

Supporting Information

A Rational Design of Carbazole-Based Host Materials With Suitable Spacer Group Towards Highly-Efficient Blue Phosphorescence

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CV curves of TMCz and DMCz:

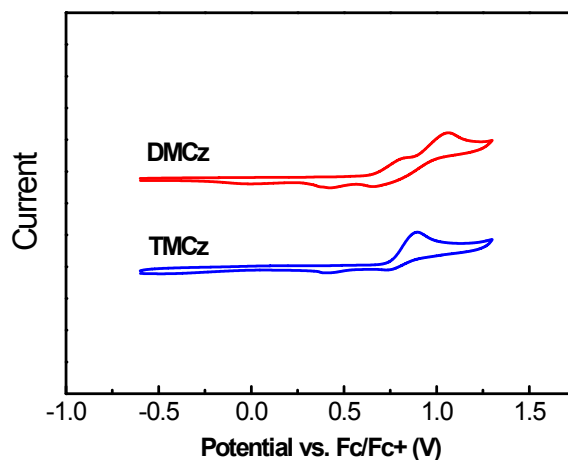


Fig. S1 Cyclic voltammograms of DMCz and TMCz in dichloromethane solution for oxidation.

TGA curves of DMCz and TMCz:

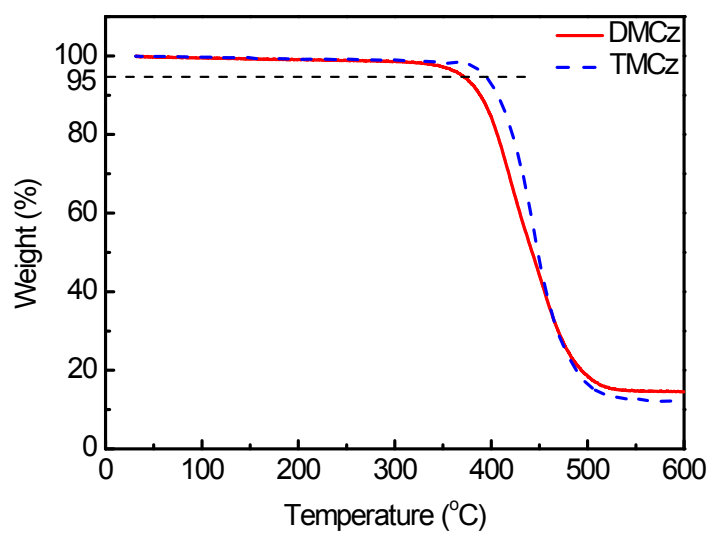


Fig. S2 TGA curves of DMCz and TMCz.

^1H NMR and ^{13}C NMR of TMCz and DMCz:

