Electronic Supplementary Information

Manipulation of sterically hindered effect to realize AIE and TADF for high-performing nondoped solution-processed OLEDs with extremely low efficiency roll-off

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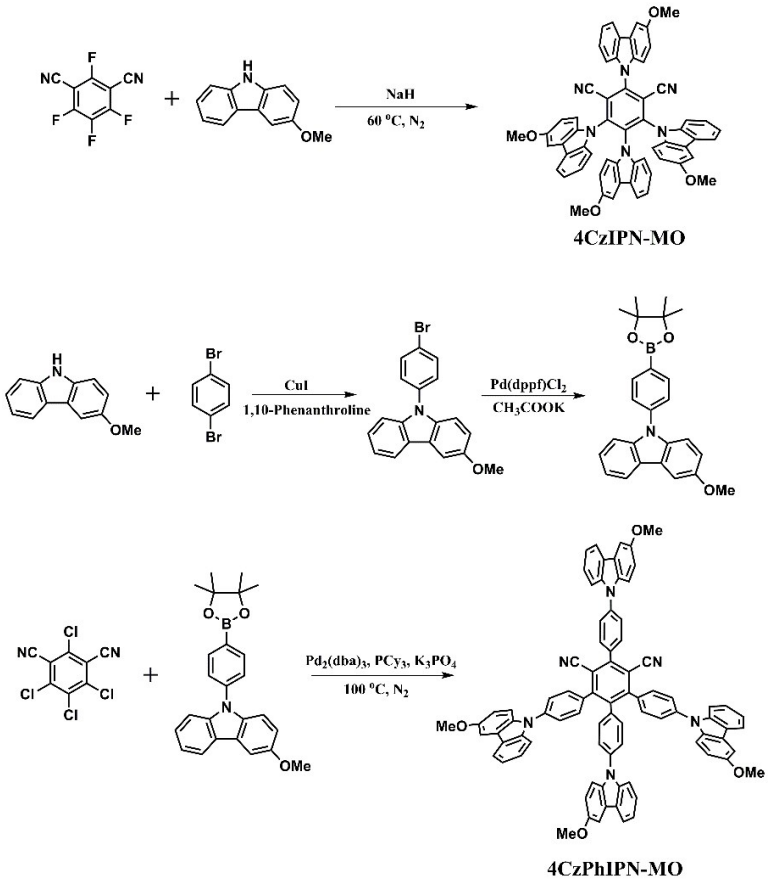
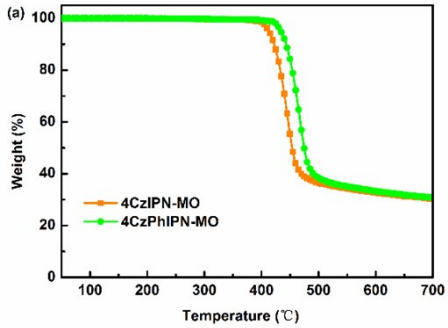
Scheme S1. Synthetic routes for 4CzIPN-MO and 4CzPhIPN-MO.





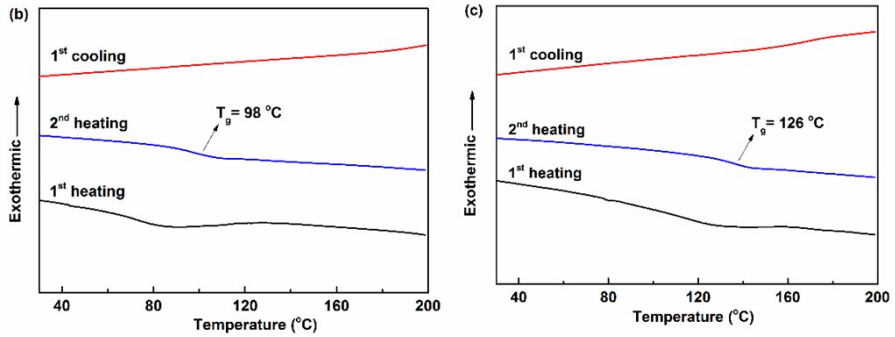


Fig. S1. (a) TGA curves and DSC curves of 4CzIPN-MO (b) and 4CzPhIPN-MO (c) recorded at a heating rate of 10 °C min^{-1}.

