Electronic Supplementary Material (ESI) for RSC Advances.

Surporting information

Molecular design approach of increasing the triplet energy of host materials using pyrrole as a core structure

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Table S1.

	PPyCz2	27PTCz	36PTCz
LUMO	-0.74 eV	-1.20 eV	-1.20 eV
HOMO	-5.52 eV	-5.20 eV	-5.17 eV
Band Gap	4.78 eV	4.00 eV	3.97 eV
Triplet energy	3.18 eV	2.89 eV	3.06 eV

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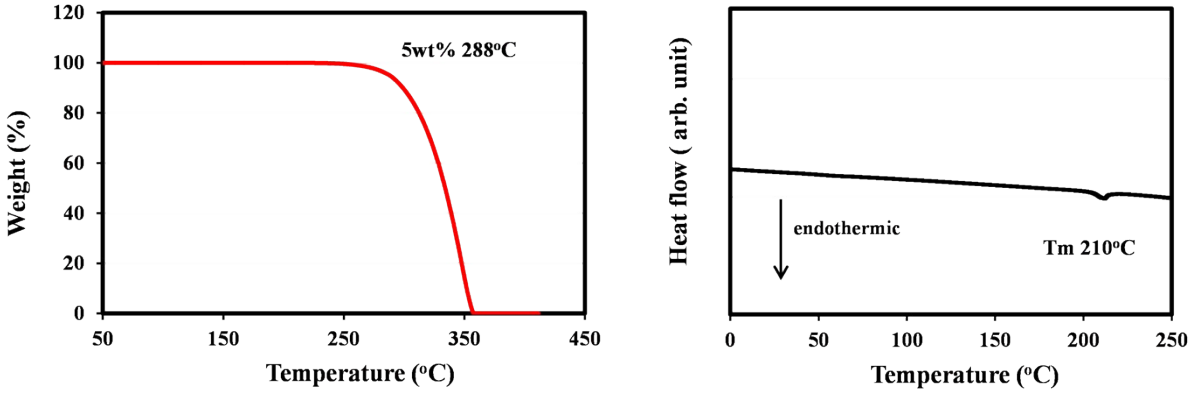
120
100
80
60
40
20
0
Weight (%)
5wt% 288°C
50
150
250
350
450
Temperature (°C)
Heat flow (arb. unit)
endothermic
Tm 210°C
0
50
100
150
200
250
Temperature (°C)

Figure S1.

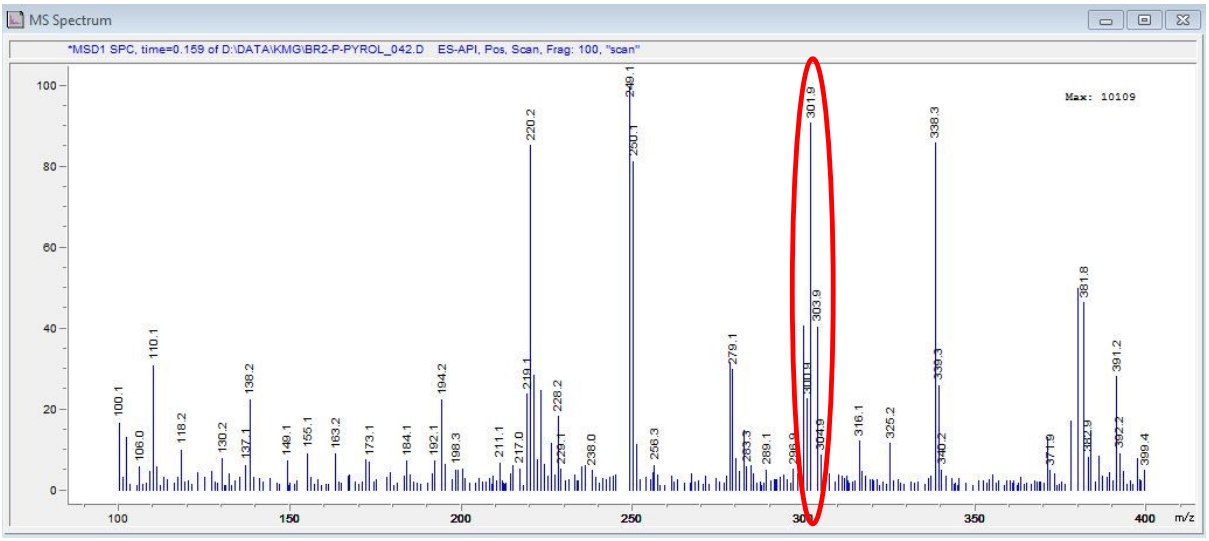
MS Spectrum
*MSD1 SPC, time=0.159 of D:\DATA\KMG\BR2-P-PYROL_042.D ES-API, Pos, Scan, Frag: 100, "scan"
Max: 10109
m/z

