Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Microporous Polycarbazole Frameworks with Large Conjugated π System for Cyclohexane Separation from Cyclohexane-Containing Mixtures

Liangji Chen,[a] Hao Zhang,[a] Yingxiang Ye,[a] Zhen Yuan,[a] Jiaqi Wang,[a] Yisi Yang,[a] Si Lin,[a] Fahui Xiang,[a] Shengchang Xiang*[a] and Zhangjing Zhang*[a]

a. Fujian Provincial Key Laboratory of Polymer Materials, College of Chemistry and Materials Science, Fujian Normal University, 32 Shangsan Road, Fuzhou 350007, PR China

CONTENTS

Figure S1. FT-IR spectra of **BCz** and **FJU-P6**.....**S2**
Figure S2. FT-IR spectra of **DCzPh** and **FJU-P7**.....**S2**
Figure S3. SEM pictures of (a) **FJU-P6** and (b) **FJU-P7**.....**S3**
Figure S4. PXRD patterns of **FJU-P6** and **FJU-P7**.....**S3**
Figure S5. TGA curves of **FJU-P6** and **FJU-P7**.....**S4**
Figure S6. BET plots for **FJU-P6**.....**S4**
Figure S7. BET plots for **FJU-P7**.....**S4**
Figure S8. The pore-size distribution (PSD) of **FJU-P6** and **FJU-P7**.....**S5**
Figure S9. CO_2 adsorption isotherms of **FJU-P6** and **FJU-P7** at 273 K.....**S5**
Figure S10. DSLF fitting of the vapors sorption data at 294 K on **FJU-P6** and **FJU-P7**.....**S6**
Figure S11. IAST selectivities for equivalent C_6H_6/C_6H_{12} and C_6H_{10}/C_6H_{12} of **FJU-P6** and **FJU-P7** at 294 K.....**S6**
Table S1. Equation parameters for the DSLF isotherm model.....**S6**
Figure S12. Electrostatic potential maps around of monomers and adsorbates..... **S7**
Figure S13. C-H···π interaction geometries for monomers with adsorbates.....**S8**

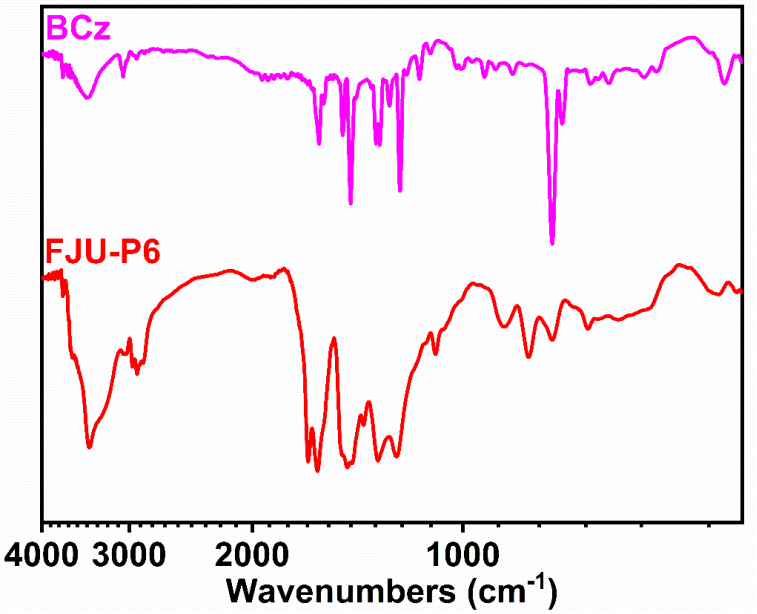

Figure S1. FT-IR spectra of **BCz** and **FJU-P6**.

