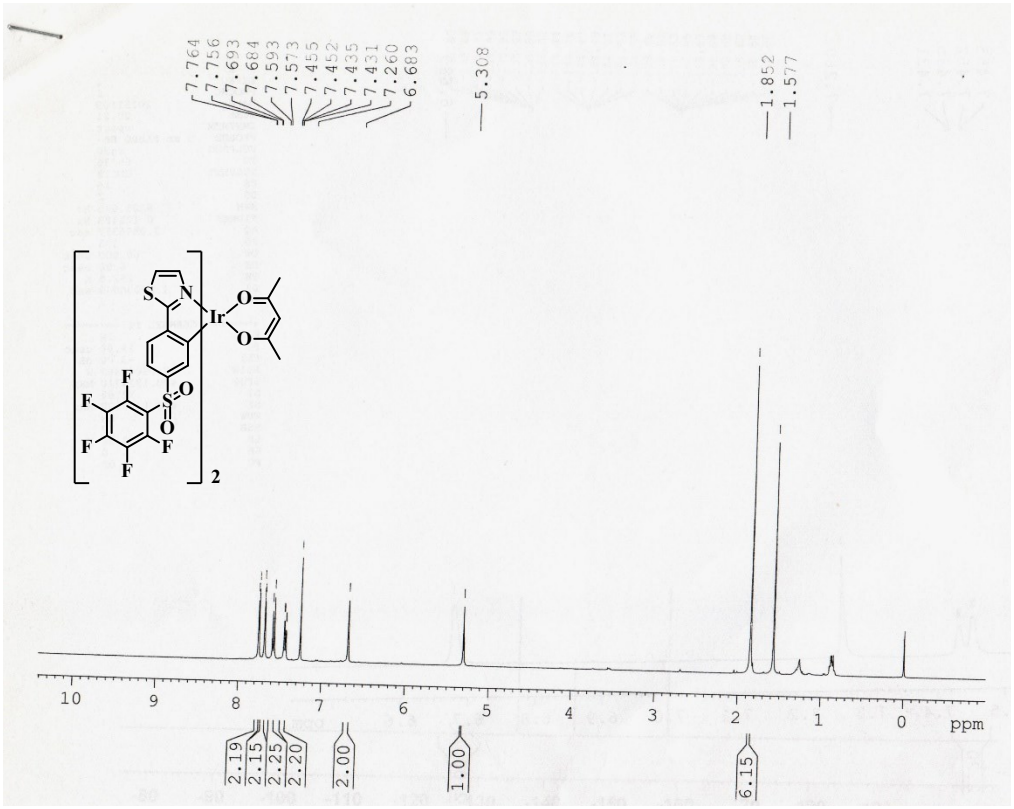
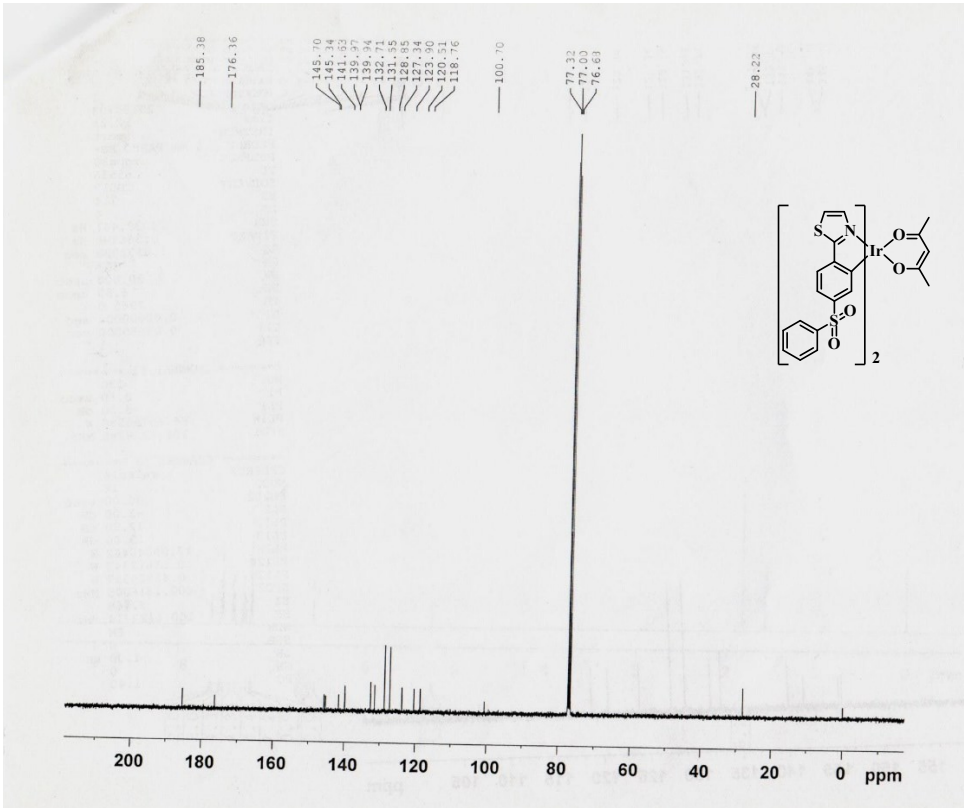
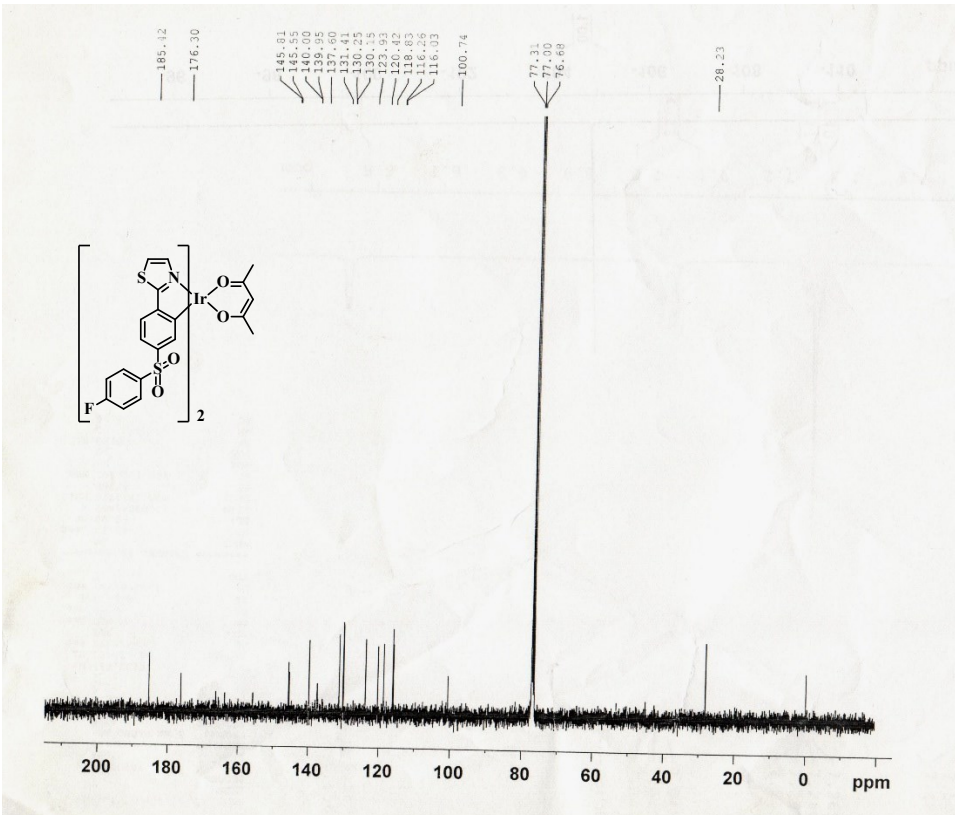


