Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

The Design, Synthesis, Characterization and Application of Novel Electron-deficient Moiety 1, 5-Diazacarbazole in High Triplet Energy Host Materials

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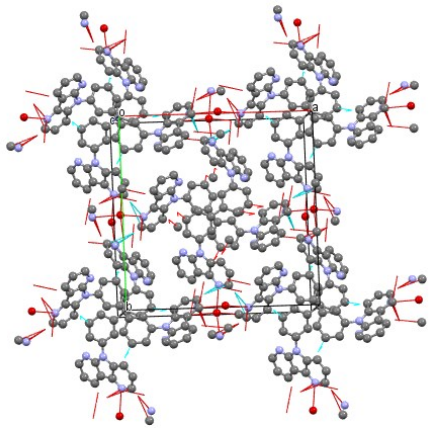

Figure S1. Packing structure of **NCzBPhNCz·0.5H_2O**

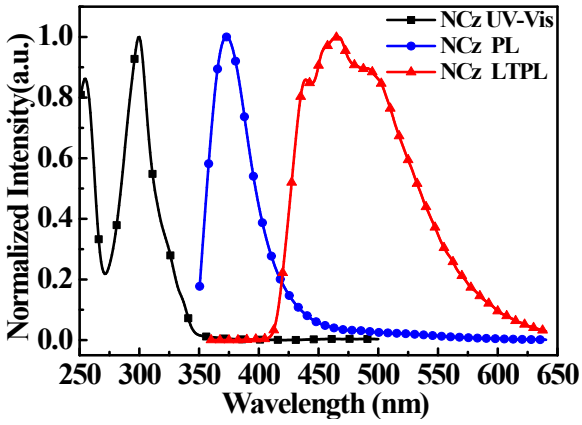

Figure S2. Photophysical properties of NCz

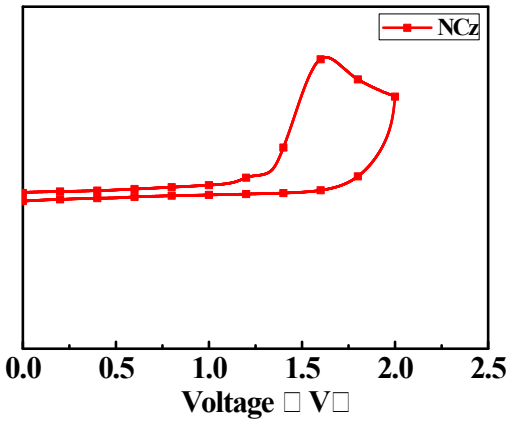

Figure S3. Cyclic voltammetry curve of NCz

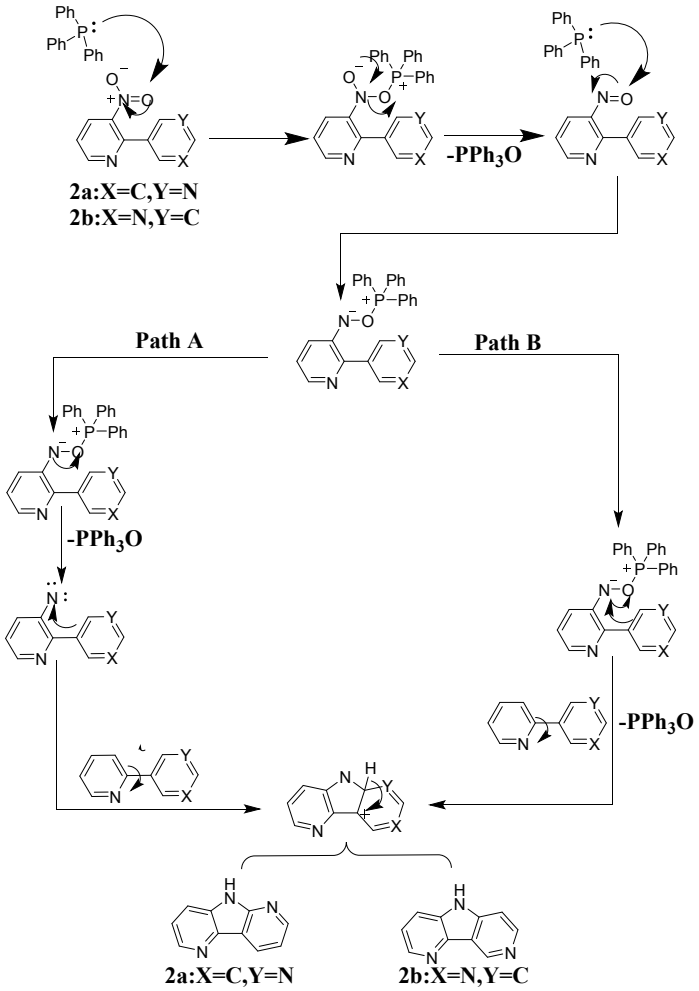

Figure S4 The possible reaction mechanism for reductive cyclization[1-3]

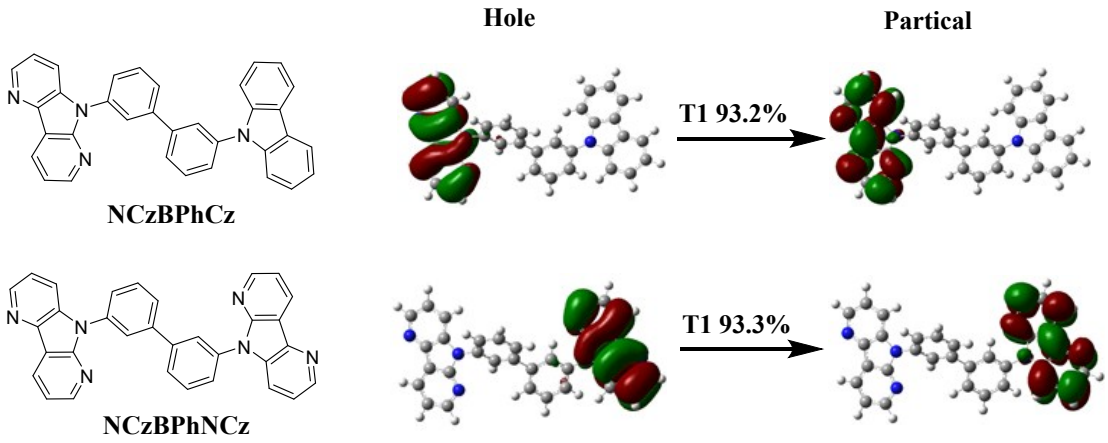

Figure S5. The $S_0 \rightarrow T_1$ NTO of NCzBPhCz and NCzBPhNCz and the weights of hole-particle are given for the $S_0 \rightarrow T_1$ excitations.

Table S1. Crystal Data and Structure Refinement for **NCzBPhNCz·0.5H$_2$O**

