

## Supporting information for the paper

### Wet-process feasible novel carbazole-type molecular host for highly efficient phosphorescent organic light emitting diodes

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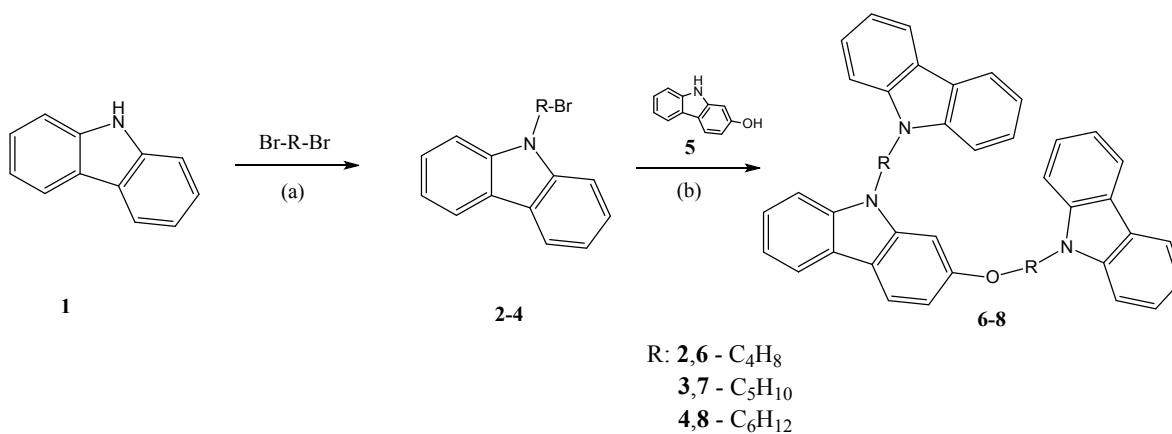
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### Experimental details for synthesis of the host materials 6-8 (Scheme1)

9H-Carbazole (**1**), 2-Hydroxycarbazole (**5**), 1,4-dibromobutane, 1,5-dibromopentane 1,6-dibromohexane, tetra-n-butylammonium hydrogen sulfate (TBAHS) and KOH were purchased from Aldrich and used as received.



**Scheme 1.** a) KOH, TBAHS, acetone; b) KOH, TBAHS, THF.

9-(4-bromobutyl)carbazole (**2**), 9-(5-bromopentyl)carbazole (**3**) and 9-(6-bromohexyl)carbazole (**4**) were synthesized according to the procedures outlined in literature<sup>1</sup>.

#### **9-(4-Bromobutyl)carbazole (2)**

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.13 (d, 2H, *J* = 7.8 Hz, Ar), 7.57-7.35 (m, 4H, Ar), 7.30-7.21 (m, 2H, Ar), 4.38 (tr, 2H, *J* = 6.9 Hz, NCH<sub>2</sub>), 3.34 (t, 2H, *J* = 6.6 Hz, BrCH<sub>2</sub>), 2.15-2.01 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>), 1.99-1.84 (m, 2H, BrCH<sub>2</sub>CH<sub>2</sub>). Yield: 55.6 % (7.6 g) of white amorphous substance.

#### **9-(5-Bromopentyl)carbazole (3)**

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.10 (d, 2H, *J* = 7.8 Hz, Ar), 7.53-7.35 (m, 4H, Ar), 7.27-7.18 (m, 2H, Ar), 4.32 (tr, 2H, *J* = 7.2 Hz, NCH<sub>2</sub>), 3.35 (tr, 2H, *J* = 6.9 Hz, BrCH<sub>2</sub>), 1.98-1.79 (m, 4H, NCH<sub>2</sub>CH<sub>2</sub>, BrCH<sub>2</sub>CH<sub>2</sub>), 1.60-1.48 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>). Yield: 57.5 % (6.5 g) of white amorphous substance.

