

## Supporting Information

### Flexible Porous Organic Polymers Constructed by C(sp<sup>3</sup>)-C(sp<sup>3</sup>) Coupling Reaction and Their High Methane-Storage Capacity

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## Experimental Procedures

### 1. Chemicals:

All reagents and anhydrous solvents of analytical purity were commercially available and used as received unless otherwise indicated, including 4-bromomethyl biphenyl (98%, Aladdin), 1,2-bis(bromomethyl)benzene (98%, Aladdin), 1,3-bis(bromomethyl)benzene (98%, Aladdin), 1,4-bis(bromomethyl)benzene (99%, 3A Chemicals), 4,4'-bis(bromomethyl)biphenyl (98%, Aladdin), 1,3,5-tris(bromomethyl)benzene (99%, Acros), 1,2,4,5-tetrakis(bromomethyl)benzene (98%, Aladdin), tetraphenylmethane (98%, Aladdin), titanium tetrabromide (98%, Aladdin), cis,cis-1,5-Cyclooctadiene (COD) (99%, Acros), 2,2'-bipyridine (99%, Acros), nickel bis(1,5-cyclooctadiene) ( $\text{Ni}(\text{COD})_2$ ) (99%, Aladdin), bromomethoxy methane (99%, Aladdin), 2,2':6',2''-terpyridine (99%, Sigma-Aldrich), hexamethylphosphoric triamide (HMPA) (99%, Sigma-Aldrich), nickel(II) chloride (98%, Aladdin), copper(I) iodide (98%, Aladdin), samarium (Sm) (99%, Acros) and zinc (Zn) (99%, Acros). Hydrochloric acid, tetrahydrofuran (THF), dimethylformamide (DMF), acetonitrile, methylene chloride and other solvents are supplied from local dealer.

### 2. Synthesis of 1,2-bis(diphenyl) ethane

**Synthesized by  $\text{Ni}(\text{COD})_2$  catalytic system:** 4-Bromomethyl biphenyl (0.124 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) ( $\text{Ni}(\text{COD})_2$ ) (0.080 g, 0.3 mmol), 2,2'-bipyridine (0.047 g, 0.3 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.033g, 0.3 mmol) in N,N-dimethylformamide (DMF) (1 mL) and tetrahydrofuran (THF) (2 mL). The reaction mixture was heated at 60 °C for 5 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 30 °C to yield 1,2-bis(diphenyl) ethane as a white powder (0.067 g, 98% yields)<sup>1</sup>

**Synthesized by  $\text{CuI}/\text{Sm}$  catalytic system:** 4-Bromomethyl biphenyl (0.124 g, 0.5 mmol) were added to a mixture solution of CuI (0.095 g, 0.5 mmol), Sm (0.075 g, 0.5 mmol) in tetrahydrofuran (THF) (2 mL). The reaction mixture was heated at 80 °C for 48 h under nitrogen protection. After cooling to room temperature, 5 M HCl/ $\text{HNO}_3$  solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 30 °C to yield 1,2-bis(diphenyl) ethane (0.013 g, 19% yields)<sup>3</sup>

**Synthesized by  $\text{NiCl}_2/\text{Sm}$  catalytic system:** 4-Bromomethyl biphenyl (0.124 g, 0.5 mmol) were added to a mixture solution of  $\text{NiCl}_2$  (0.065 g, 0.5 mmol), Sm (0.075 g, 0.5 mmol), hexamethylphosphoric triamide (HMPA) (0.09g, 0.5mol) in tetrahydrofuran (THF) (2 mL). The reaction mixture was heated at 40 °C for 48 h under nitrogen protection. After cooling to room temperature, 3 M HCl/ $\text{HNO}_3$  solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 30 °C to yield 1,2-bis(diphenyl) ethane (0.008 g, 13% yields)<sup>4</sup>

**Synthesized by  $\text{NiCl}_2/\text{Zn}$  catalytic system:** 4-Bromomethyl biphenyl (0.124 g, 0.5 mmol) were added to a mixture solution of  $\text{NiCl}_2$  (0.065 g, 0.5 mmol), Zn (0.033 g, 0.5 mmol), tpy (0.177g, 0.5mmol) in N,N-dimethylformamide (DMF) (2ml). The reaction mixture was heated at 40 °C for 48 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the

solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 30 °C to yield 1,2-bis(diphenyl) ethane (0.032 g, 48% yields)<sup>5</sup>

### 3. Synthesis of polymers

**P1** was synthesized by following method: 1,2-Bis(bromomethyl)benzene (0.132 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.160 g, 0.6 mmol), 2,2'-bipyridine (0.094 g, 0.6 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.065g, 0.6 mmol) in N,N-dimethylformamide (DMF) (3 mL) and tetrahydrofuran (THF) (5 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 30 °C to yield **P1** as a white powder (0.054 g, 85% yields)

**P2** was synthesized by following method: 1,3-Bis(bromomethyl)benzene (0.132 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.160 g, 0.6 mmol), 2,2'-bipyridine (0.094 g, 0.6 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.065g, 0.6 mmol) in N,N-dimethylformamide (DMF) (3 mL) and tetrahydrofuran (THF) (5 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water and ethanol. The products were then dried under vacuum for 12 h at 50 °C to yield **P2** as a white powder (0.044 g, 93% yields)

**P3** was synthesized by following method: 1,4-Bis(bromomethyl)benzene (0.132 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.160 g, 0.6 mmol), 2,2'-bipyridine (0.094 g, 0.6 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.065g, 0.6 mmol) in N,N-dimethylformamide (DMF) (3 mL) and tetrahydrofuran (THF) (5 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water, acetonitrile and methanol and subsequently dried under vacuum for 12 h at 80 °C to yield **P3** as a white powder (0.045 g, 95% yields)

**P4** was synthesized by following method: 4,4'-Bis(bromomethyl)biphenyl (0.170 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.160 g, 0.6 mmol), 2,2'-bipyridine (0.094 g, 0.6 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.065g, 0.6 mmol) in N,N-dimethylformamide (DMF) (3 mL) and tetrahydrofuran (THF) (5 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water, acetonitrile and methanol. The products were then purified by Soxhlet extraction with dichloromethane for 48 h and subsequently dried under vacuum for 12 h at 80 °C to yield **P4** as a white powder (0.088 g, 98% yields)

**PAF-64** was synthesized by following method: 1,3,5-Tris(bromomethyl)benzene (0.119 g, 0.33 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.160 g, 0.6 mmol), 2,2'-bipyridine (0.094 g, 0.6 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.065g, 0.6 mmol) in N,N-dimethylformamide (DMF) (3 mL) and tetrahydrofuran (THF) (5 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water, acetonitrile and methanol. The products were then purified by Soxhlet extraction with dichloromethane for 48 h and subsequently dried under vacuum for 12 h at 80 °C to yield **PAF-64** as a white powder (0.038 g, 97% yields)