Fig. S1 NMR H^1 spectra of these 2-phenylthiazole Ir(III) complexes.

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176.30
145.81
145.55
140.00
139.95
137.60
131.41
130.25
123.63
120.42
118.83
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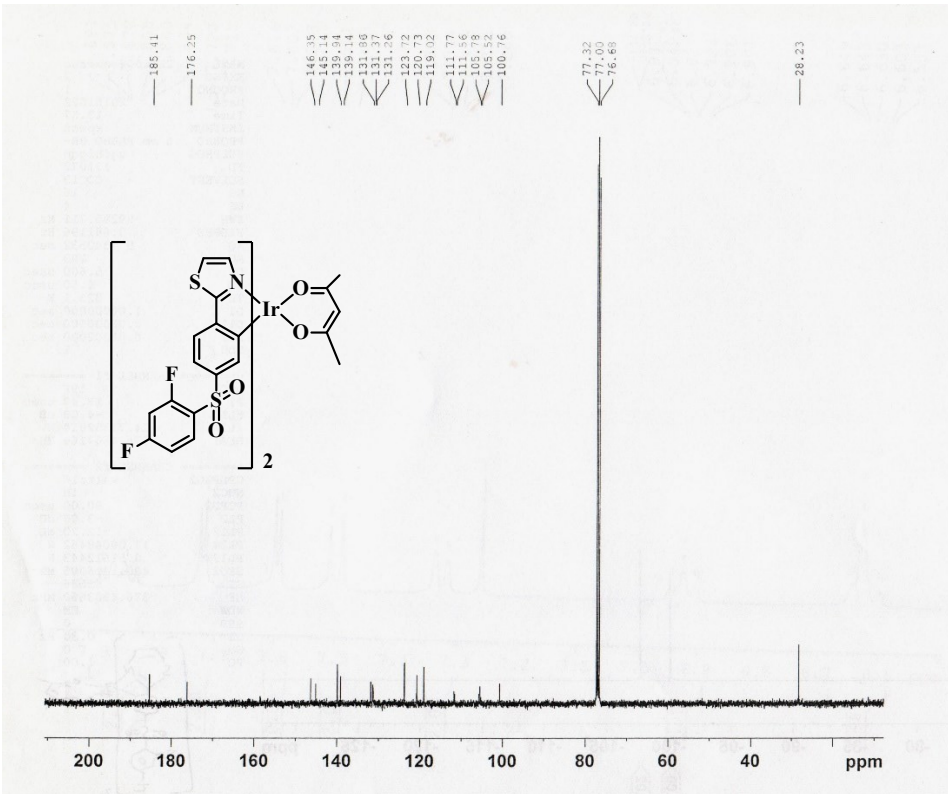
116.03
100.74
77.31
77.00
76.68
28.23
200
180
160
140
120
100
80
60
40
20
0
ppm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176.25
146.35
145.14
139.34
139.14
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123.72
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119.02
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111.56
105.78
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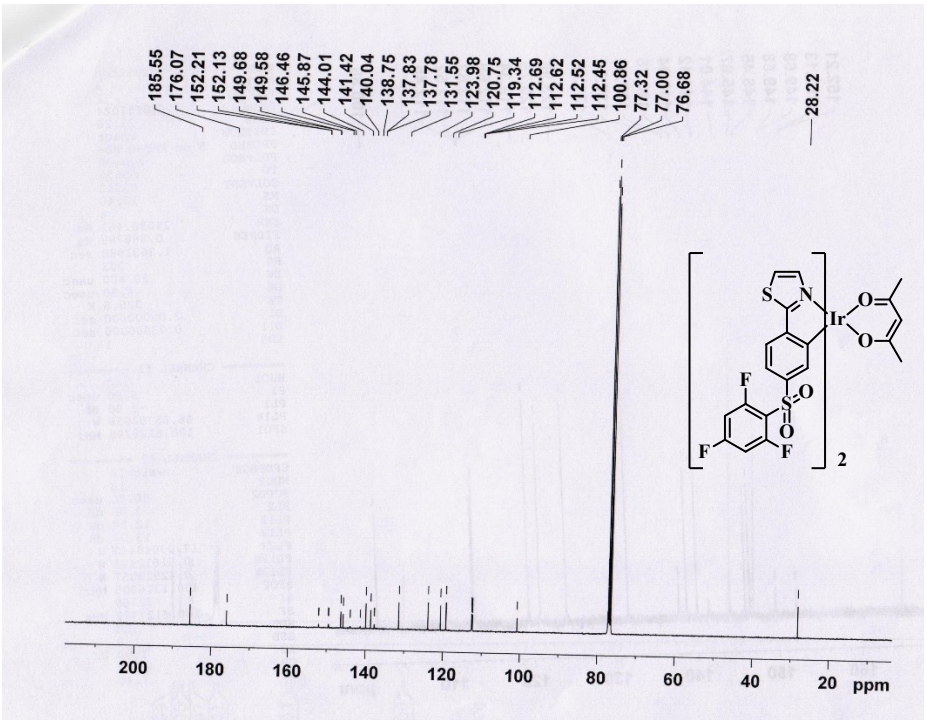
77.32
77.00
76.68
28.23
200
180
160
140
120
100
80
60
40
ppm