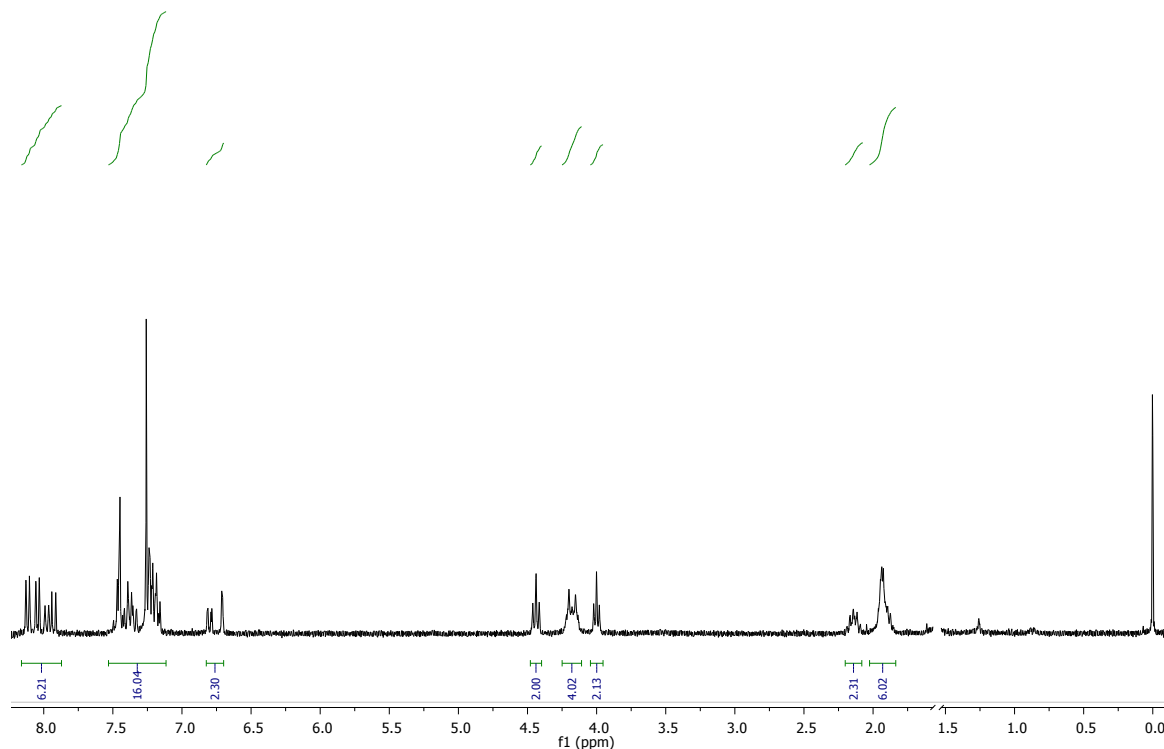
#### **9-(6-Bromohexyl)carbazole (4)**

MS (APCI<sup>+</sup>, 20 V): 443,6 ([M+H], 100 %). <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.11 (d, 2H, *J*=7.5, Ar), 7.50–7.38 (m, 4H, Ar), 7.24 (tr, 2H, *J*=7.5, Ar), 4.33 (tr, 2H, *J*=7.5, NCH<sub>2</sub>), 3.36 (tr, 2H, *J*=6.6, BrCH<sub>2</sub>), 1.95-1.82 (m, 4H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br), 1.59-1.48 (m, 4H, NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br). Yield: 40.3 % (6.35 g) of white amorphous substance.

**2-[4-(carbazol-9-yl)butyloxy]-9-[4-(carbazol-9-yl)butyl]carbazole (6)** was prepared by the reaction of 2-hydroxycarbazole (**5**) with excess of 9-(4-bromobutyl)carbazole (**2**) under basic conditions in the presence of phase transfer catalyst. 1.65 g (5.5 mmol) of the compound **2** and 0.25 g (1.4 mmol) of 2-hydroxycarbazole (**5**) were heated till reflux in 40 ml of THF. Then 0.23 g (4.1 mmol) of powdered potassium hydroxide and a catalytic amount of TBAHS were added to the mixture, and it was refluxed for 2 h. After TLC control the mixture was filtered, the solvent was evaporated and the product was purified by column chromatography with silica gel using the mixture of ethyl acetate and hexane (vol. ratio 1:20) as an eluent. Yield: 61.2 % (0.52 g) of white crystals.

MS (APCI<sup>+</sup>, 20 V): 626.32 ([M+H], 100 %). <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.15-7.90 (m, 6H, Ar), 7.49-7.15 (m, 16H, Ar), 6.87-6.74 (m, 2H, Ar), 4.45 (tr, 2H, *J* = 7.2 Hz,

NCH<sub>2</sub>), 4.25-4.13 (m, 4H, 2×NCH<sub>2</sub>), 4.01 (tr, 2H, *J* = 6.3 Hz, OCH<sub>2</sub>), 2.21-2.08 (m, 2H, OCH<sub>2</sub>CH<sub>2</sub>), 1.99-1.85 (m, 6H, 2×NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>, OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>).