**PAF-65** was synthesized by following method: 1,2,4,5-Tetrakis (bromomethyl)benzene (0.225 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.320 g, 1.2 mmol), 2,2'-bipyridine (0.186 g, 1.2 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.13g, 1.2 mmol) in N,N-dimethylformamide (DMF) (4 mL) and tetrahydrofuran (THF) (6 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After

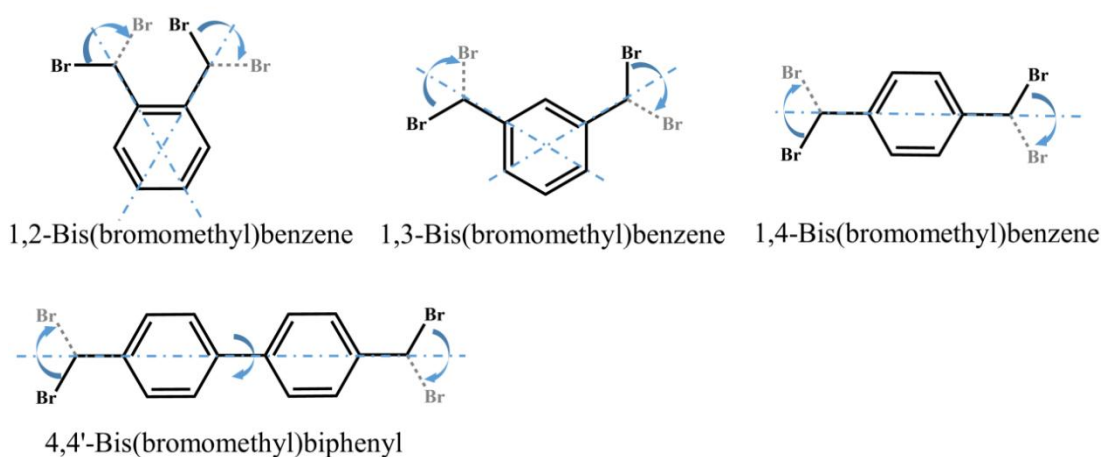
cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water, acetonitrile and methanol. The products were then purified by Soxhlet extraction with dichloromethane for 48 h and subsequently dried under vacuum for 12 h at 80 °C to yield **PAF-65** as a white powder (0.064 g, 98% yields)

**Tetrakis(4-(bromomethyl)phenyl)methane:** To a stirred solution of tetraphenylmethane (0.644 g, 2.00 mmol) and titanium tetrabromide (4.40 g, 12.0 mmol) in dichloromethane (20 mL), cooled in an ice-bath, than added dropwise bromomethoxymethane (2.5 g, 20.0 mmol). The mixture was stirred at room temperature for 24 h and then added bromomethoxymethane (2.5 g, 20.0 mmol) again for 48h. Lastly, water (20 mL) was added dropwise. The organic phase was separated and the aqueous phase was extracted with dichloromethane (20 mL×2). The organic phases were combined and washed with water (20 mL×2) and brine (20 mL), and dried over sodium sulfate. Upon removal of the solvent with a rota-vapor, the resulting residue was subjected to column chromatography (petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> 1:5) to give tetrakis(4-(bromomethyl)phenyl)methane as white solid (0.80 g, 57%).<sup>2</sup>

**PAF-66** was synthesized by following method: Tetrakis(4-(bromomethyl)phenyl)methane (0.346 g, 0.5 mmol) were added to a mixture solution of nickel bis(1,5-cyclooctadiene) (Ni(COD)<sub>2</sub>) (0.320 g, 1.2 mmol), 2,2'-bipyridine (0.186 g, 1.2 mmol), cis,cis-1,5-cyclooctadiene (COD) (0.13g, 1.2 mmol) in N,N-dimethylformamide (DMF) (6 mL) and tetrahydrofuran (THF) (12 mL). The reaction mixture was heated at 60 °C for 24 h under nitrogen protection. After cooling to room temperature, 2 M HCl solution were added to remove impurities from catalysts, and the solid products were filtered and washed with water, acetonitrile and methanol. The products were then purified by Soxhlet extraction with dichloromethane for 48 h and subsequently dried under vacuum for 12 h at 80 °C to yield **PAF-66** as a white powder (0.178 g, 96% yields)

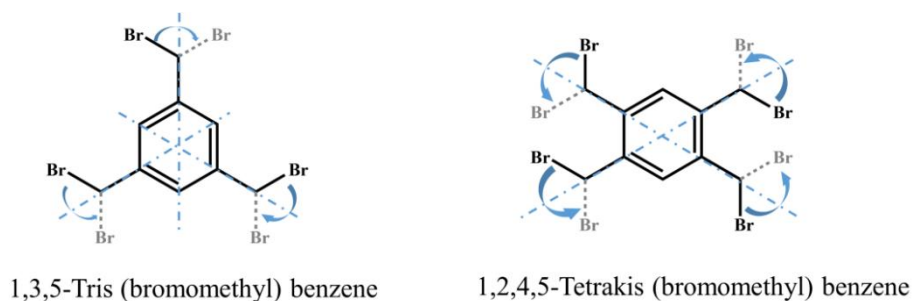
#### 4. Calculation of the flexibilization degree (D<sub>F</sub>)

##### D<sub>F</sub> calculation of one or two benzene monomers for linear polymers



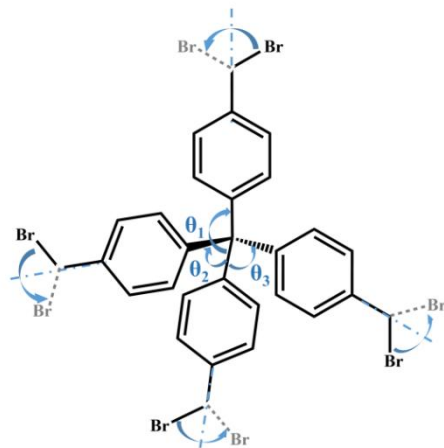
The relative flexibilization degree (D<sub>F</sub>) of the monomers of P1, P2, P3 and P4 containing one or two benzene rings are easy to determine. The diBr<sub>s</sub> of the monomers (1,2-bis(bromomethyl)benzene, 1,3-bis(bromomethyl)benzene, 1,4-bis(bromomethyl)benzene and 4,4'-bis(bromomethyl)biphenyl) can wave in a wide-angle range, offering them flexibility, respectively. The benzene rings in 4,4'-Bis(bromomethyl)biphenyl also can rotate around the central axis and offering it the higher flexibility.