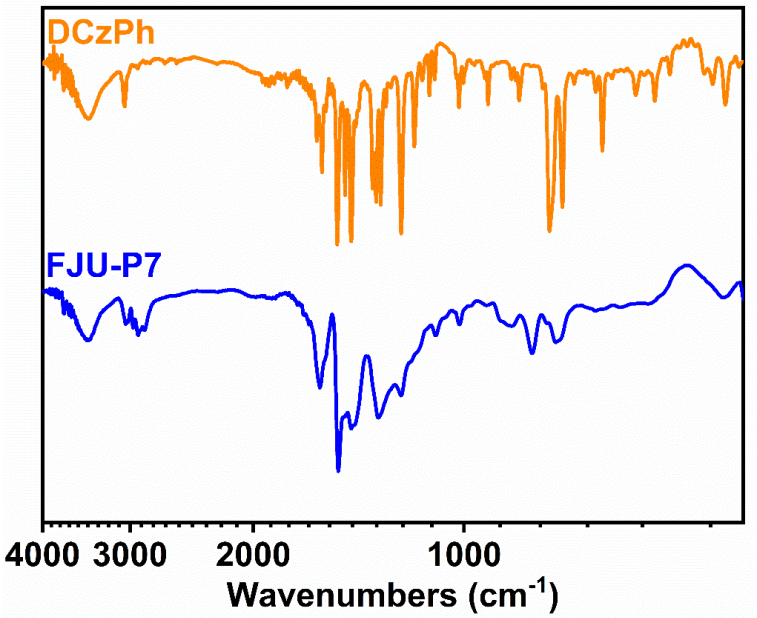

Figure S2. FT-IR spectra of **DCzPh** and **FJU-P7**.

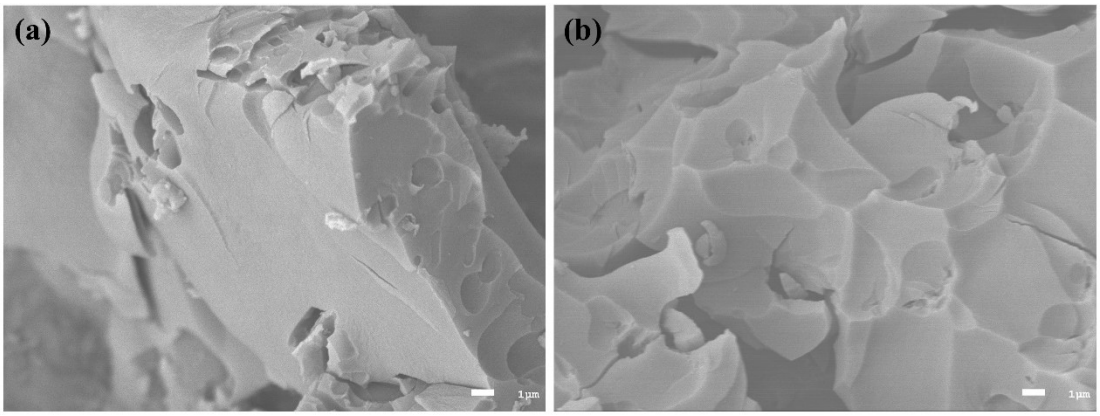

Figure S3. SEM pictures of (a) **FJU-P6** and (b) **FJU-P7**.