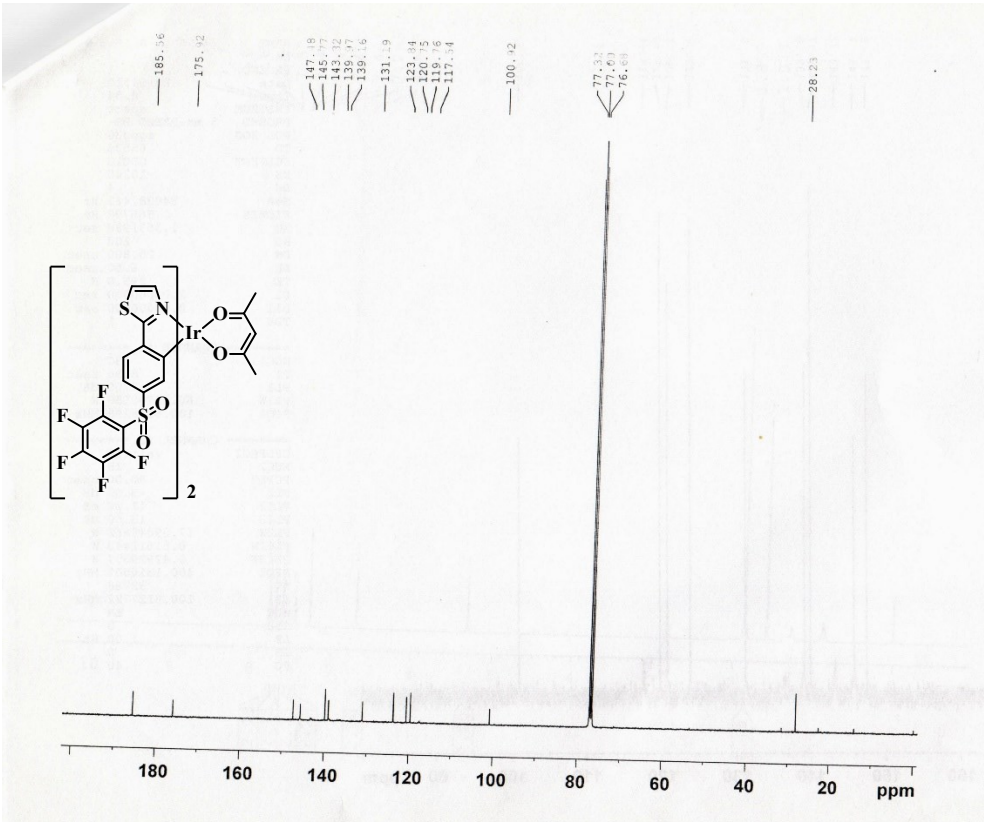
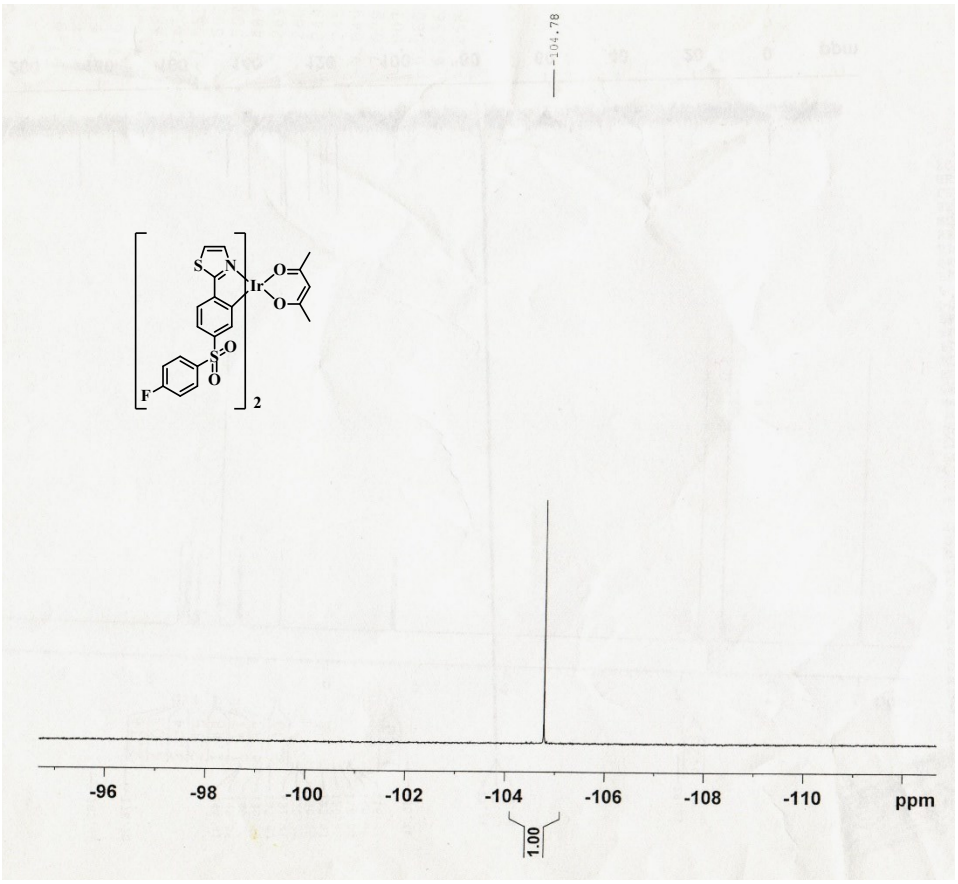