##### D<sub>F</sub> calculation of one benzene monomers for three-dimensional porous polymers



The relative flexibilization degree ( $D_F$ ) of the monomers of PAF-64 and PAF-65 containing one benzene ring offering them the higher flexibility compare with linear polymers. Because more TrisBrs and TetraBrs of the monomers (1,3,5-Tris (bromomethyl) benzene) and 1,2,4,5-Tetrakis (bromomethyl) benzene) can wave in a wide-angle range, offering them the high and higher flexibility, respectively.

#### $D_F$ calculation of tetrahedral-like monomers for three-dimensional porous polymers



Tetrabromomethyl tetraphenyl methane

The relative flexibilization degree ( $D_F$ ) of the monomers of PAF-66 containing four benzene rings offering it highest flexibility, respectively. The flexibilization degree is 4, the same as the 1,3,5-Tris (bromomethyl) benzene or 1,2,4,5-Tetrakis (bromomethyl) benzene. Beyond that, another flexibilization degree ( $D_F$ ) of tetrahedral-like monomers is calculated by the following formula:

$$D_F = \sum_{i=1}^n \theta_i = \theta_1 + \theta_2 + \theta_3 + \dots + \theta_n$$

where  $\theta_i$  is the bond angle that can determine the spatial position of the benzene rings in building blocks. Specifically, the maximum vibration ranges of isolated benzene rings in tetrabromomethyl tetraphenyl methane are defined by three key bond angles, i.e.,  $\theta_1$ ,  $\theta_2$  and  $\theta_3$ .

$$D_F (\text{tetrabromomethyl tetraphenyl methane}) = \theta_1 + \theta_2 + \theta_3 = 328.12^\circ$$

#### 5 Packing density measurements

The packing density ( $\rho_p$ , also called tapped bulk density) of PAF-66 was calculated from the ratio of weight to volume. Briefly, a 1.5 ml measuring container with known mass was filled with the PAF-66 powder. After being tapped vertically 100 times, the volume and weight were recorded to calculate the packing density. As a result, the  $\rho_p$  for PAF-64 is 0.46 g/cm<sup>3</sup>. Similarly, the  $\rho_p$  for PAF-65 is 0.47 g/cm<sup>3</sup> and the  $\rho_p$  for PAF-66 is 0.50 g/cm<sup>3</sup> (Figure S22).

#### 6 Framework (skeletal) density measurements

The framework densities ( $d$ ) of PAF-64, PAF-65, PAF-66 were tested by XEMIS at room temperature and 10, 20, 30, 40, 50, 60, 70, 80, 90, 100 bar on the base of helium-buoyancy measurement. The  $d$  is 1.16 g/cm<sup>3</sup> for PAF-64, is 1.25 g/cm<sup>3</sup> for PAF-65 and is 1.32 g/cm<sup>3</sup> for PAF-66.

The volumetric uptake expressed as the volume of the ideal gas over the volume occupied by the same amount at a certain pressure was measured as follows  $V/V_0 = (V_0/g) * [1/(V_0 + 1/d)]$  where  $V_0$  corresponds to the pore volume known by N<sub>2</sub> adsorption at 77 K, and  $d$  corresponds to the sample density as mentioned above (Figure S26).

#### 7 Apparatuses and Procedures

The CH<sub>4</sub> absorption experiments were carried out using a XEMIS gravimetric microbalance at high pressure (up to 100 MPa). High pressure measurements (up to ~100 MPa) were conducted using a high-pressure view cell. The gravimetric microbalances (XEMIS) only require a small amount of sample (50-100mg) which was loaded into a

Pyrex sample container and dried under high vacuum prior to each experiment at 473 K for 12 h. XEMIS balance is controlled via magnetic coupling which can be studied precisely at high temperature and high pressures.

### Characterizations of linear polymers

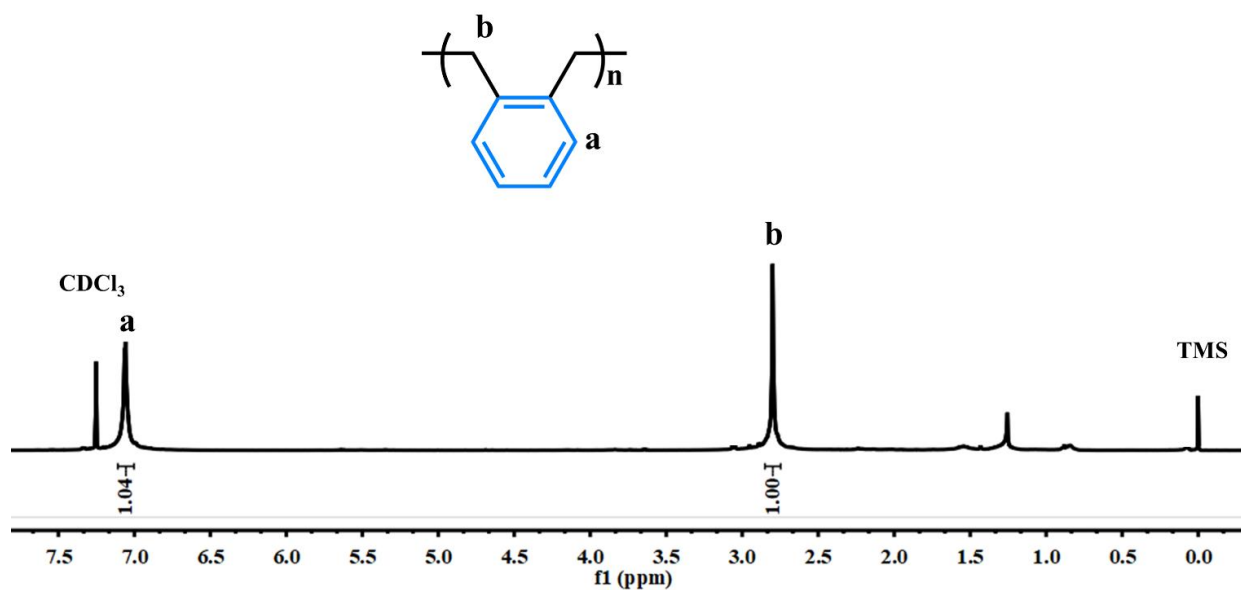


Figure S1. <sup>1</sup>H NMR spectrum of P1.