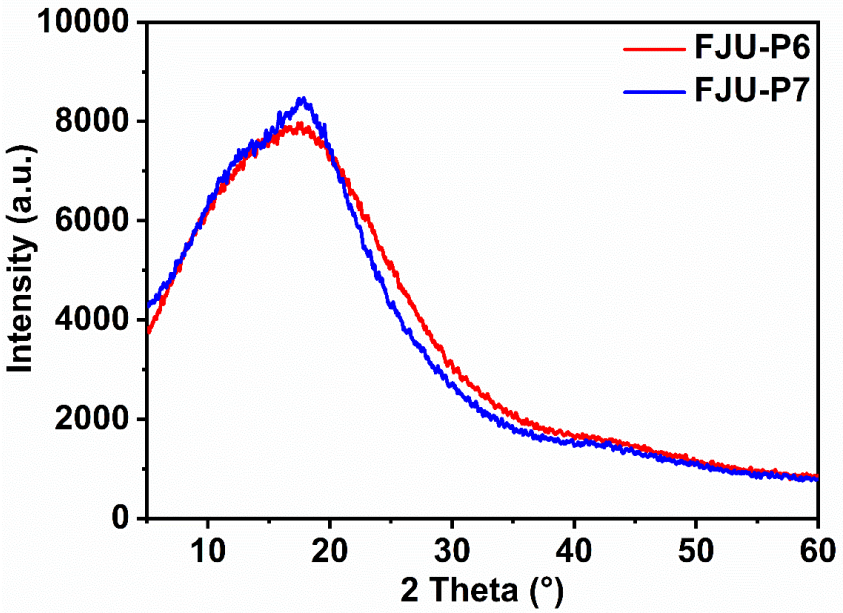

Figure S4. PXRD patterns of **FJU-P6** and **FJU-P7**.

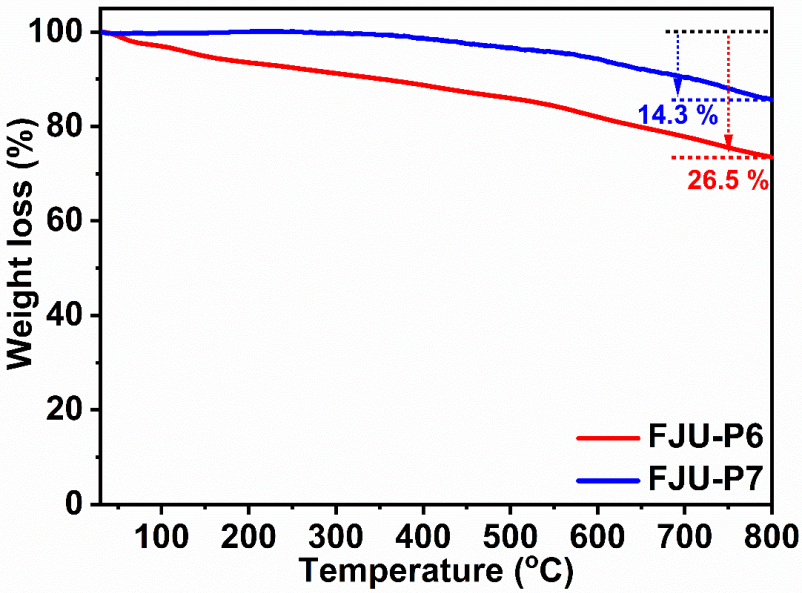

Figure S5. TGA curves of **FJU-P6** and **FJU-P7**.