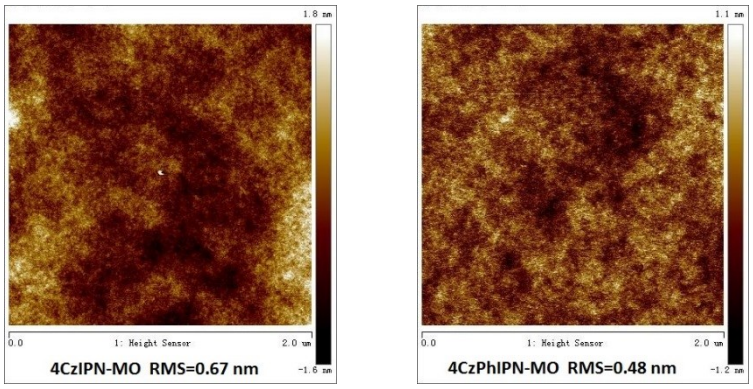
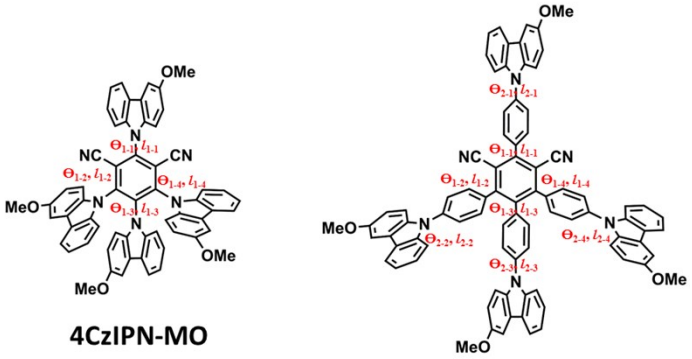


Fig. S2. AFM images of 4CzIPN-MO (left) and 4CzPhIPN-MO (right) thin films.

Table S1. Molecular structures and calculated HOMO, LUMO, Bandgap, S_1, T_1, ΔE_{st}, *f*, Dihedral angles (Θ) and Bond lengths (*l*) values from DFT and TD-DFT at B3LYP/6-31g(d) level.



Emitter	HOMO [eV]	LUMO [eV]	Bandgap [eV]	S_1 [eV]	T_1 [eV]	ΔE_{st} [eV]	*f*	$\Theta_{1\text{-}1}$-$\Theta_{1\text{-}4}$	$\Theta_{2\text{-}1}$-$\Theta_{2\text{-}4}$	$l_{1\text{-}1}$-$l_{1\text{-}4}$ (Å)	$L_{2\text{-}1}$-$l_{2\text{-}4}$ (Å)
4CzIPN-MO	-5.28	-2.45	2.83	2.28	2.17	0.11	0.0122	79°, 64°, 63°, 66°	/	1.41094, 1.40745, 1.40995, 1.40653	/
4CzPhIPN-MO	-5.03	-2.24	2.79	2.52	2.49	0.03	0.0549	60°, 70°, 66°, 69°	51°, 60°, 53°, 52°	1.48775, 1.49508, 1.49718, 1.49522	1.41260, 1.41700, 1.41311, 1.41944

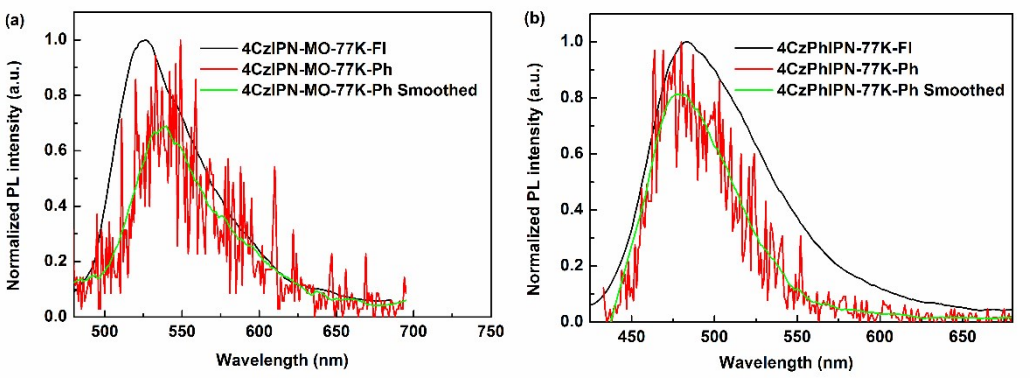


Fig. S3. Fluorescence and phosphorescence spectra (measured at 77K) of (a) 4CzIPN-MO and (b) 4CzPhIPN-MO in toluene.

