Manipulation of Connecting Topology in Carbazole/Benzimidazole Universal Bipolar Hosts for RGB and White PhOLEDs

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Supporting Information

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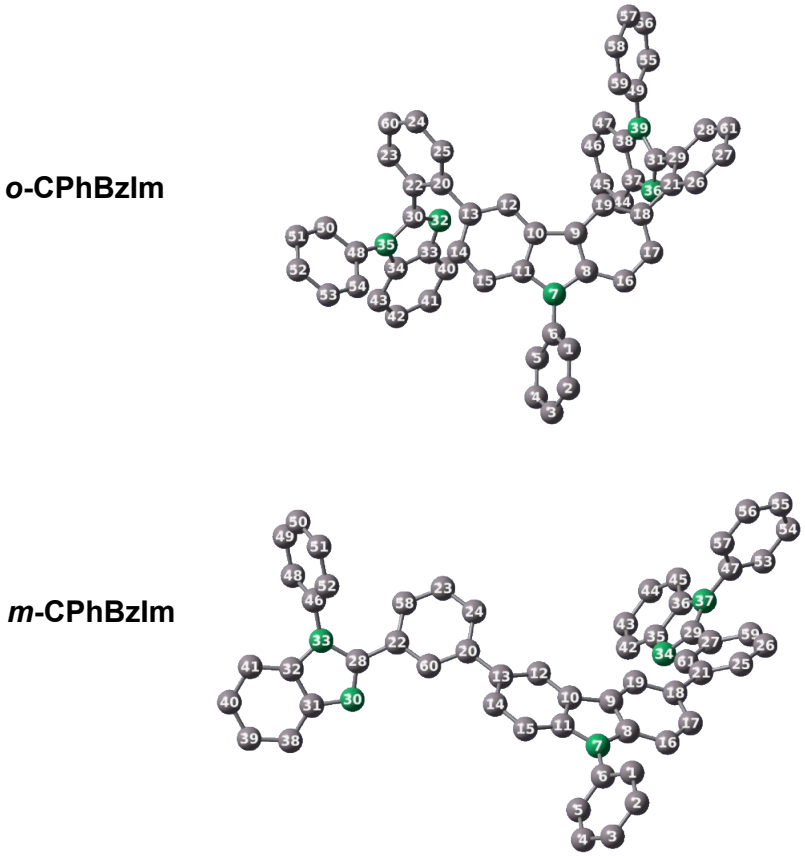

Fig. S1 Atomic numbers of ***o*-CPhBzIm** and ***m*-CPhBzIm** in the geometry of S_0 optimized by B3LYP/6-31G(d). All the protons are excluded.

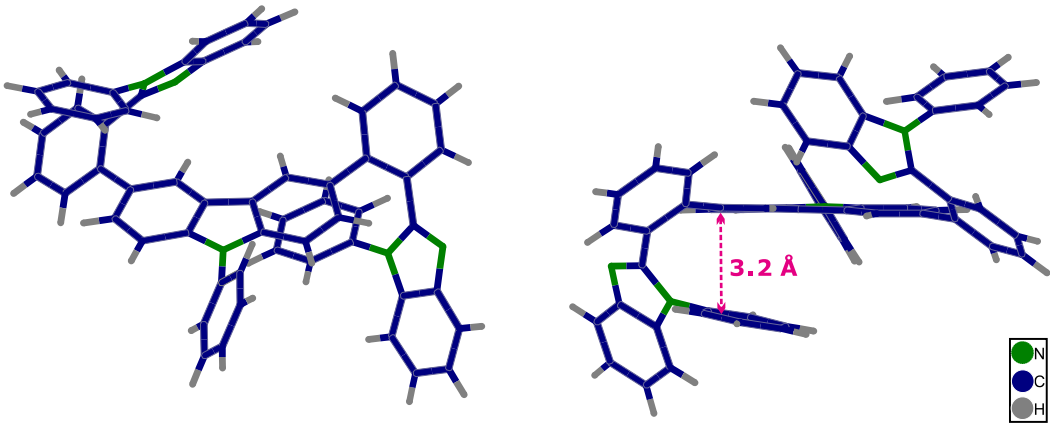

Fig. S2 Crystal structure of ***o*-CPhBzIm**. The solvente molecules are omitted for clarity. The crystal was obtained by the slow evaporation from the hexane/chloroform co-solvent system.