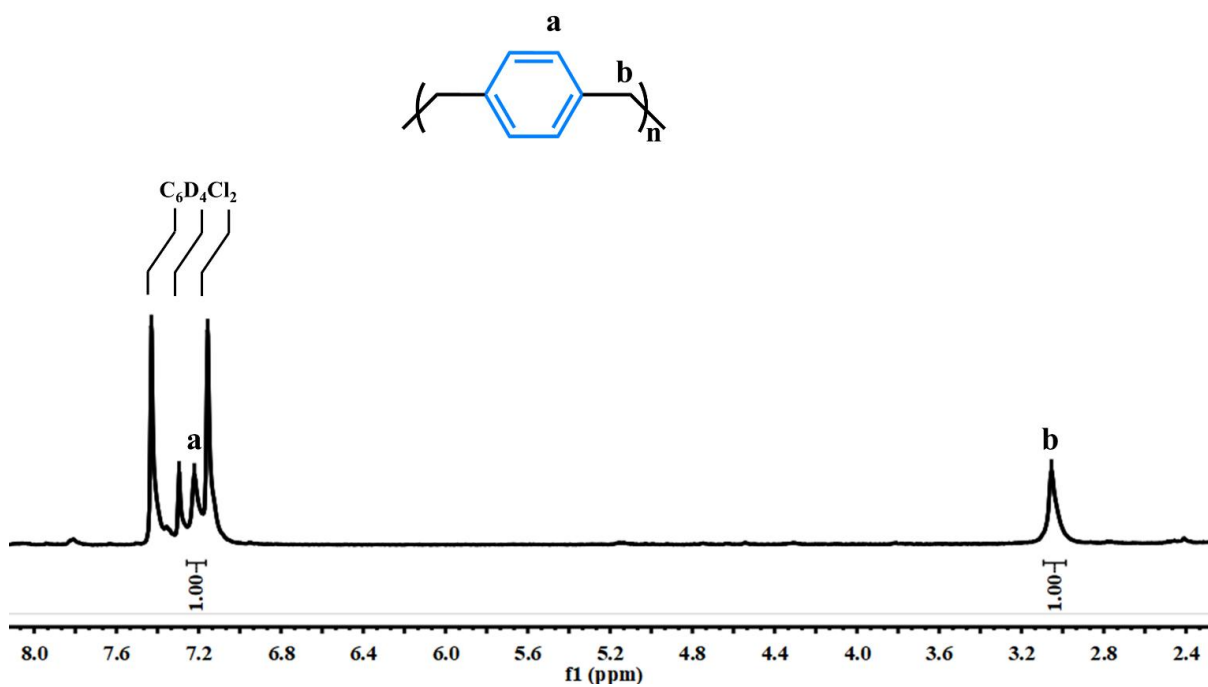


Figure S2.  $^1\text{H}$  NMR spectrum of P3.

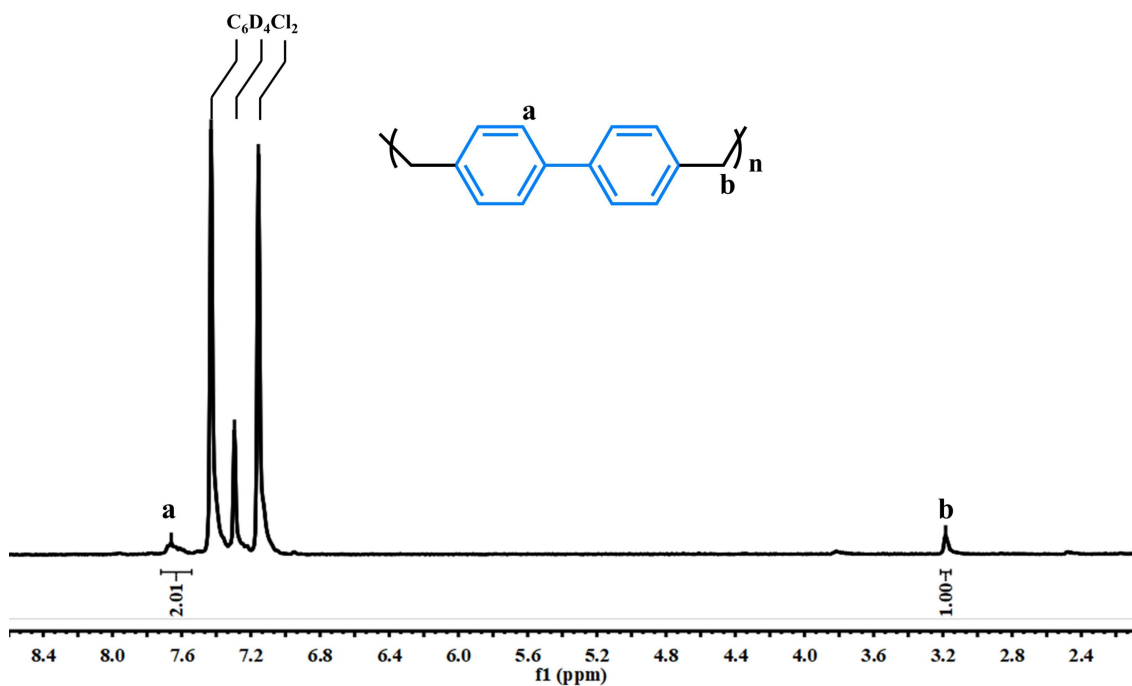
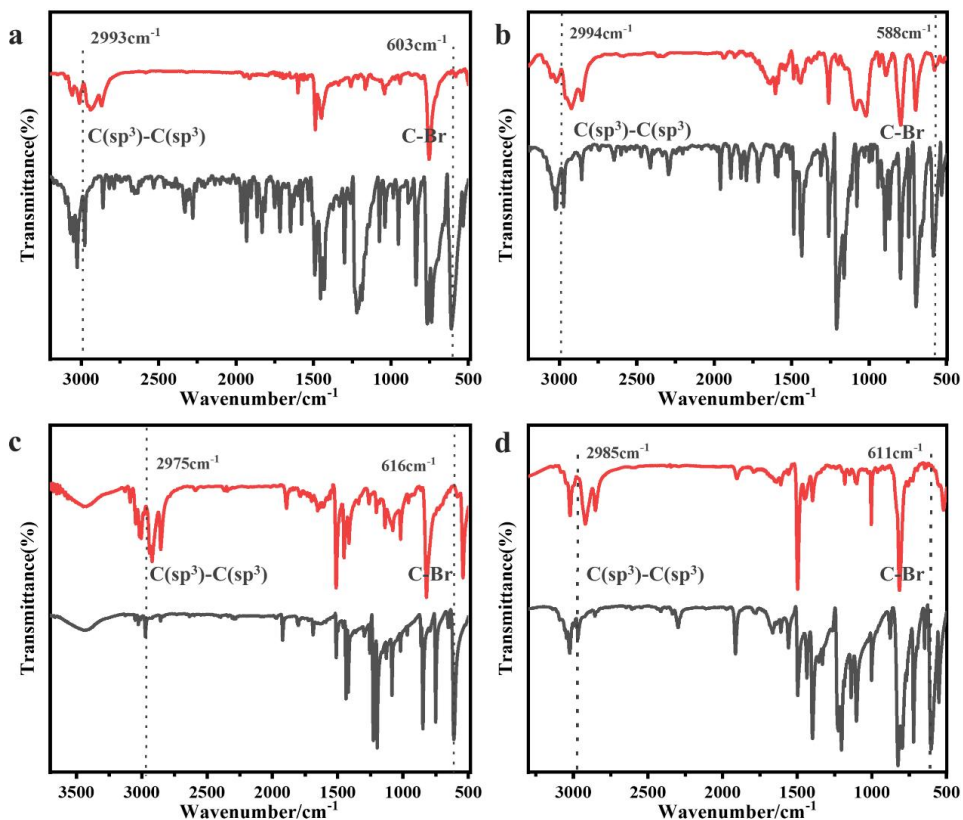
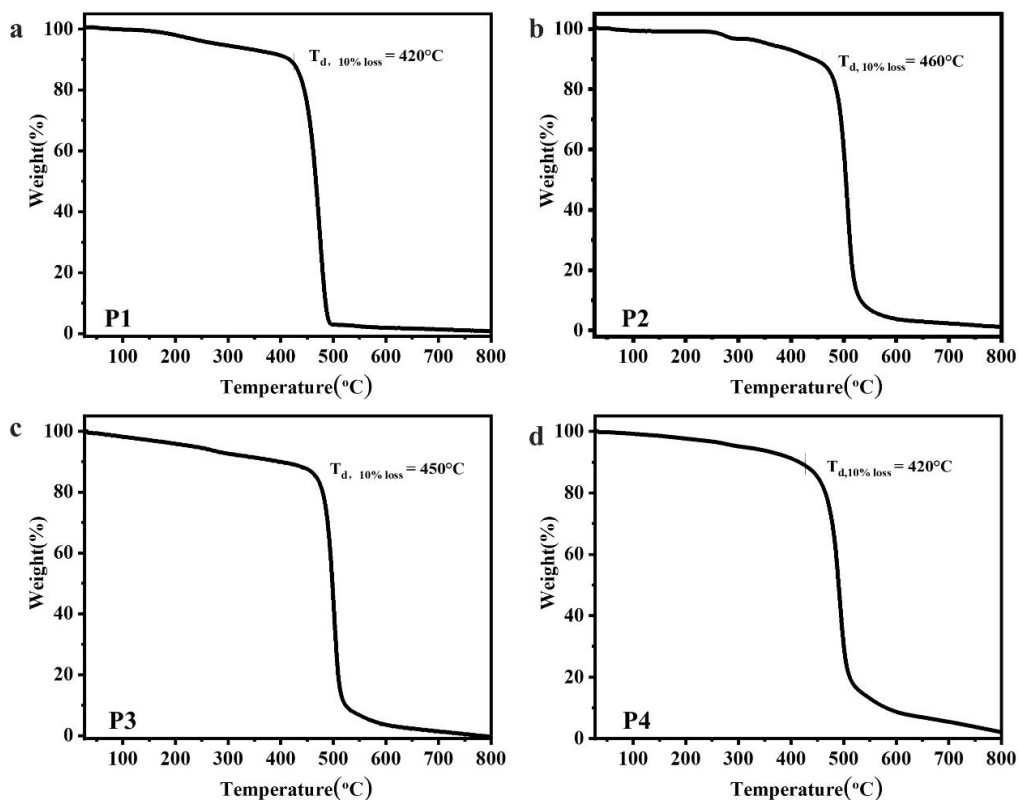