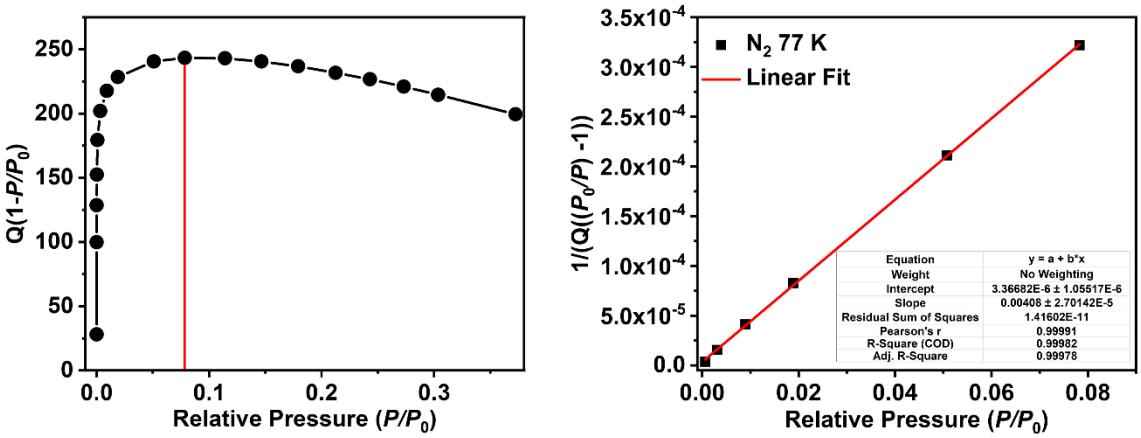

Figure S6. BET plots for **FJU-P6**. Points are selected based on the first consistency criterion.

S_{BET}=1/(3.36682×10^{-6}+0.00408)/22414×6.023×10^{23} ×0.162×10^{-18} =1066 m^2 g^{-1}

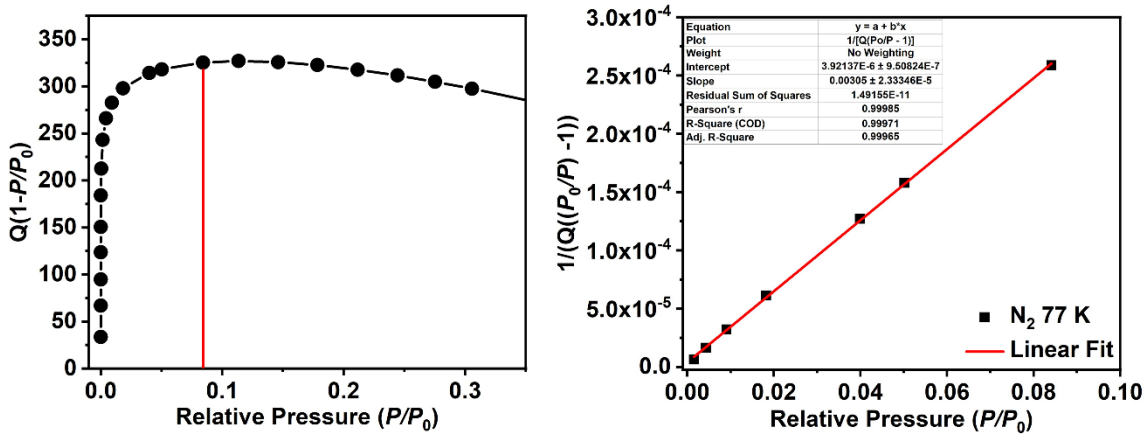

Figure S7. BET plots for **FJU-P7**. Points are selected based on the first consistency criterion.

S_{BET}=1/(3.92137×10^{-6}+0.00305)/22414×6.023×10^{23} ×0.162×10^{-18} =1425 m^2 g^{-1}