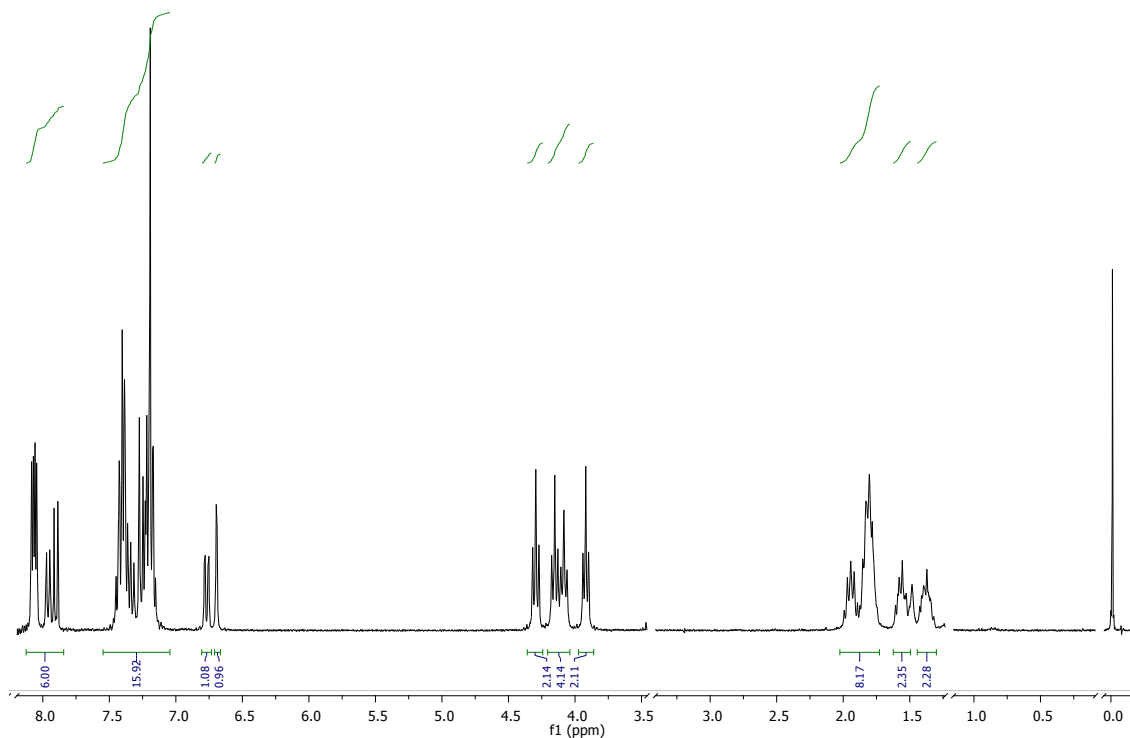


**Figure S1.** NMR spectra of compound **6**.

**2-[5-(carbazol-9-yl)pentyl]oxy]-9-[5-(carbazol-9-yl)pentyl]carbazole (**7**)** was prepared by the reaction of 2-hydroxycarbazole (**5**) with excess of 9-(5-bromopentyl)carbazole (**3**) under basic conditions in the presence of TBAHS phase transfer catalyst. 1.24 g (5.4 mmol) of the compound **3** and 0.25 g (1.4 mmol) of 2-hydroxycarbazole (**5**) were heated till reflux in 50 ml of THF. Then 0.23 g (4.1 mmol) of powdered potassium hydroxide and a catalytic amount of TBAHS were added to the mixture, and it was refluxed for 2 h. After TLC control the mixture was filtered, the solvent was evaporated and the product was purified by column chromatography with silica gel using the mixture of ethyl acetate and hexane (vol. ratio 1:15) as an eluent. Yield: 65.2 % (0.58 g) of white crystals.

MS (APCI<sup>+</sup>, 20 V): 654.34 ([M+H], 100 %). <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.20-8.14 (m, 3H, Ar), 8.09-7.98 (m, 2H, Ar), 7.59-7.43 (m, 6H, Ar), 7.39-7.27 (m, 7H, Ar), 6.87 (dd, 1H, *J*<sub>1</sub> = 2.1 Hz, *J*<sub>2</sub> = 6.6 Hz, Ar), 6.79 (d, 1H, *J* = 1.8 Hz, Ar), 4.40 (tr, 2H, *J* = 7.2 Hz, NCH<sub>2</sub>),

4.32-4.14 (m, 4H, 2×NCH<sub>2</sub>), 4.02 (tr, 2H, *J* = 6.3 Hz, OCH<sub>2</sub>), 2.14-1.84 (m, 8H, 3×NCH<sub>2</sub>CH<sub>2</sub>, OCH<sub>2</sub>CH<sub>2</sub>), 1.71-1.46 (m, 4H, 2×NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>).