Fig. S2 NMR C^{13} spectra of these 2-phenylthiazole Ir(III) complexes.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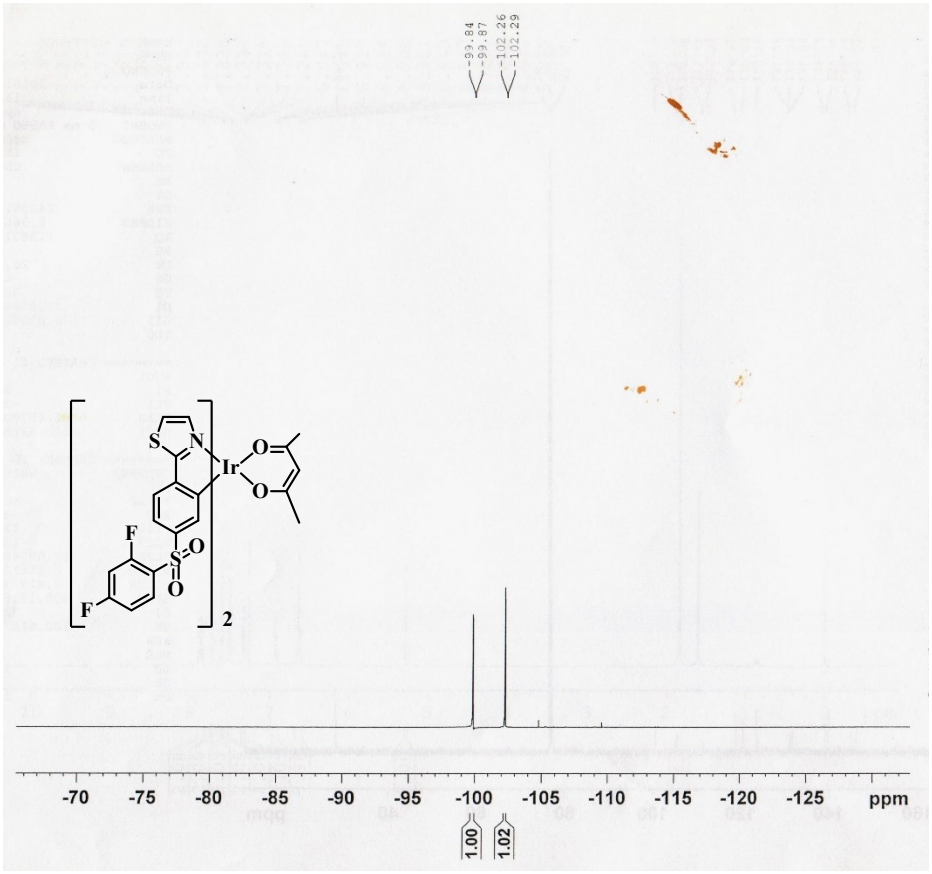
S
N
Ir
O
O
S
O
O
F
2
-96
-98
-100
-102
-104
-106
-108
-110
ppm
1.00