Figure S3.  $^1\text{H}$  NMR spectrum of P4.

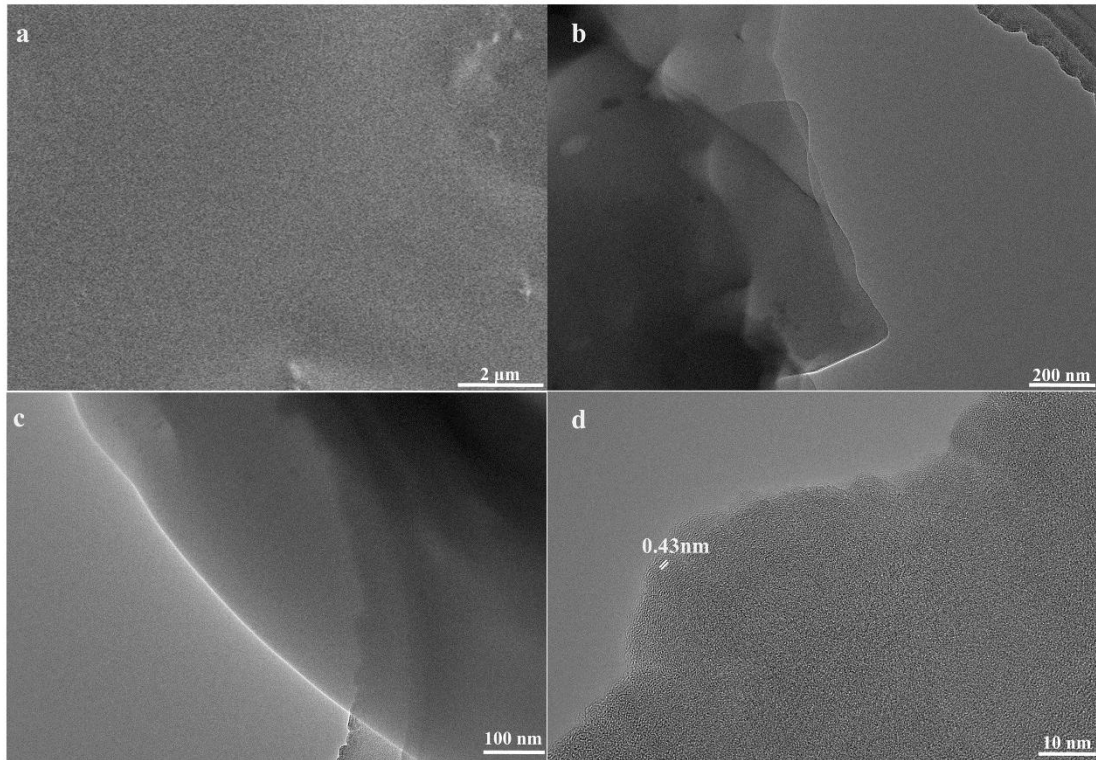


**Figure S4.** FTIR spectra of P1 (a), P2 (b), P3 (c) and P4 (d) and their monomer.

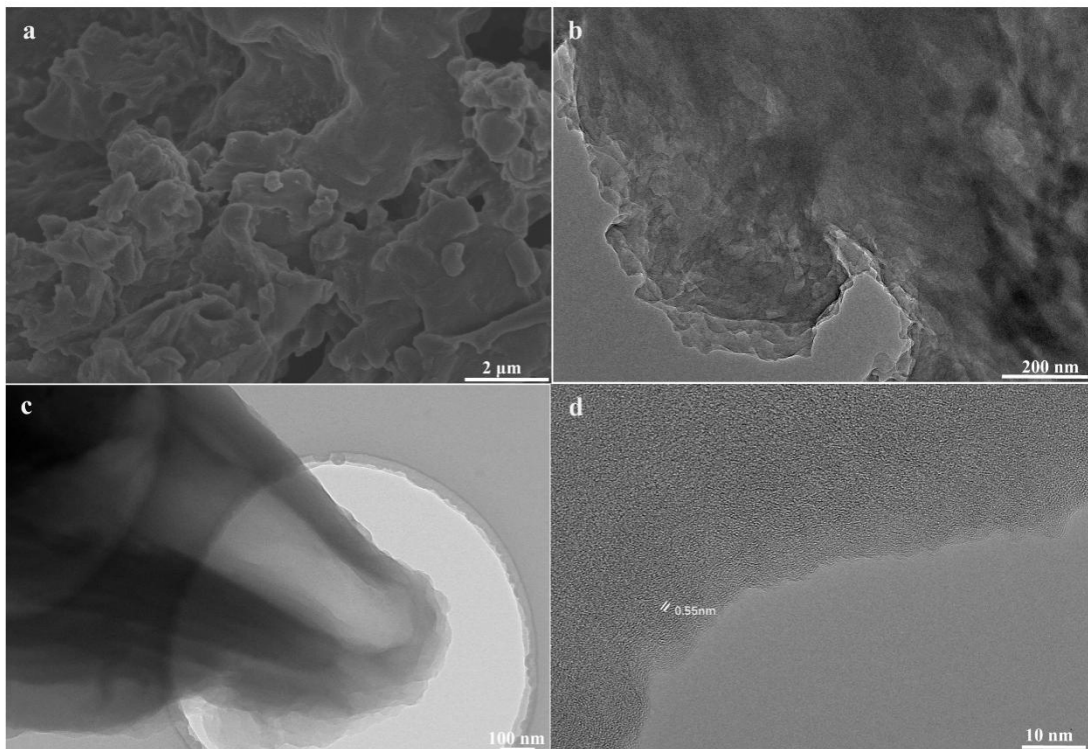