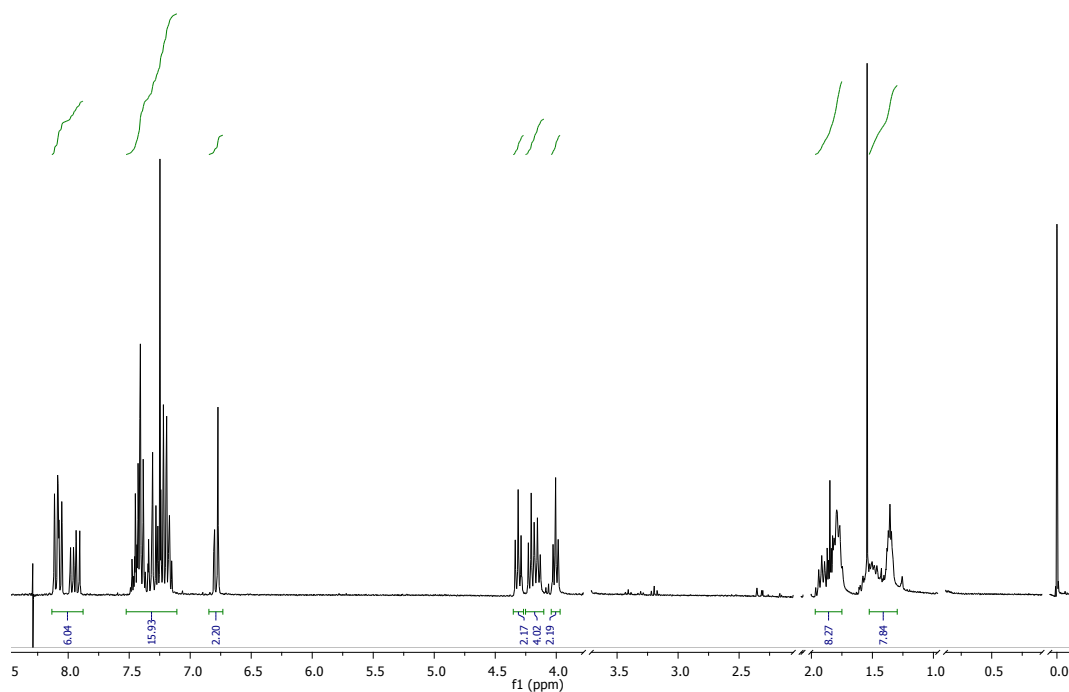


**Figure S2.** NMR spectra of compound **7**.

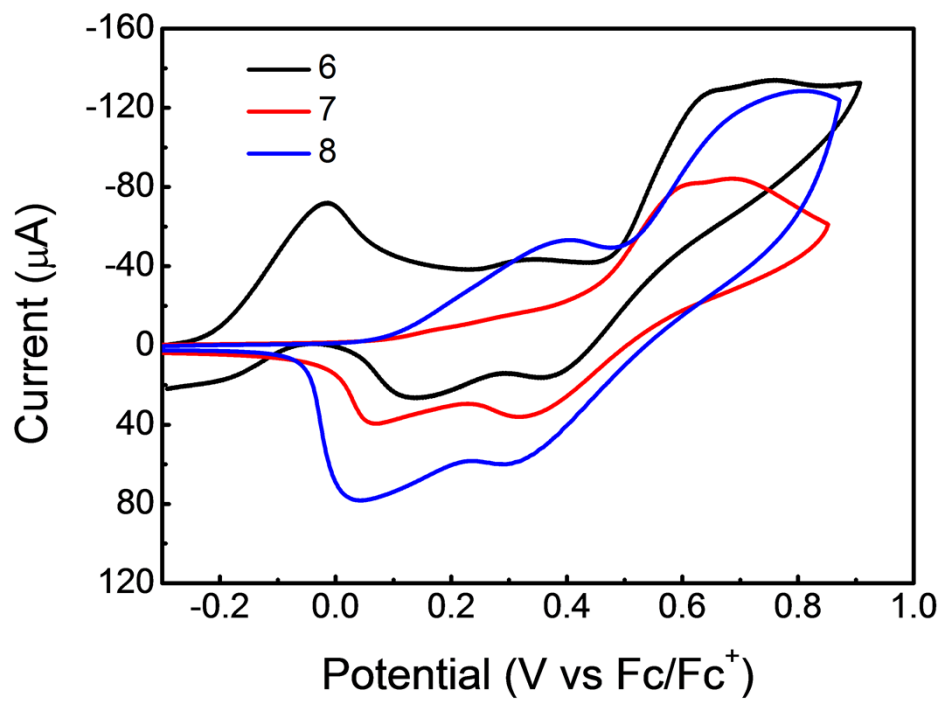
**2-[6-(carbazol-9-yl)hexyloxy]-9-[6-(carbazol-9-yl)hexyl]carbazole (8)** was prepared by the reaction of 2-hydroxycarbazole (**5**) with excess of 9-(6-bromohexyl)carbazole (**4**) under basic conditions in the presence of TBAHS phase transfer catalyst. 1.8 g (5.5 mmol) of the compound **4** and 0.25 g (1.4 mmol) of 2-hydroxycarbazole (**5**) were heated till reflux in 50 ml of THF. Then 0.23 g (4.1 mmol) of powdered potassium hydroxide and a catalytic amount of TBAHS were added to the mixture, and it was refluxed for 3 h. After TLC control the mixture was filtered, the solvent was evaporated and the product was purified by column chromatography with silica gel using the mixture of ethyl acetate and hexane (vol. ratio 1:30) as an eluent. Yield: 67.7 % (0.63 g) of white amorphous substance.