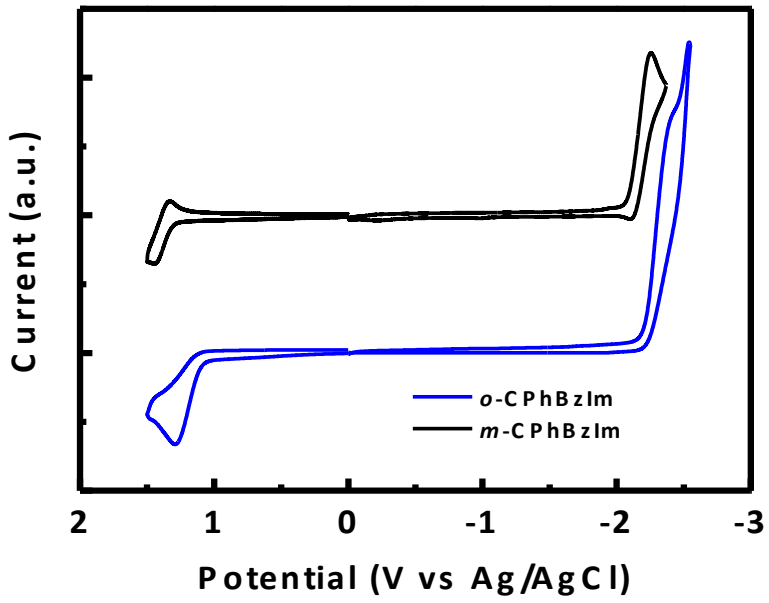

Fig. S3 Cyclic voltammograms of ***o*-CPhBzIm** and ***m*-CPhBzIm**; 0.1 M TBAP (reduction) in DMF and 0.1 M $TBAPF_6$ (oxidation) in CH_2Cl_2 were used as supporting electrolytes.

Table S1 Bond lengths (*r*) and dihedral angles (*Φ*) for DFT//B3LYP/6-31G(d) ground states (S_0) and CIS/6-31G(d) excited states (S_1) of ***o*-CPhBzIm** and ***m*-CPhBzIm**.

***o*-CPhBzIm**	B3LYP/6-31G(d) S_0	CIS/6-31G(d) S_1	***m*-CPhBzIm**	B3LYP/6-31G(d) S_0	CIS/6-31G(d) S_1
r (7,11)	1.39862	1.39178	r(7,11)	1.39885	1.38692
r (11,10)	1.4171	1.41642	r(11,10)	1.41713	1.39817
r (10,12)	1.39718	1.39134	r(10,12)	1.39667	1.38942
r (12,13)	1.3993	1.39357	r(12,13)	1.40057	1.38604
r (13,20)	1.48941	1.49179	r(13,20)	1.48568	1.492
r (20,22)	1.41425	1.41182	r(20,60)	1.40109	1.37503
r (22,23)	1.40225	1.39733	r(60,22)	1.40383	1.44086
r (22,30)	1.48697	1.47907	r(22,28)	1.4739	1.40078
r (30,35)	1.40413	1.38466	r(28,33)	1.40078	1.41155
r (35,48)	1.42917	1.42169	r(33,46)	1.42823	1.42291
Φ(11,7,6,1)	-124.68925	-125.01504	A(11,7,6,1)	-124.92623	-106.97394
Φ(12,13,20,22)	127.94239	-53.89147	A(12,13,20,24)	-36.09328	-44.96407
Φ(19,18,21,29)	-53.89147	-135.53848	A(19,18,21,25)	142.70764	135.03988
Φ(20,22,30,35)	110.93178	-60.69919	A(58,22,28,33)	-29.12682	-4.82923
Φ(21,29,31,39)	135.20356	62.38141	A(59,27,29,37)	-30.49351	-38.7755
Φ(31,39,49,59)	-53.3322	55.35748	A(22,28,33,46)	-10.25591	-20.90794
Φ(30,35,48,54)	-111.52553	-49.02867	A(27,29,37,47)	-10.50612	-9.43388
Φ(47,38,39,49)	0.54649	6.08442	A(28,33,46,52)	-57.65537	-60.47038
Φ(43,34,35,48)	8.83564	-1.07163	A(29,37,47,57)	-56.79822	-61.55644

Table S2 The crystal data of ***o*-CPhBzIm**.

	***o*-CPhBzIm**
Empirical formula	$C_{56}H_{37}N_5$
Formula weight	949.16
Temperature	150(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 14.0188(2) Å $\alpha = 90^o$
	b= 14.5960(2) Å $\beta = 106.5080(10)^o$
	c = 20.5850(3) Å $\gamma = 90^o$
Cell Volume, z	4038.45(10) $Å^3$, 4
Density (calc.)	1.283 Mg/m^3
F(000)	1632
Reflections collected	16583
Independent reflections	7355 (R_{int} = 0.0354)
Final R indices [I>2σ(I)]	R1 = 0.0471, *wR2* = 0.1188
R indices (all data)	R1 = 0.0782, *wR2* = 0.1336