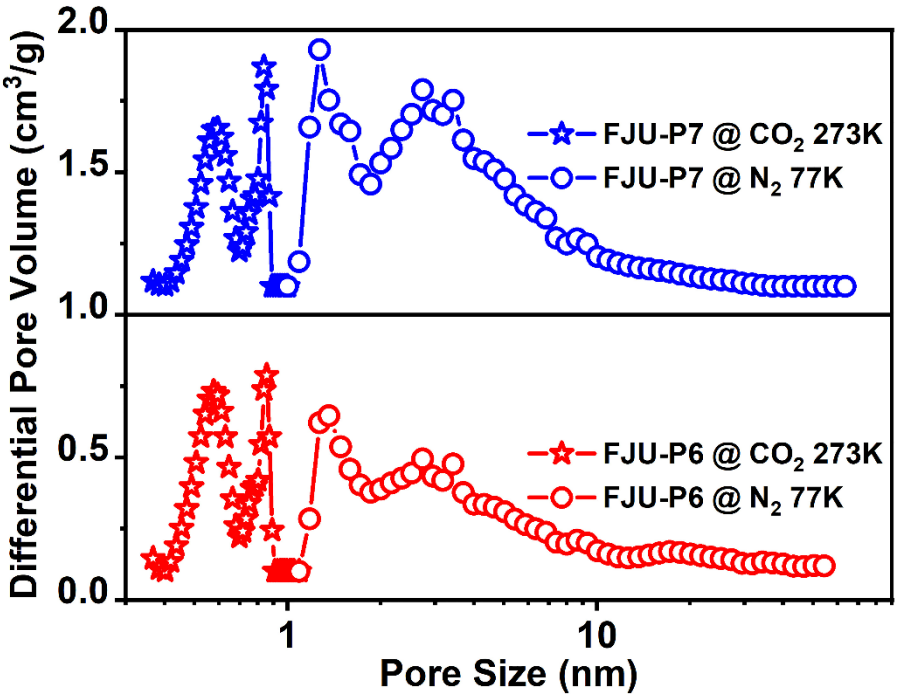

Figure S8. The pore-size distribution (PSD) of **FJU-P6** and **FJU-P7** from the 273 K CO_2 and 77 K N_2 isotherms based on the no-local density functional theory (NLDFT) model.

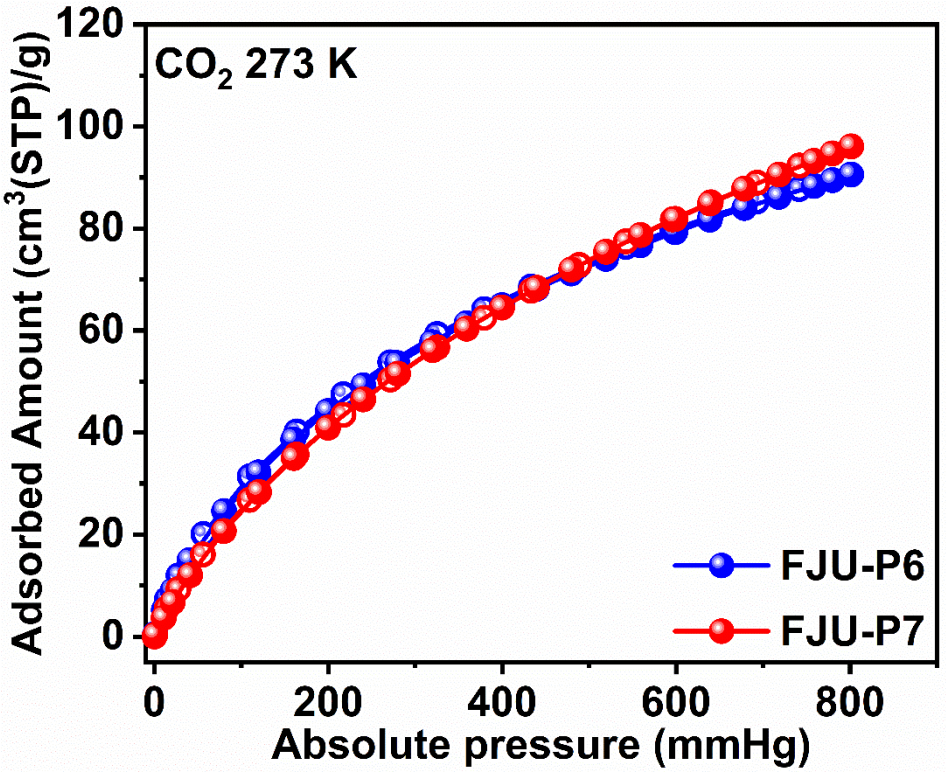

Figure S9. CO_2 adsorption isotherms of **FJU-P6** (red) and **FJU-P7** (blue) at 273 K.