-99.84
-99.87
-102.26
-102.29
S
N
Ir
O
O
F
S
O
O
F
2
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-90
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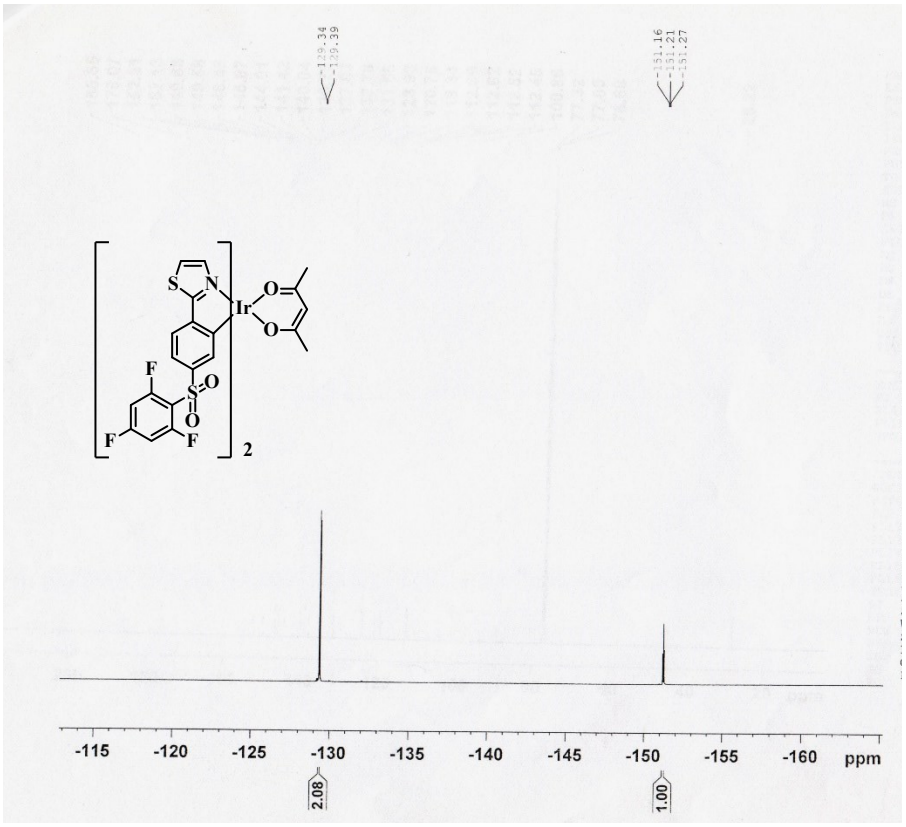
-105
-110
-115
-120
-125
ppm
1.00
1.02



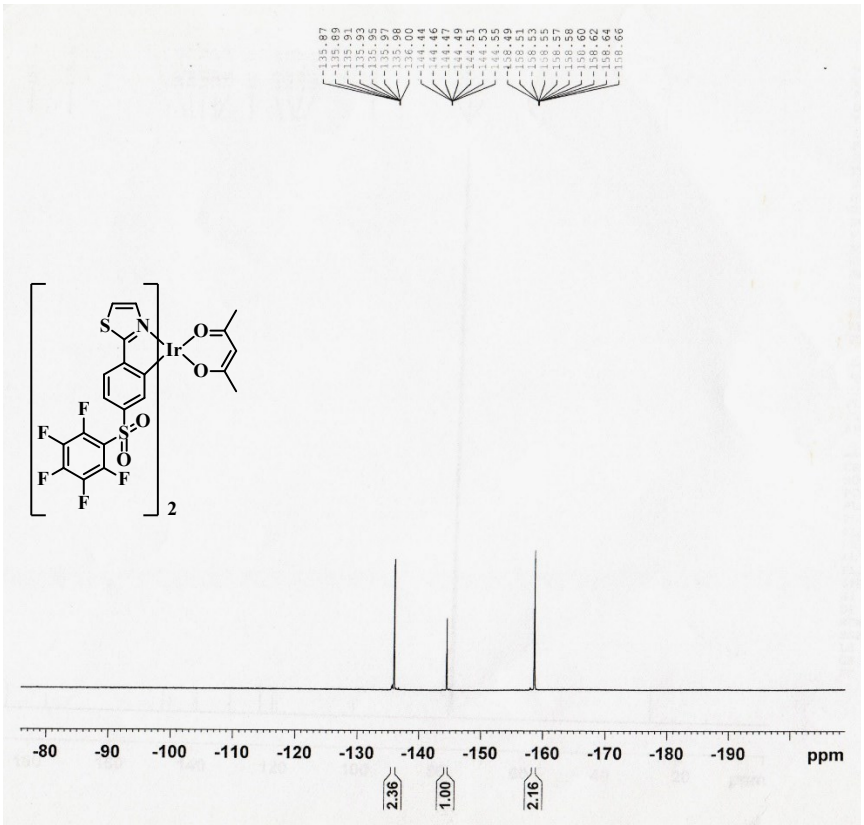


Fig. S3 NMR F^{19} spectra of these 2-phenylthiazole Ir(III) complexes.

Table S1 Single crystal data for **IrST-0F**

Complex	**IrST-0F**
CCDC No.	1817403
formula	$C_{35}H_{27}IrN_2O_6S_4$
formula weight	1011.39
crystal system	Triclinic
space group	*P*
a /Å	11.983(2)
b /Å	12.525(2)
c /Å	14.611(2)
α /deg	76.766(8)
β /deg	68.353(9)
γ /deg/	77.376(9)
V /Å^3	1962.2(5)
Z	2
D_{calcd} /g·cm^{-3}	1.712
crystal size /mm^3	0.042×0.156×0.293
F /000	996
μ/mm^{-1}	3.866
ϑ range /deg	1.52 - 25.14
diffrn reflns number	6804
reflns number total	14245
no. of parameters	471
*R*1, *wR*2 [$I > 2.0\sigma(I)$][a]	0.0354,0.0981
*R*1, *wR*2 (all data)	0.0423,0.1081
GOF on F^2 [b]	1.092

[a] $R1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$. $wR2 = \{\Sigma[w(F_0^2 - Fc^2)^2]/\Sigma[w(F_0^2)^2]\}^{1/2}$. [b] GOF = $[(\Sigma w|F_0| - |F_c|)^2/(N_{obs} - N_{param})]^{1/2}$.