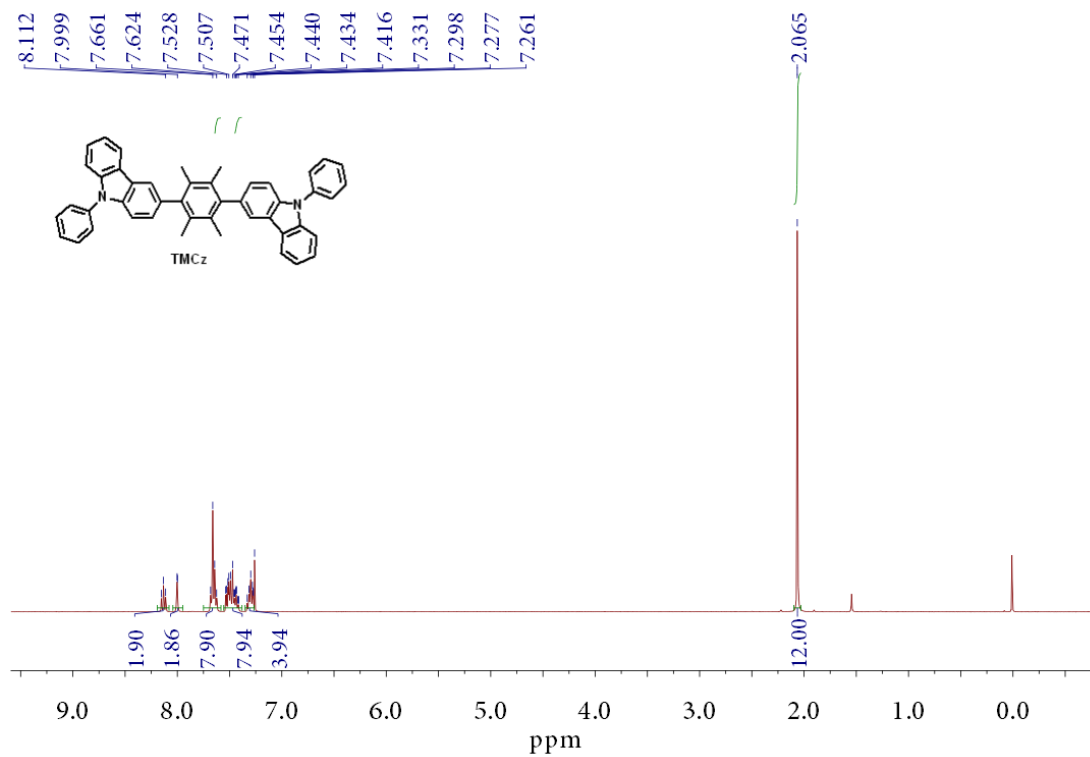


Fig. S3 400 MHz ^1H NMR spectrum of TMCz in CDCl_3 .

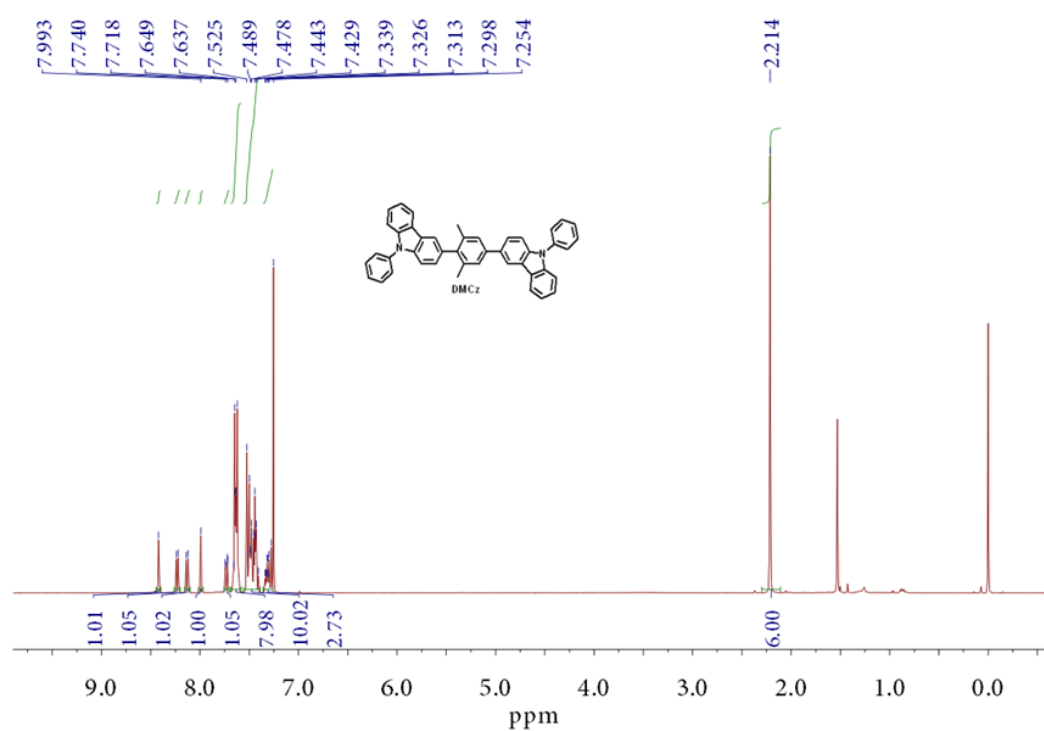


Fig. S4 400 MHz ¹H NMR spectrum of DMCz in CDCl₃.