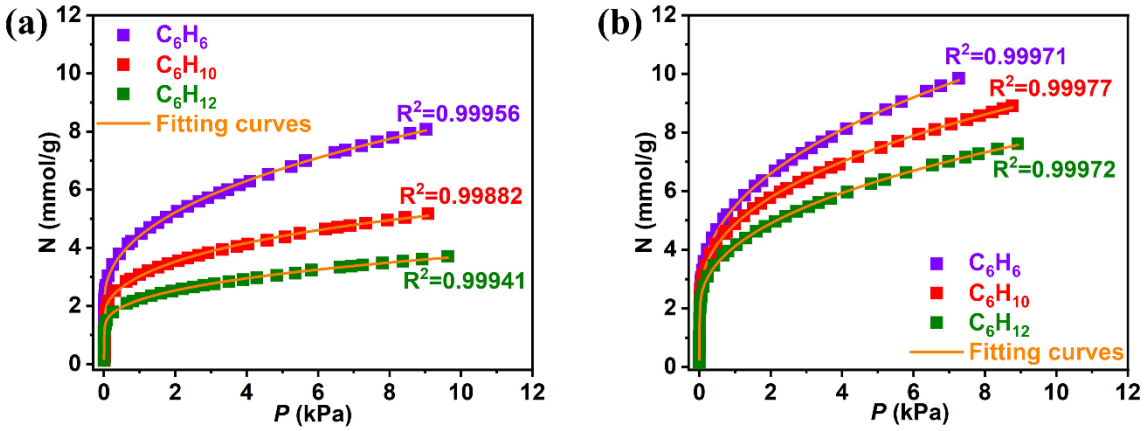

Figure S10. DSLF fitting of the C_6H_6 (violet), C_6H_{10} (red) and C_6H_{12} (olive) sorption data at 294 K on **FJU-P6** (a) and **FJU-P7** (b).

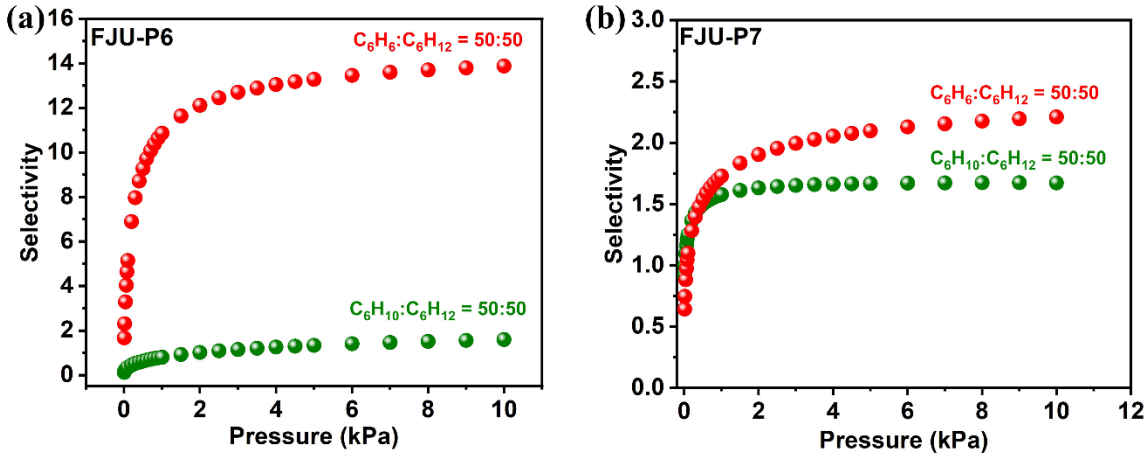

Figure S11. IAST selectivities for equivalent C_6H_6/C_6H_{12} (red) and C_6H_{10}/C_6H_{12} (olive) of **FJU-P6** (a) and **FJU-P7** (b) at 294 K.

Table S1. Equation parameters for the DSLF isotherm model.