Equations S1: [1-3]

$\Phi_{prompt} = \Phi_{PL} R_{prompt}$ (1)

$\Phi_{delayed} = \Phi_{PL} R_{delayed}$ (2)

$k_F = \Phi_{prompt}/\tau_{prompt}$ (3)

$\Phi_{PL} = k_F/(k_F + k_{IC})$ (4)

$\Phi_{prompt} = k_F/(k_F + k_{IC} + k_{ISC})$ (5)

$\Phi_{IC} = k_{IC}/(k_F + k_{IC} + k_{ISC})$ (6)

$\Phi_{ISC} = k_{ISC}/(k_F + k_{IC} + k_{ISC}) = 1 - \Phi_{prompt} - \Phi_{IC}$ (7)

$\Phi_{RISC} = \Phi_{delayed}/\Phi_{ISC}$ (8)

$k_{RISC} = (k_p k_d \Phi_{delayed})/(k_{ISC} \Phi_{prompt})$ (9)

$k_p = 1/\tau_{prompt}$; $k\mathrm{d} = 1/\tau_{delayed}$ (10)

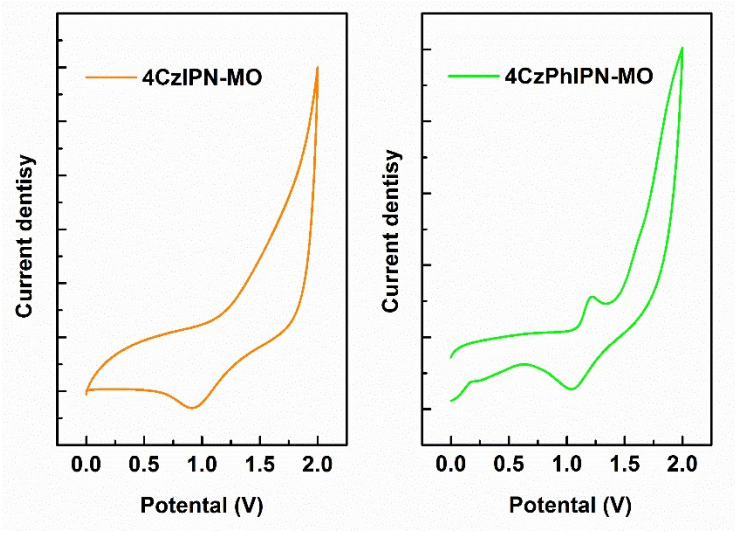


Fig. S4. Cyclic voltammograms of 4CzIPN-MO and 4CzPhIPN-MO in dichloromethane.

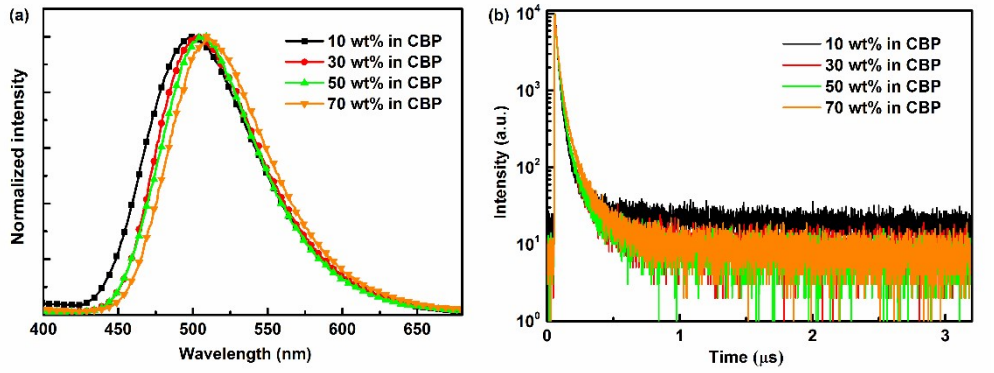


Fig. S5. PL spectra (a) and Transient PL spectra (b) of 4CzPhIPN-MO-based doped films.