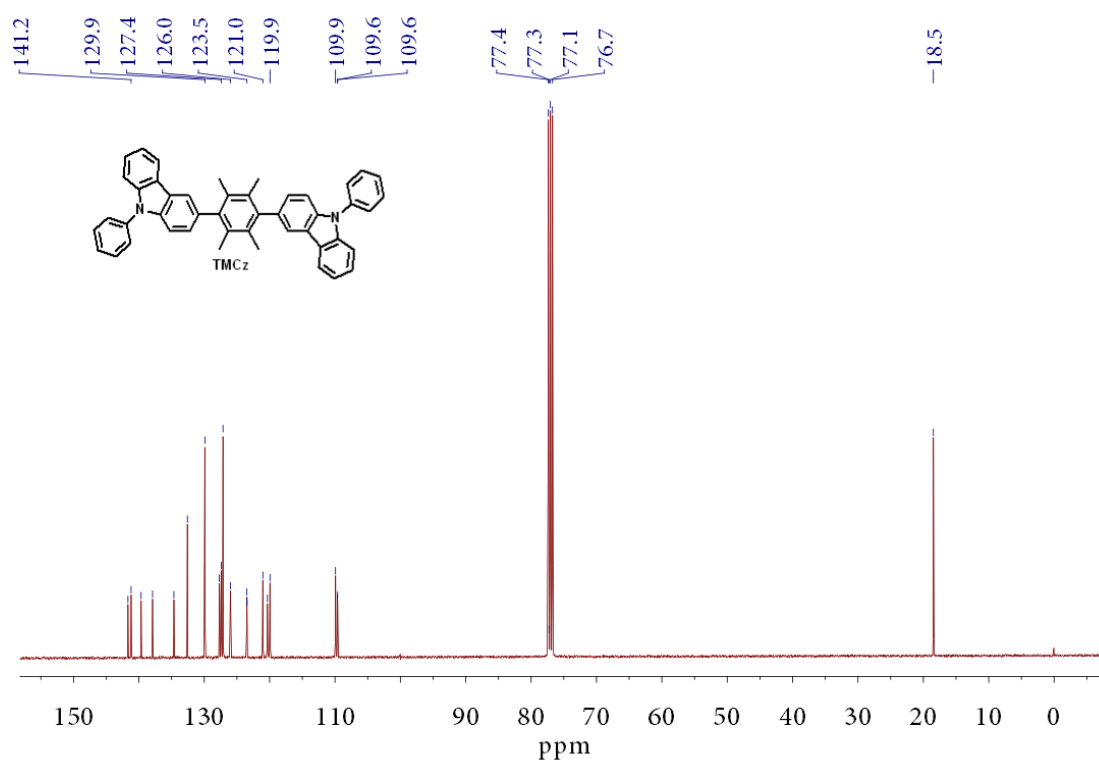


Fig. S5 400 MHz ¹³C NMR spectrum of TMCz in CDCl₃.

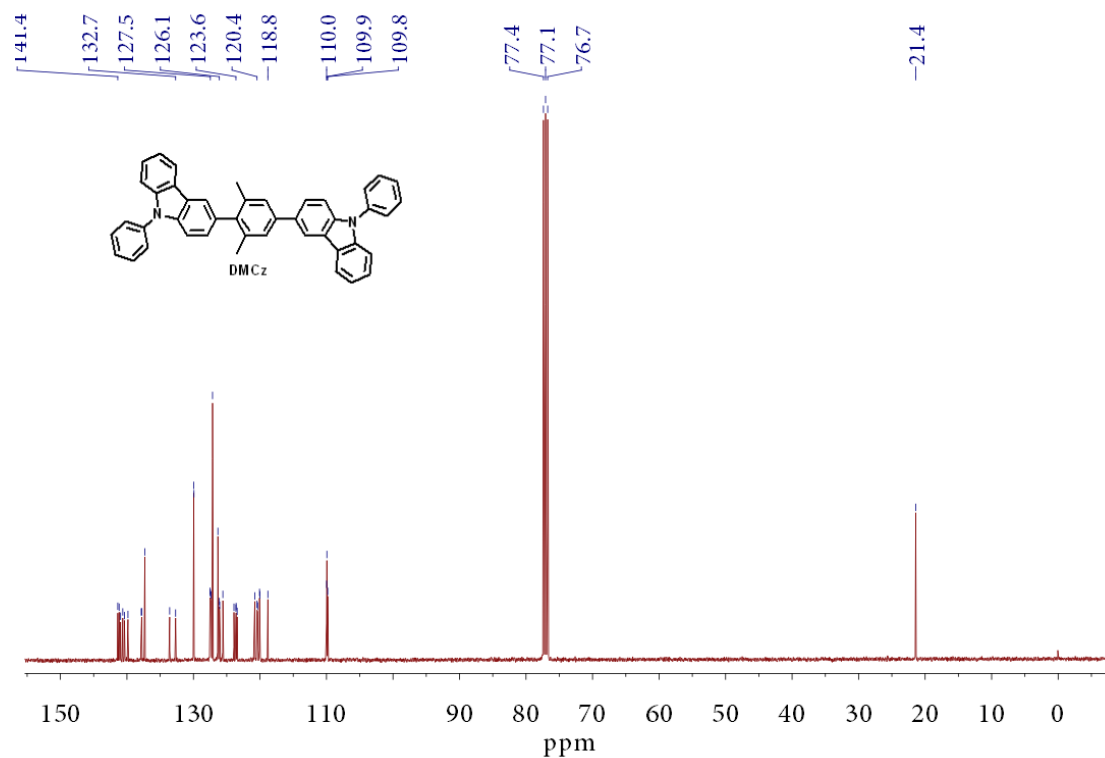


Fig. S6 400 MHz ¹³C NMR spectrum of DMCz in CDCl₃.