**Figure S5.** TGA curve of P1 (a), P2 (b), P3 (c) and P4 (d) under N<sub>2</sub>

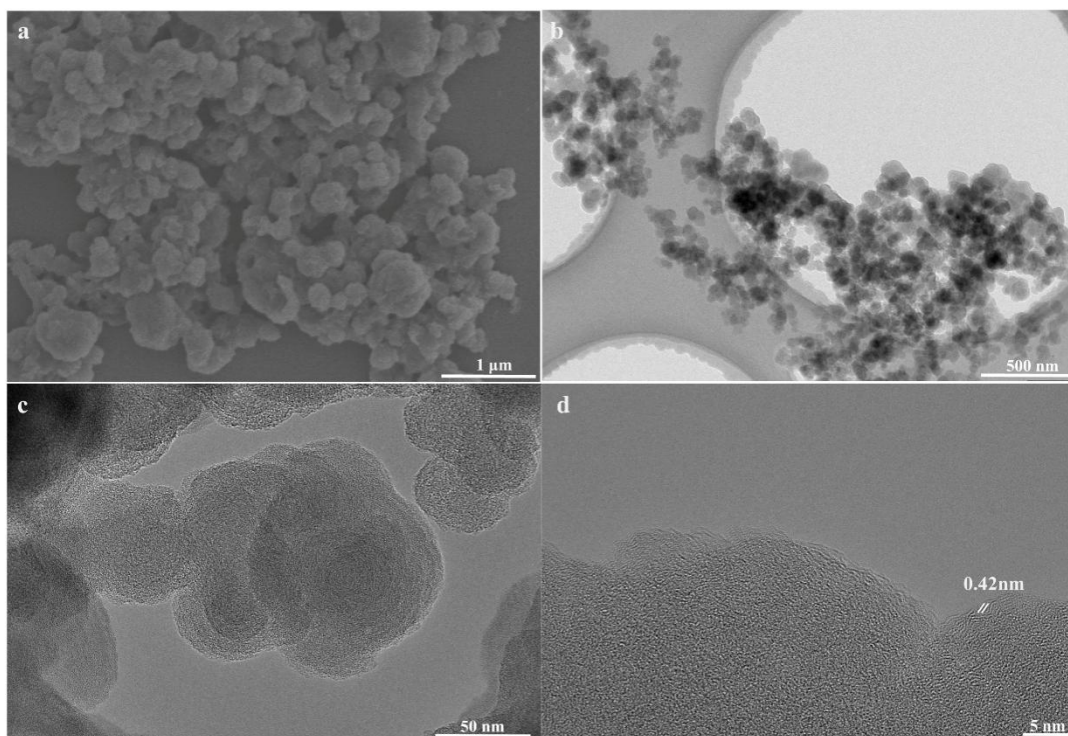




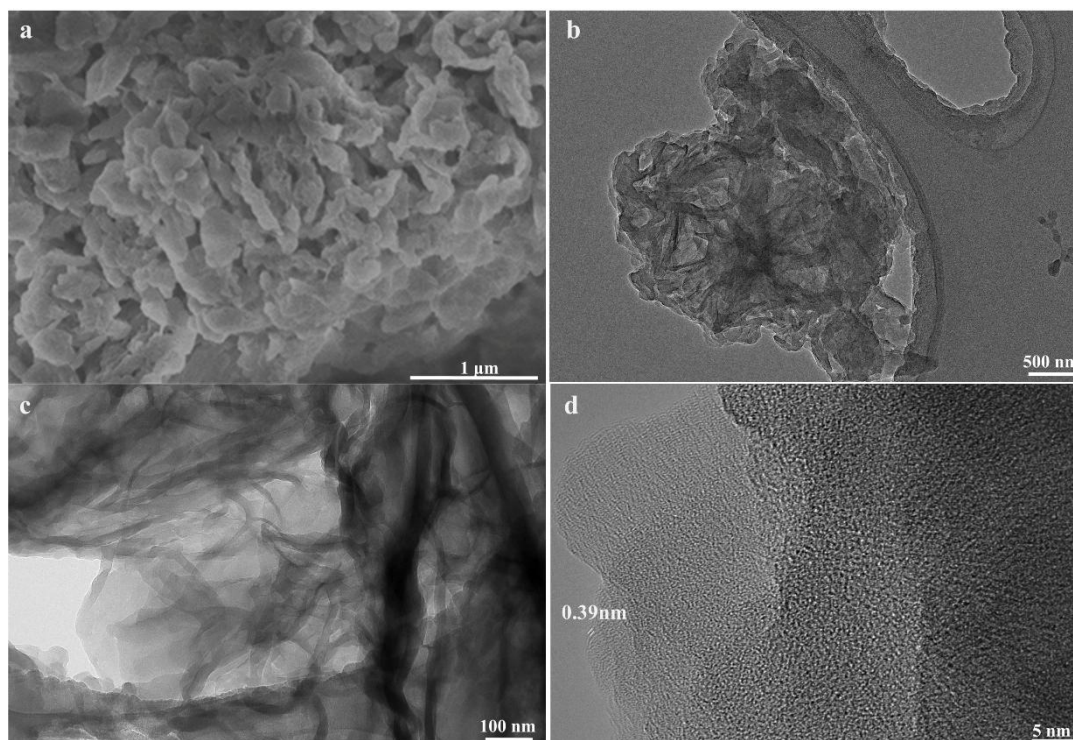
**Figure S6.** SEM images (a) and TEM images (b-d) for P1.