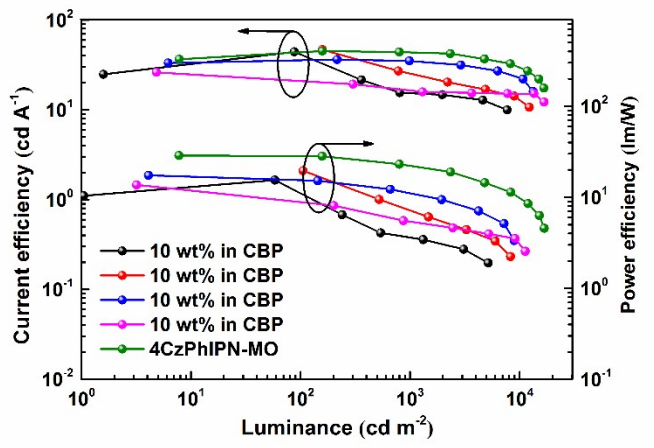
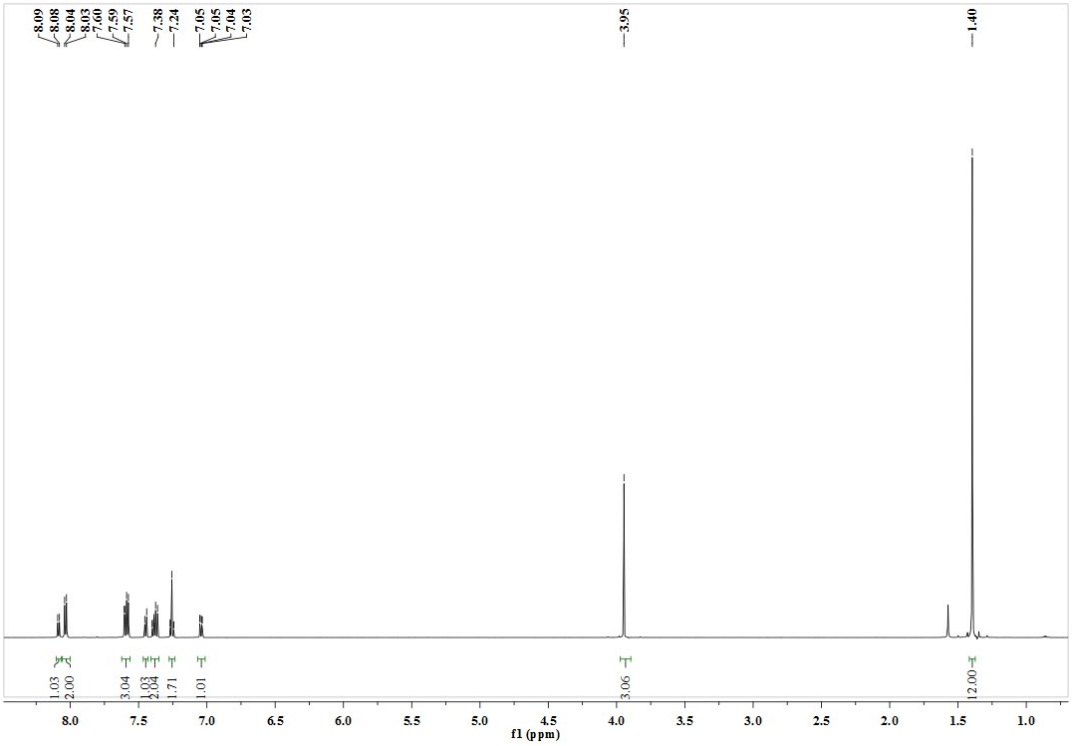
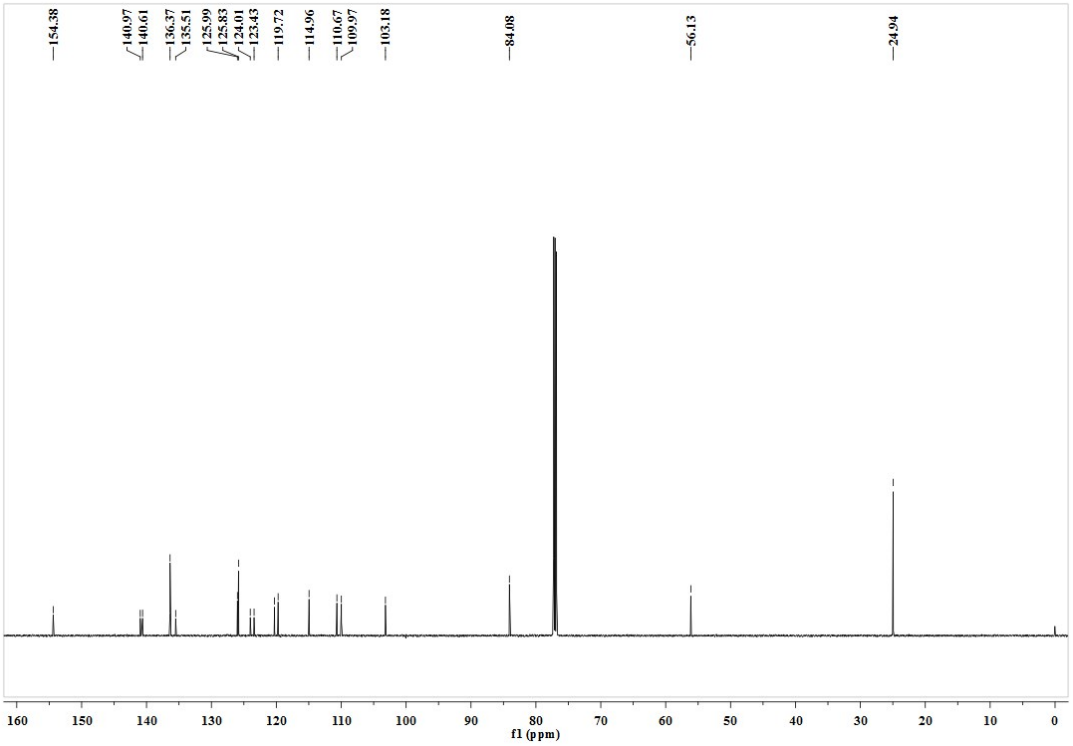