formula	$C_{32}H_{21}N_6O_{0.5}$
fw	497.55
cryst size, mm	0.21 × 0.16 × 0.14
T, K	153(2)
cryst syst	tetragonal
space group	I-4
a, Å	18.5174(19)
b, Å	18.5174(19)
c, Å	7.2125(15)
α, deg	90.00
β, deg	90.00
γ, deg	90.00
V, Å^3	2473.1(7)
Z	4
ρ, g cm^{-3}	1.336
μ, mm^{-1}	0.083
F(000)	1036
data/restraints/parameters	3062/0/174
quality-of-fit indicator	1.020
final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0542$, $wR_2 = 0.1309$
R indices (all data)	$R_1 = 0.0772$, $wR_2 = 0.1420$

Table S2. Calculation energy level of Cz、Cb、NCz and hosts

	HOMO	LUMO	bandgap	Triplet energy
Cz	-5.44	-0.64	4.8	3.19
Cb	-5.77	-1.02	4.75	3.14
NCz	-6.10	-1.33	4.77	3.19
NCzBPhCz	-5.41	-1.37	4.04	3.18
NCzBPhNCz	-5.83	-1.43	4.4	3.18

References

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3 G. Zotti, G. Schiavon, S. Zecchin, J. F. Morin and L. Mario, *Macromolecules.* 2002, **35**, 2122-2128.