Table S2 Selected structural parameters of **IrST-0F**

Complex	Bond Angles/°				Bond Lengths/Å	
IrST-0F	C(25)-Ir(1)-C(10)	89.2(2)	N(1)-Ir(1)-O(2)	87.92(18)	Ir(1)-C(25)	1.964(6)
	C(25)-Ir(1)-N(2)	80.0(2)	C(25)-Ir(1)-O(1)	91.8(2)	Ir(1)-C(10)	2.003(5)
	C(10)-Ir(1)-N(2)	93.1(2)	C(10)-Ir(1)-O(1)	175.10(19)	Ir(1)-N(1)	2.037(5)
	C(25)-Ir(1)-N(1)	97.10(19)	N(2)-Ir(1)-O(1)	91.80(19)	Ir(1)-N(2)	2.040(5)
	C(10)-Ir(1)-N(1)	80.3(2)	N(1)-Ir(1)-O(1)	94.81(18)	Ir(1)-O(1)	2.140(4)
	N(2)-Ir(1)-N(1)	172.88(17)	O(2)-Ir(1)-O(1)	88.83(19)	Ir(1)-O(2)	2.136(4)
	C(25)-Ir(1)-O(2)	174.87(19)				
	C(10)-Ir(1)-O(2)	90.7(2)				
	N(2)-Ir(1)-O(2)	94.9(2)				

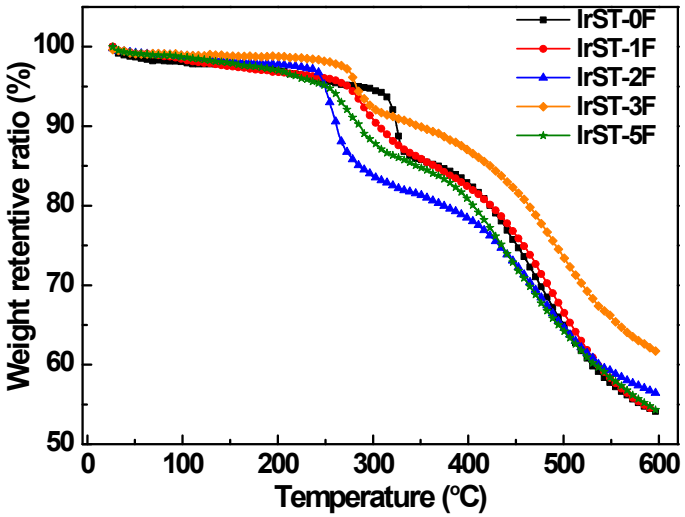


Fig. S4 TG carves for these 2-phenylthiazole-type Ir(III) complexes.

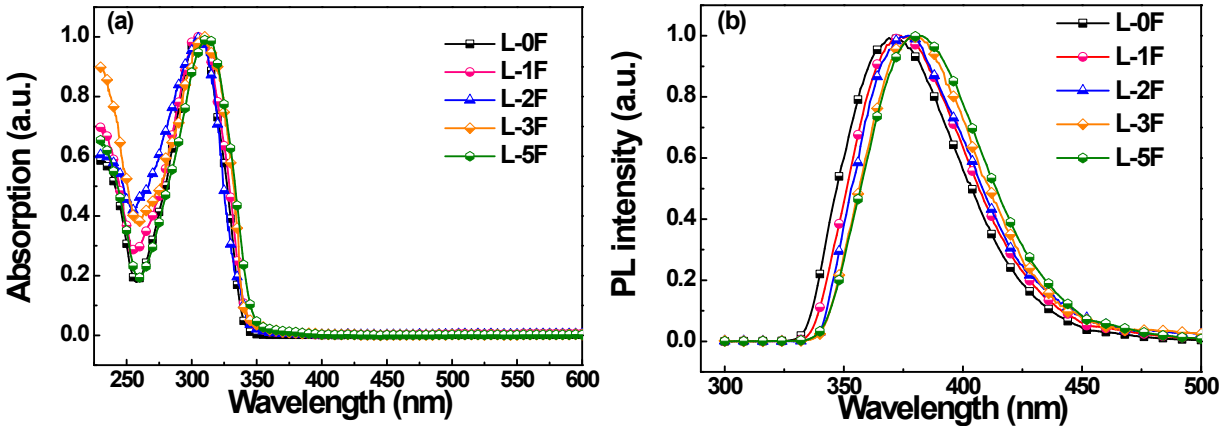


Fig. S5 UV-Vis and PL spectra for these 2-phenylthiazole ligands.

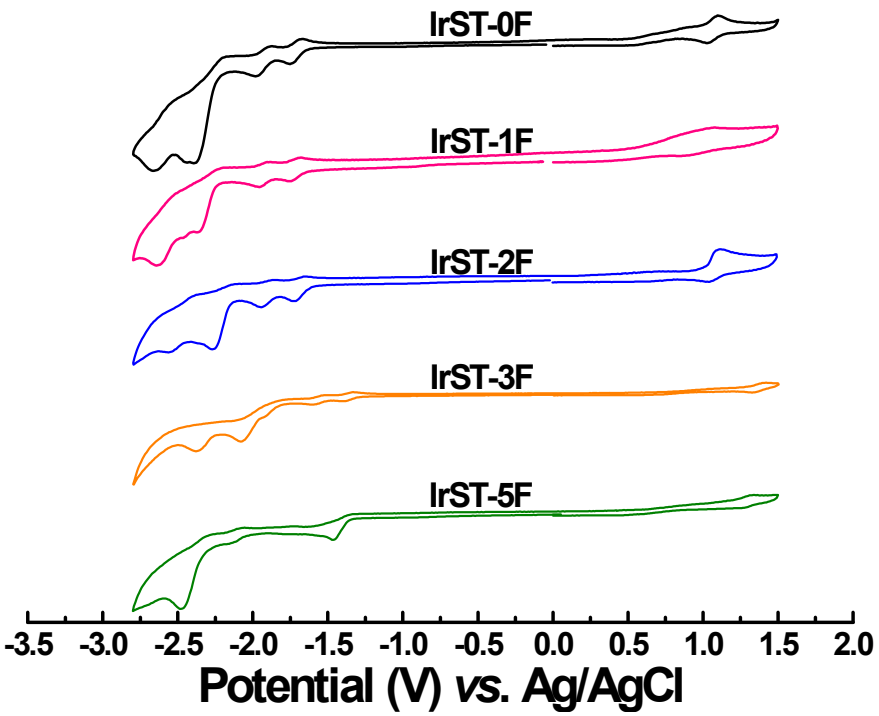


Fig. S6 CV carves for these 2-phenylthiazole-type Ir(III) complexes.