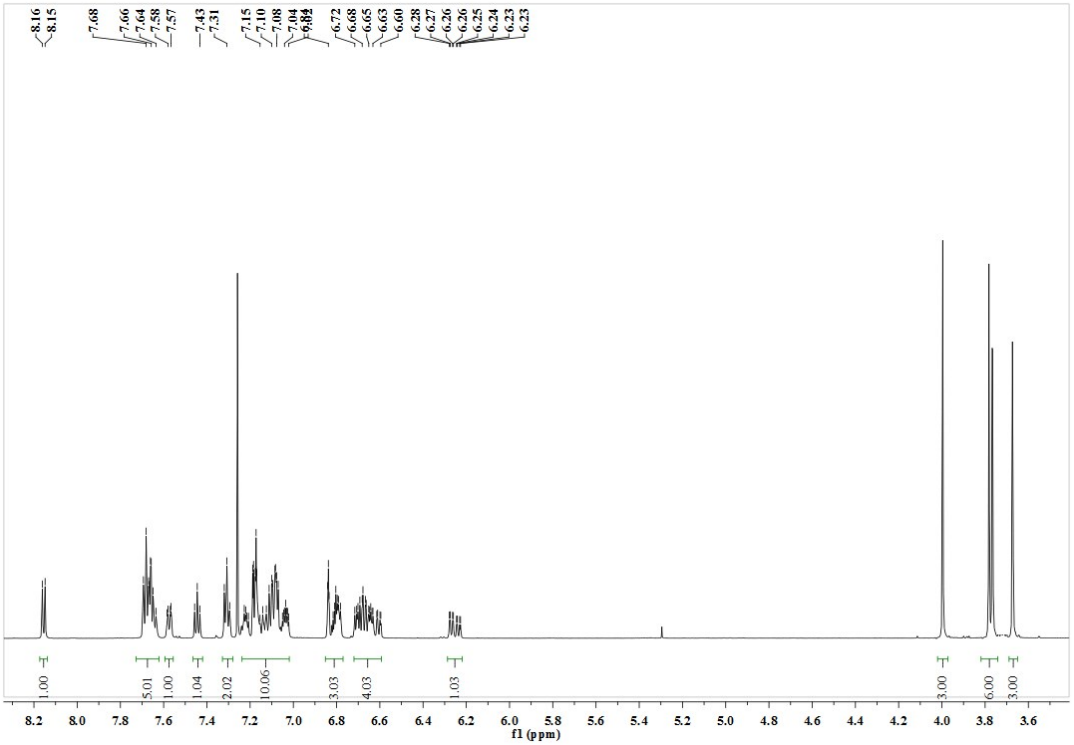
Fig. S6. Current efficiencies and power efficiencies versus brightness characteristics of 4CzPhIPN-MO-based devices.