Polymers	Adsorbates	N_1^{max} (mmol g^{-1})	b_1 (kPa^{-1})	$1/n_1$	N_2^{max} (mmol g^{-1})	b_2 (kPa^{-1})	$1/n_2$
FJU-P6	benzene	2.02758	9122.53765	1.71824	212.92323	0.01131	0.42889
	cyclohexene	1.68155	3.47291E8	5.64168	10.64258	0.14395	0.54079
	cyclohexane	1.12413	946.0946	1.24002	144.52421	0.00758	0.37874
FJU-P7	benzene	2.24083	10744.94006	2.04497	168.13274	0.01962	0.44012
	cyclohexene	2.17533	2181.68026	1.56111	166.3786	0.01962	0.4296
	cyclohexane	1.83063	1685.06854	1.41181	219.64403	0.01053	0.42814

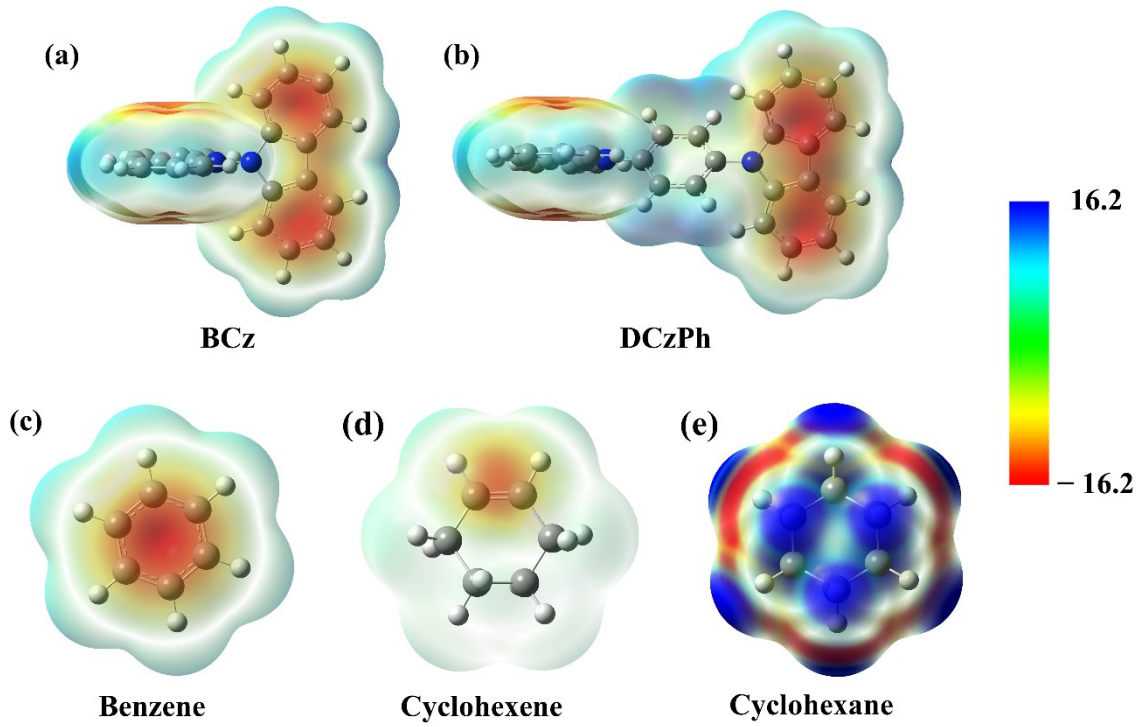

Figure S12. Electrostatic potential maps around of (a) **BCz**, (b) **DCzPh**, (c) benzene, (d) cyclohexene and (e) cyclohexane. The gradation on the scale bar is in kcal mol^{-1}.