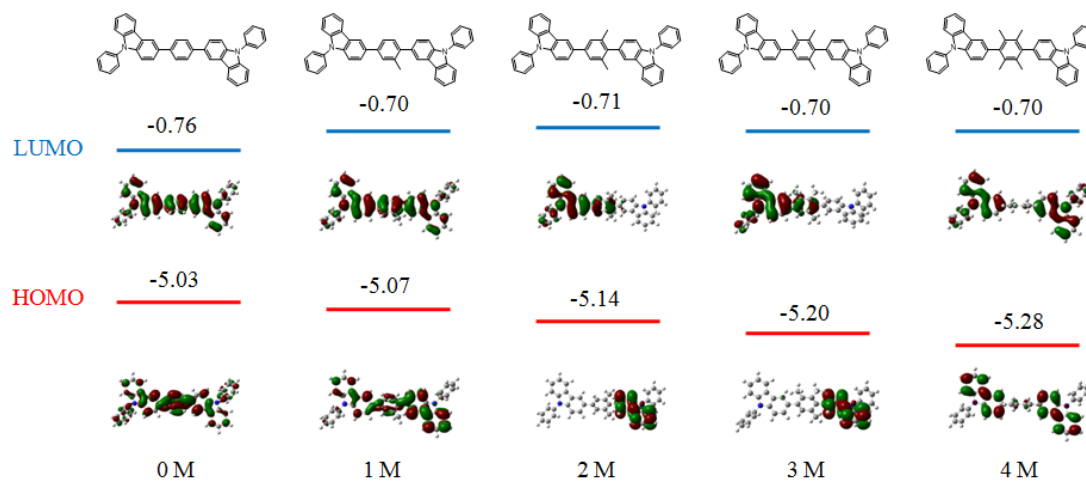


Fig. S7 Energy level diagrams of X M materials. The density functional theory (DFT) calculations were performed using the TD-DFT/B3LYP/6-31G(d) method with Gaussian 09 package. X = 0, 1, 2, 3, 4, represents the amount of methyl group in the center phenyl group.

Table S1. Electroluminescence characteristics of the devices using DMCz as the host.

Host: DMCz	V^a [V]	$\eta^{b_{ce}}$ [cd A ⁻¹]		$\eta^{b_{ce}}$ [lm W ⁻¹]		$\eta^{b_{ext}}$ [%]		CIE ^c
1 ^d	3.77	43.10	42.17	36.71	27.57	19.36	17.32	0.16, 0.39
2 ^d	3.95	44.30	43.56	35.23	27.40	17.66	17.93	0.16, 0.39
Average	3.86	43.7	42.86	35.97	27.48	18.51	17.62	0.16, 0.39

^a Voltages at 100 cd m⁻². ^b Efficiencies in the order of the maxima and at 1000 cd m⁻². ^c Commission International de l'Eclairage coordinates measured at 5 mA cm⁻². ^d Two devices with the same structure as mentioned in the discussion section.

Table S2. Electroluminescence characteristics of the devices using TMCz as the host.

Host: TMCz	V^a [V]	$\eta^{b_{ce}}$ [cd A ⁻¹]		$\eta^{b_{ce}}$ [lm W ⁻¹]		$\eta^{b_{ext}}$ [%]		CIE ^c
1 ^d	4.46	39.10	37.88	26.13	20.75	16.08	15.55	0.15, 0.37
2 ^d	4.49	32.70	32.55	23.98	17.67	13.37	13.35	0.16, 0.39
Average	4.48	35.9	35.22	25.06	19.21	14.72	14.45	0.16, 0.38

^a Voltages at 100 cd m⁻². ^b Efficiencies in the order of the maxima and at 1000 cd m⁻². ^c Commission International de l'Eclairage coordinates measured at 5 mA cm⁻². ^d Two devices with the same structure as mentioned in the discussion section.

Table S3. Electroluminescence characteristics of the devices using mCP as the host.

Host: mCP	V^a [V]	$\eta^{b_{ce}}$ [cd A ⁻¹]		$\eta^{b_{ce}}$ [lm W ⁻¹]		$\eta^{b_{ext}}$ [%]		CIE ^c
1 ^d	4.55	34.50	32.14	23.18	17.18	15.43	15.03	0.17, 0.38
2 ^d	4.36	37.60	37.01	25.69	17.60	13.67	13.25	0.16, 0.38
Average	4.46	36.05	34.58	24.44	17.39	14.55	14.14	0.16, 0.38

^a Voltages at 100 cd m⁻². ^b Efficiencies in the order of the maxima and at 1000 cd m⁻². ^c Commission International de l'Eclairage coordinates measured at 5 mA cm⁻². ^d Two devices with the same structure as mentioned in the discussion section.