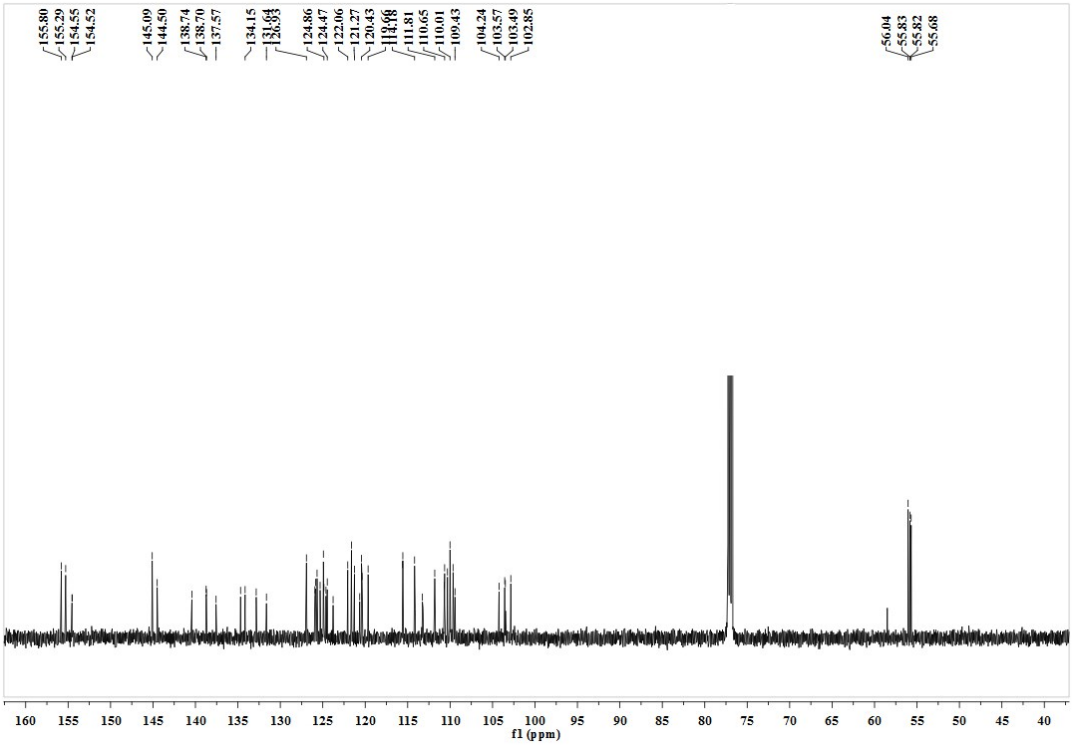
Inset: ^{1}H-NMR spectrum of 3-methoxy-9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole.



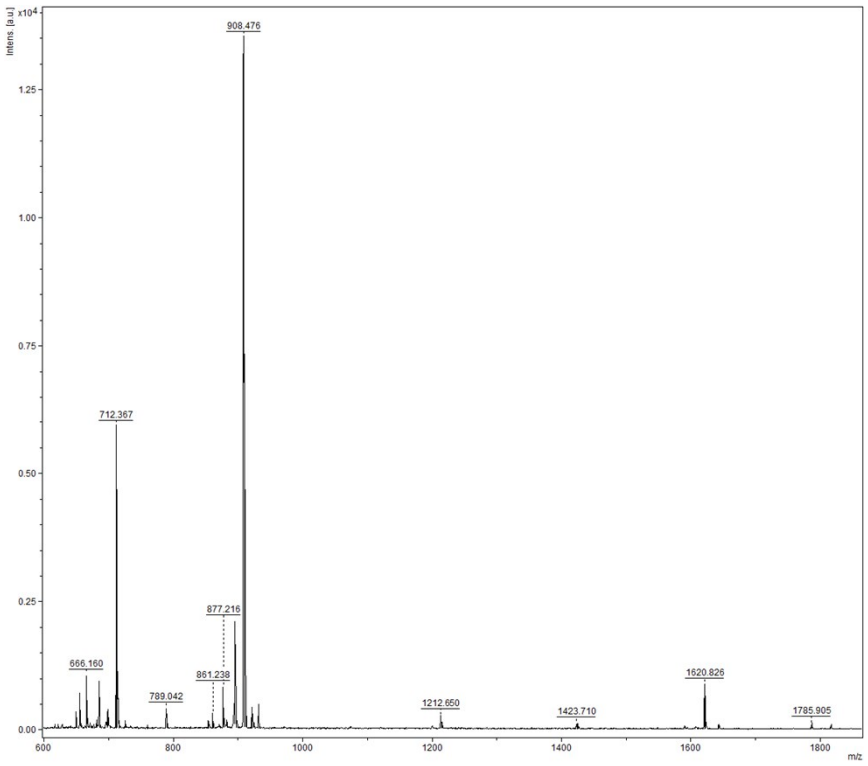
Inset: ^{13}C-NMR spectrum of 3-methoxy-9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole.