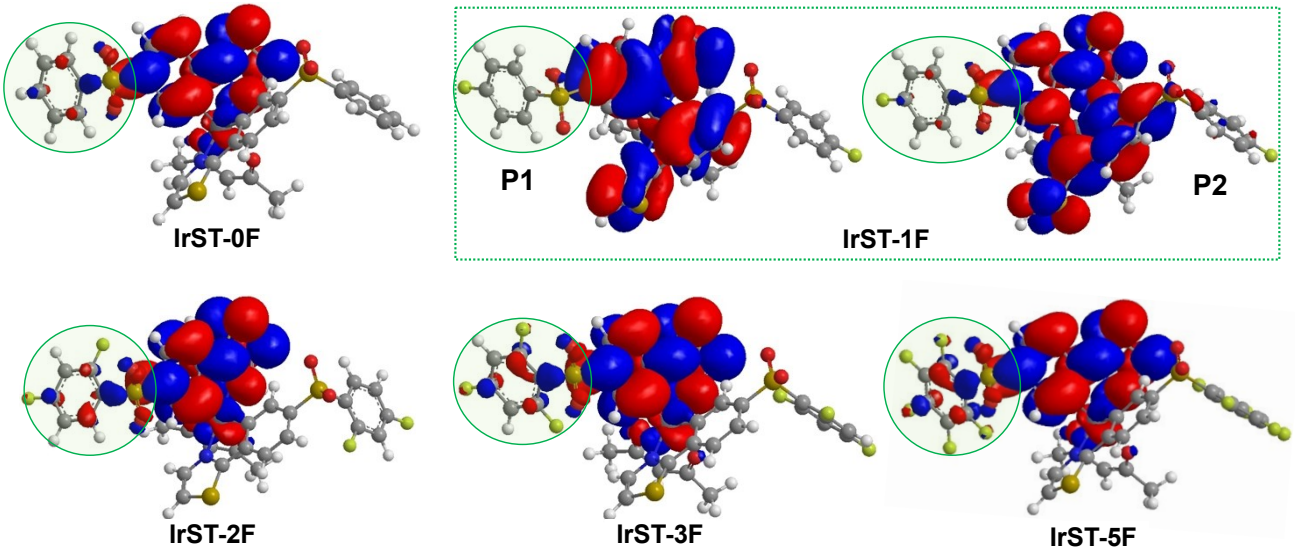


Fig. S7 Exlarged view of the NTO particle orbitals for these 2-phenylthiazole-type Ir(III) complexes, the isocontour is 0.2, the arylsulfonyl units are marked with green circles.

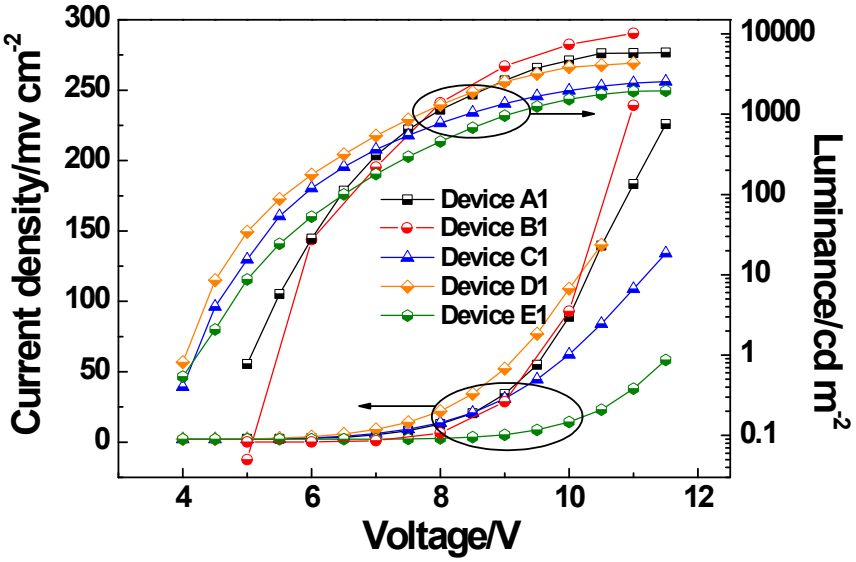
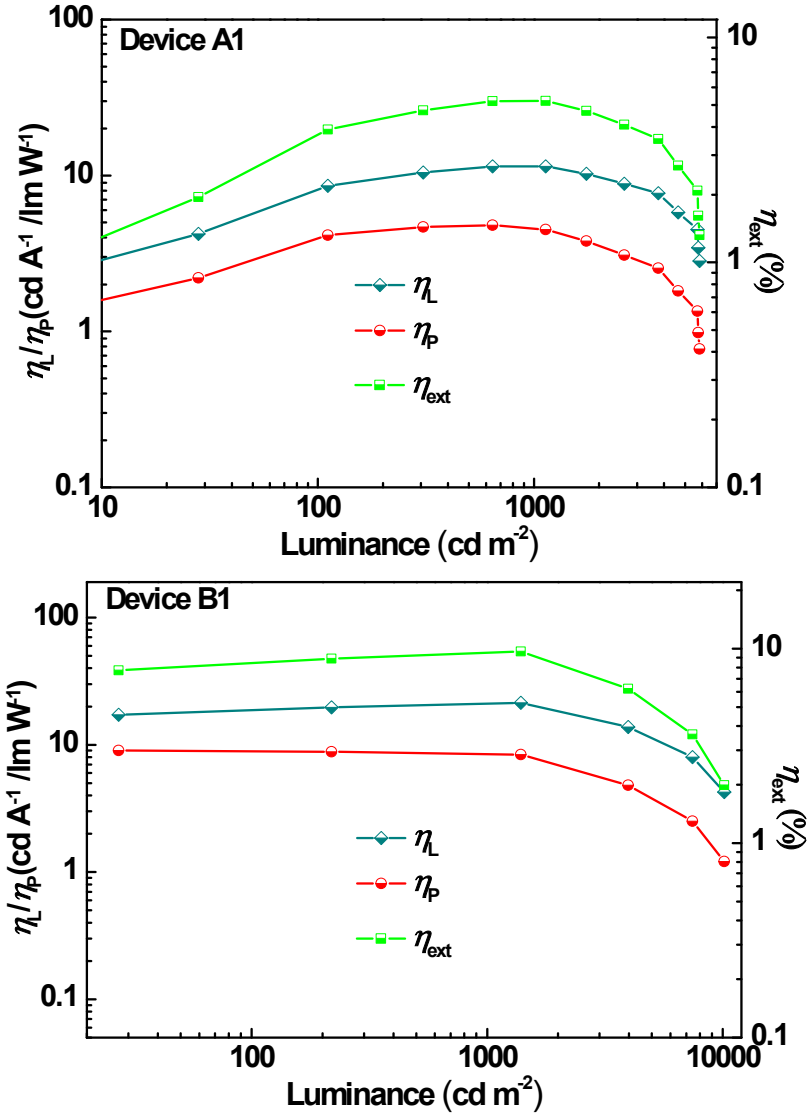