**Figure S7.** SEM images (a) and TEM images (b-d) for P2.



**Figure S8.** SEM images (a) and TEM images (b-d) for P3.



**Figure S9.** SEM images (a) and TEM images (b-d) for P4.

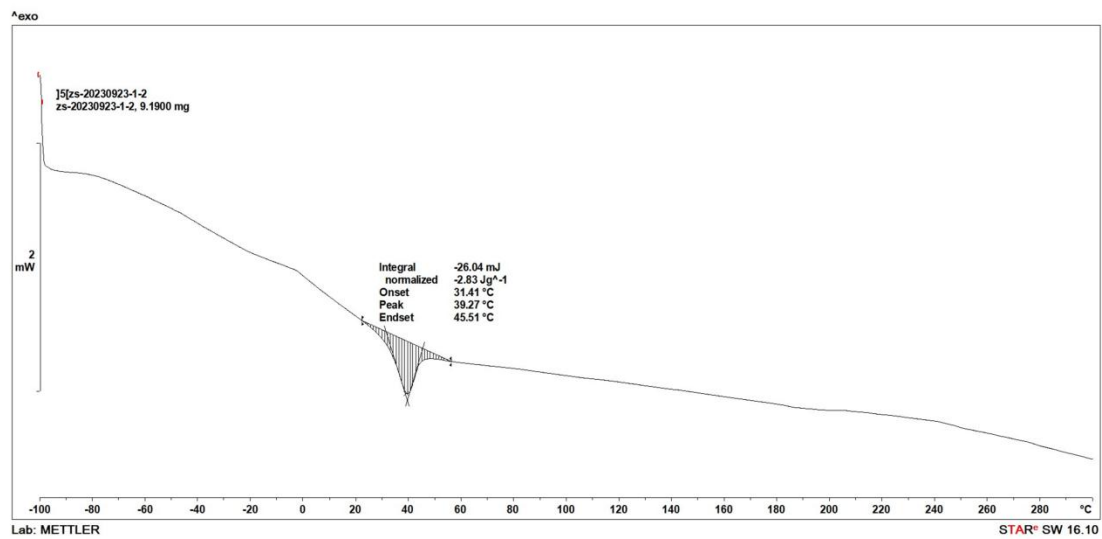


Figure S10. DSC curve of P1.