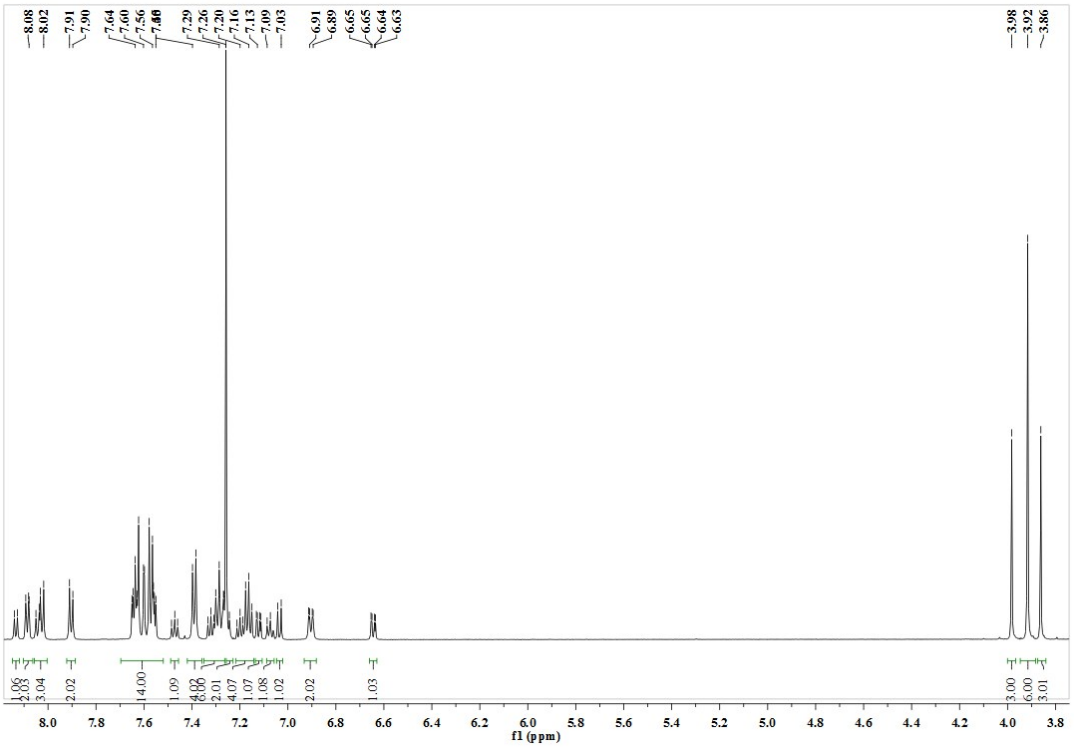
Inset: ^{1}H-NMR spectrum of 4CzIPN-MO.



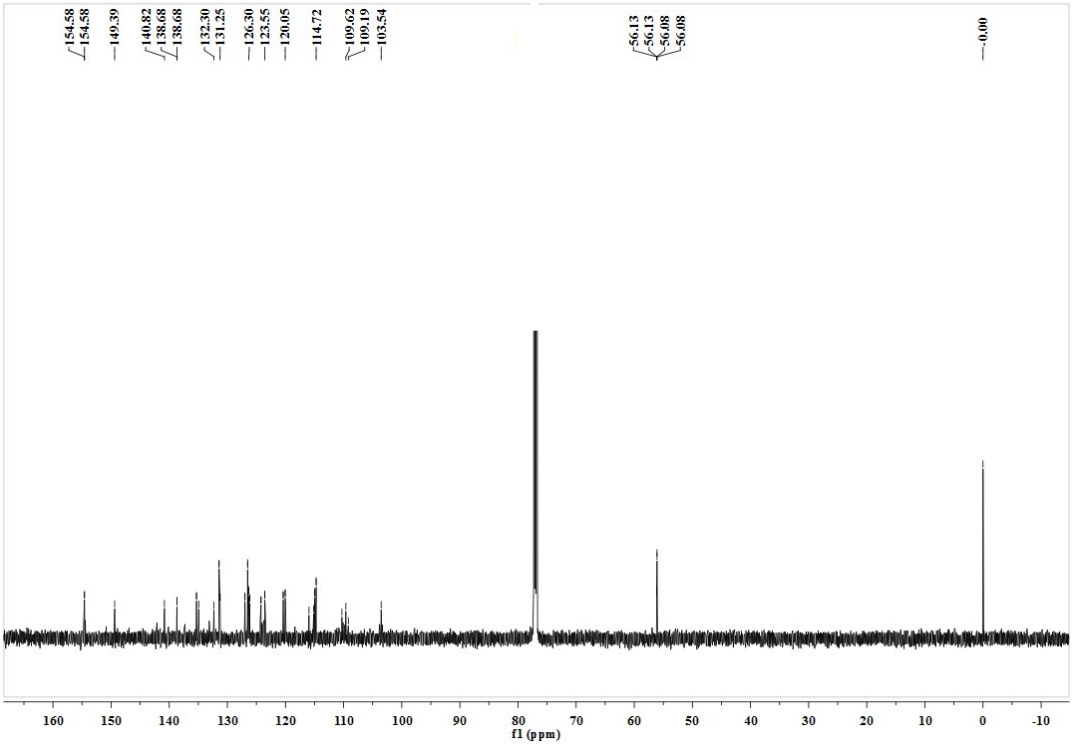
Inset: ^{13}C-NMR spectrum of 4CzIPN-MO.