Figure S8. Current density–voltage–luminance (*J*–*V*–*L*) relationships of the OLEDs.



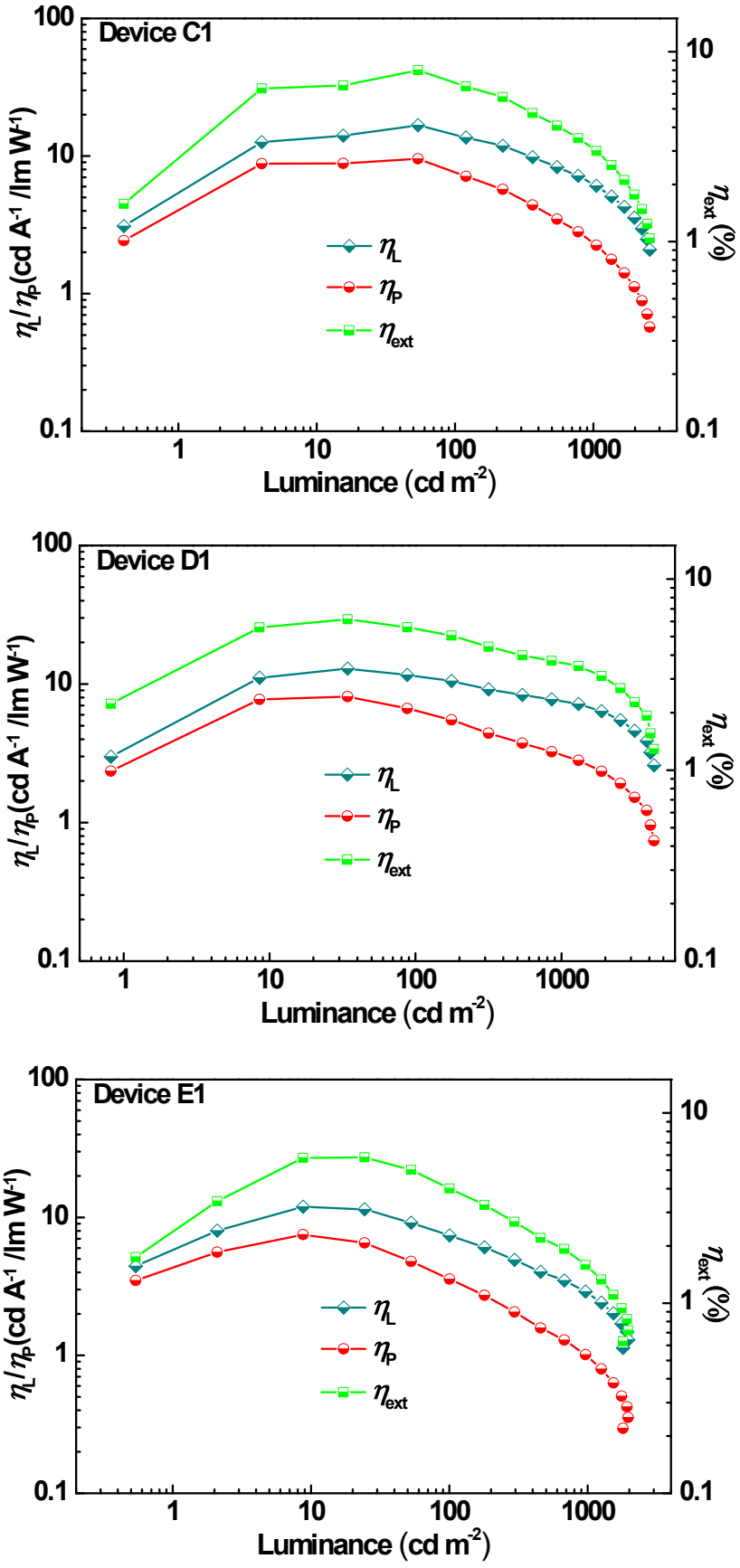


Figure S9. EL efficiencies luminance curves for the OLEDs