MS (APCI<sup>+</sup>, 20 V): 682.38 ([M+H], 100 %). <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, δ, ppm): 8.10-7.85 (m, 6H, Ar), 7.49-7.08 (m, 16H, Ar), 6.81-6.72 (m, 2H, Ar), 4.28 (tr, 2H, *J* = 7.2 Hz,

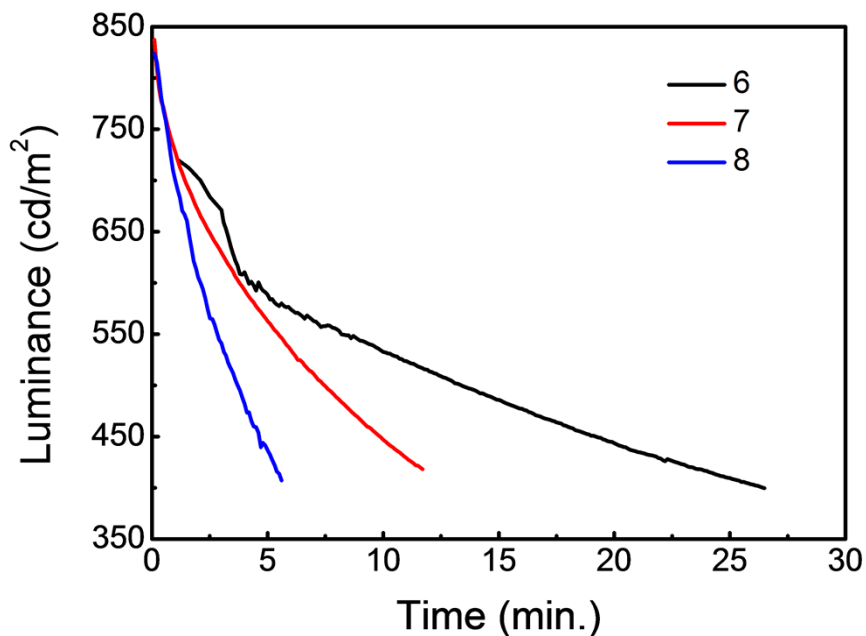
NCH<sub>2</sub>), 4.21-4.08 (m, 4H, 2×NCH<sub>2</sub>), 3.97 (tr, 2H, *J*=6.3Hz, OCH<sub>2</sub>), 1.93-1.70 (m, 8H, 3×NCH<sub>2</sub>CH<sub>2</sub>, OCH<sub>2</sub>CH<sub>2</sub>), 1.50-1.26 (m, 8H, 3×NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>, OCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>).



**Figure S3.** NMR spectra of compound **8**.



**Figure S4.** Cyclic voltammetric scans of the host compounds **6**, **7** and **8** in acetonitrile with an electrolyte containing a  $10^{-2}$  M silver nitrate, and a  $10^{-1}$  M tetra-butyl ammonium phosphate as the supporting electrolyte.



**Figure S5.** Devices operational lifetime by employing the compounds **6**, **7** and **8** as host. The operational lifetime of all devices were investigated without encapsulation. The operational lifetime of compound **6** and **7** based devices were investigated at  $800 \text{ cdm}^{-2}$ , while compound **6** based device was investigated at  $740 \text{ cdm}^{-2}$ . Here, we have plotted the real operational lifetime of compounds, **6** and **7**, while interpolated plot of compound **6**.

## References

1. X. Wang, R. Yue, B. Lu, Z. Wei, J. Xu, *J. Mater. Sci.* 45 (2010) 1963.