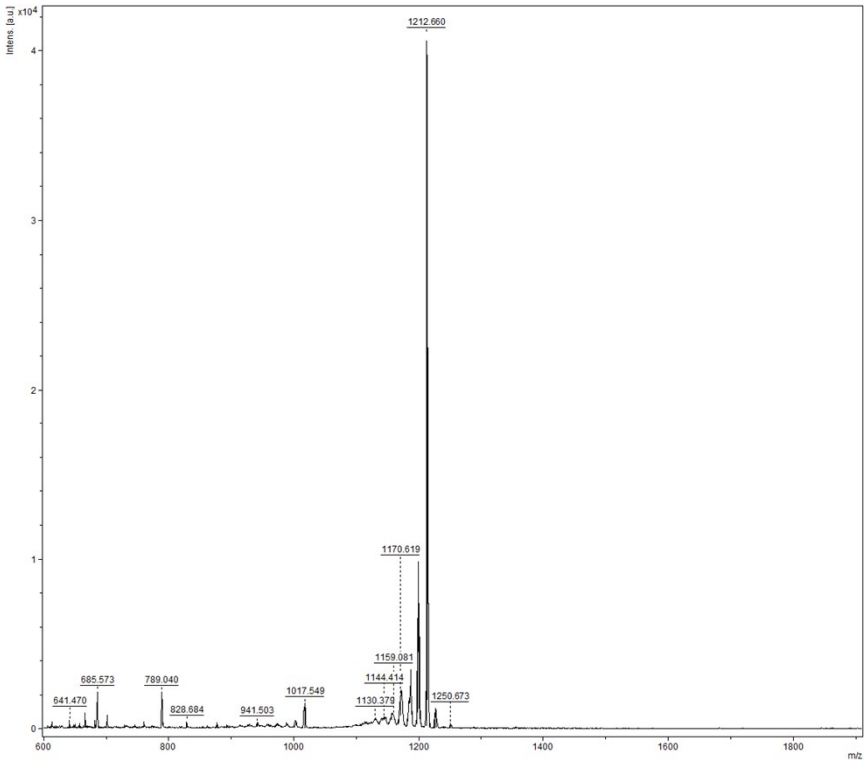
Inset: MALDI-TOF-MS spectrum of 4CzIPN-MO.



Inset: ^{1}H-NMR spectrum of 4CzPhIPN-MO.



Inset: ^{13}C-NMR spectrum of 4CzPhIPN-MO.



Inset: MALDI-TOF-MS spectrum of 4CzPhIPN-MO.

1	Summarize Results					
2	Date :	2019/5/24	14:19:52			
3	Method Name :	NCHS				
4	Method Filename :	N C H S system.mth				
5						
6						
7	Group No : 1	Element %				
8	Sample Name	Nitrogen	Carbon	Hydrogen	Sulphur	
9	LH11	9.172854061	78.69116	4.405603619	0	
10	LH12	9.310190315	79.87576	4.499294319	0	
11						
12	2 Sample(s) in Group No : 1					
13	Component Name	Average	Std. Dev.	% Rel. S. D.	Variance	
14	Nitrogen	9.241522183	0.097111	1.3174	0.0094	
15	Carbon	79.28346863	0.837639	0.1075	0.7016	
16	Hydrogen	4.45244896	0.066249	1.4879	0.0044	
17	Sulphur	0	0	0	0	
18						
19	Group No : 2	Element %				
20	Sample Name	Nitrogen	Carbon	Hydrogen	Sulphur	
21	21	6.980296612	83.34564	4.610781956	0	
22	22	6.901795425	82.98296	4.683946591	0	
23						
24	2 Sample(s) in Group No : 2					
25	Component Name	Average	Std. Dev.	% Rel. S. D.	Variance	
26	Nitrogen	6.941045773	0.055509	0.7997	0.0031	
27	Carbon	83.16429855	0.256451	0.3084	0.0658	
28	Hydrogen	4.647364274	0.051735	1.1132	0.0027	
29	Sulphur	0	0	0	0	

Inset: The element analysis data sheets of 4CzIPN-MO (NO.1) and 4CzPhIPN-MO (NO.2).

References

(1) H. Liu, J. Zeng, J. Guo, H. Nie, Z. Zhao, B. Tang, *Angew. Chem. Int. Ed.* 2018, **57**, 9290.

(2) T. Hosokai, H. Matsuzaki, H. Nakanotani, K. Tokumaru, T. Tsutsui, A. Furube, K. Nasu, H. Nomura, M. Yahiro, C. Adachi, *Sci. Adv.* 2017, **3**, e1603282.

(3) D. Zhang, L. Duan, C. Li, Y. Li, H. Li, D. Zhang, Y. Qiu, *Adv. Mater.* 2014, **26**, 5050.