Figure S2.

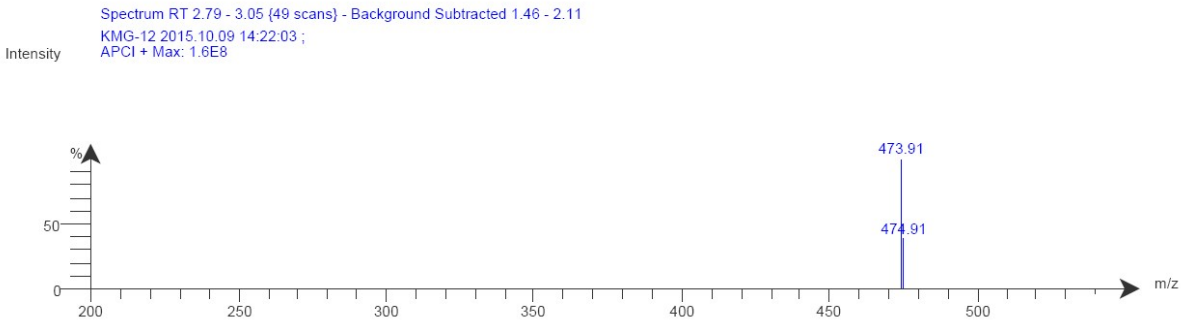
Spectrum RT 2.79 - 3.05 {49 scans} - Background Subtracted 1.46 - 2.11
KMG-12 2015.10.09 14:22:03 ;
APCI + Max: 1.6E8
Intensity
%
50
0
473.91
474.91
200
250
300
350
400
450
500
m/z

Figure S3.

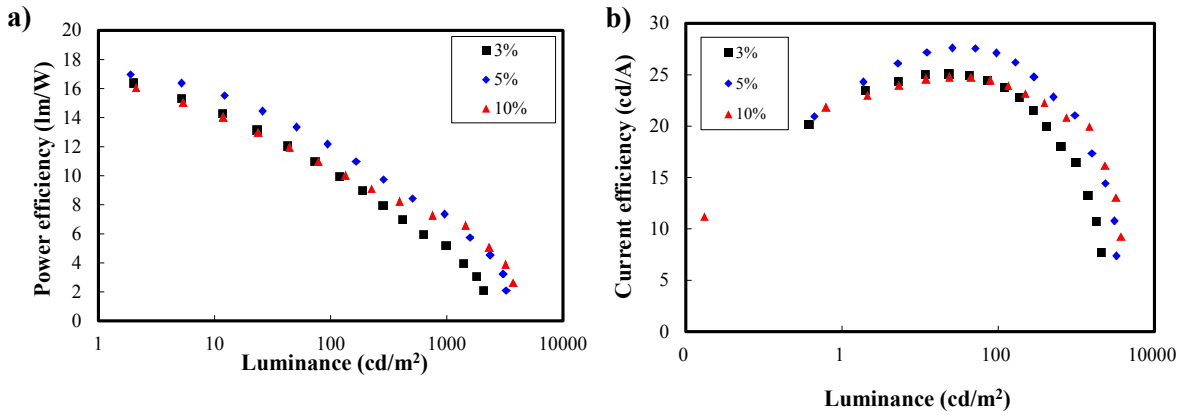
a)
Power efficiency (lm/W)
Luminance (cd/m²)
3%
5%
10%
b)
Current efficiency (cd/A)
Luminance (cd/m²)
3%
5%
10%

Figure S4.