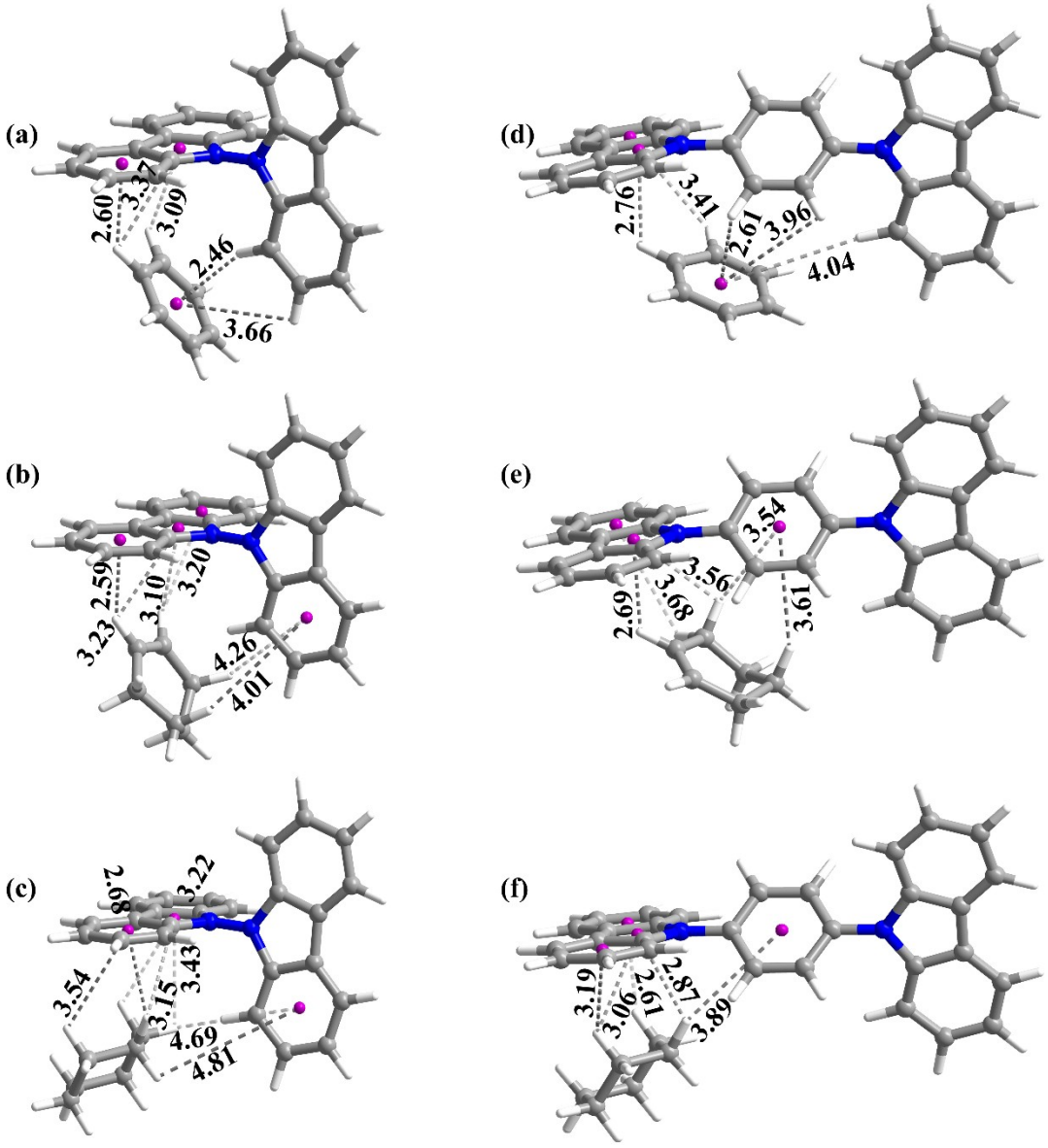

Figure S13. C-H···π interaction geometries for **BCz** with (a) benzene, (b) cyclohexene, (c) cyclohexane, and **DCzPh** with (d) benzene, (e) cyclohexene, (f) cyclohexane. Dot lines indicate C−H···π interactions, the unit of distance is Å. (C gray, N blue, H white, dummy atom: center of the arene ring, violet).