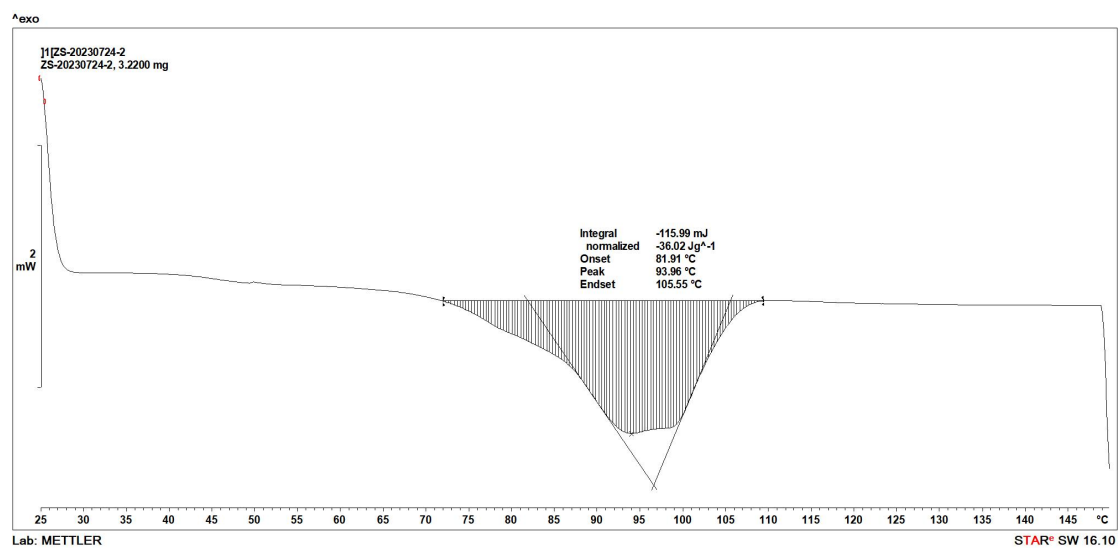
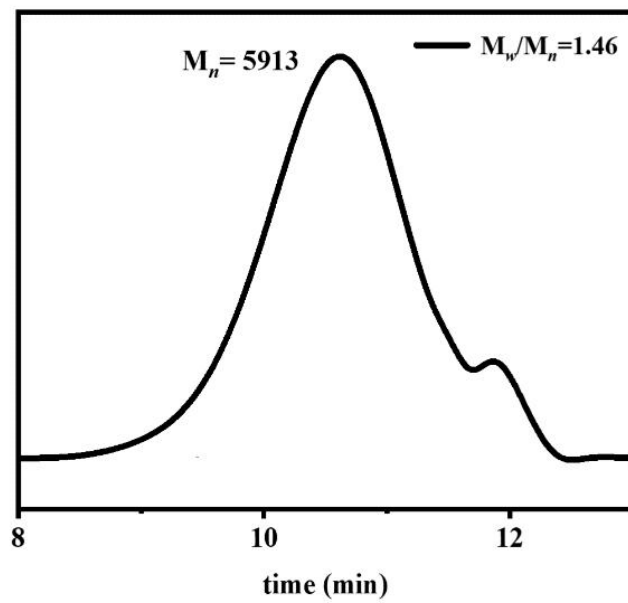
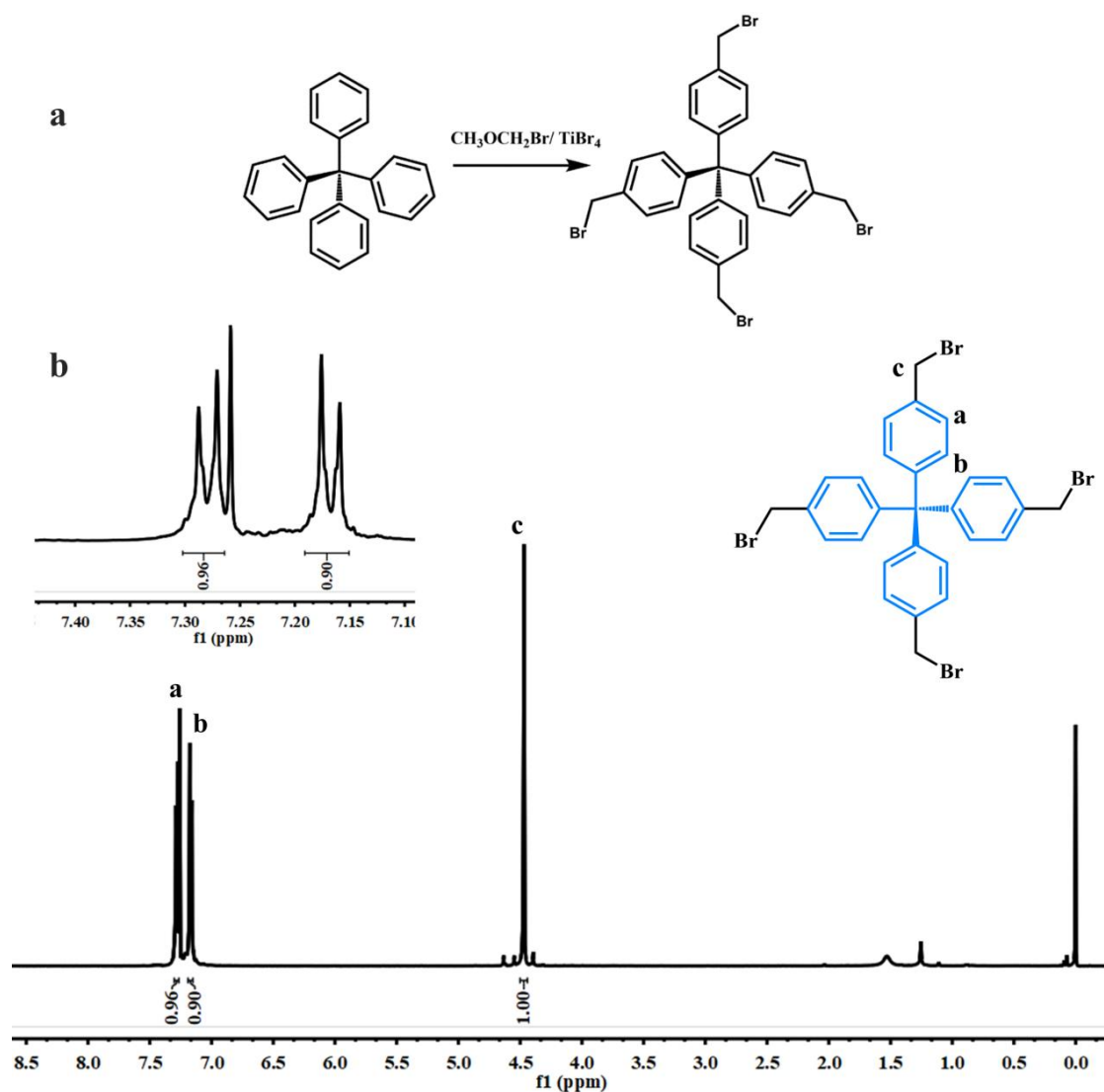


Figure S11. DSC curve of P2.

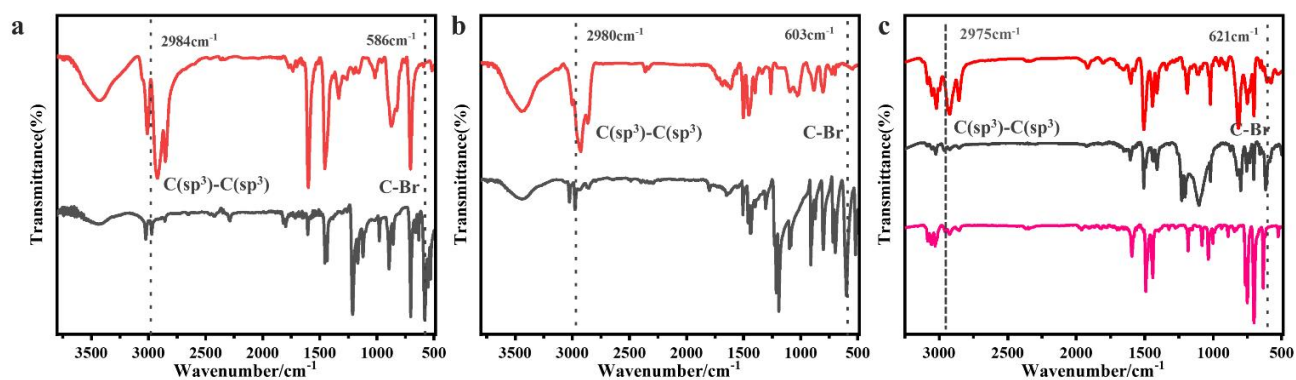


**Figure S12.** GPC curve of P1.

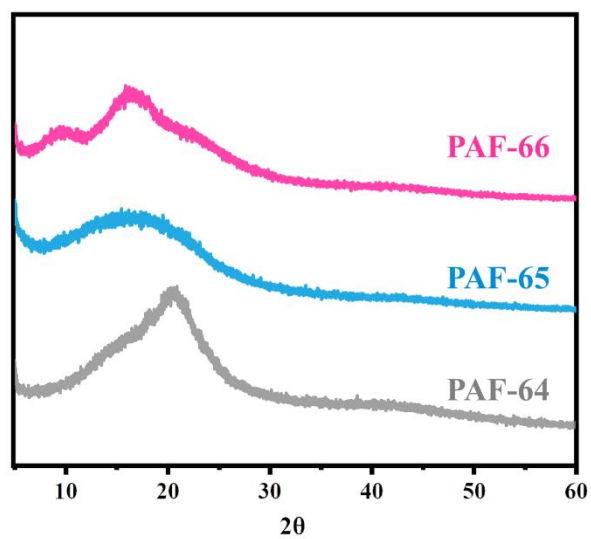
## Characterizations of porous polymers



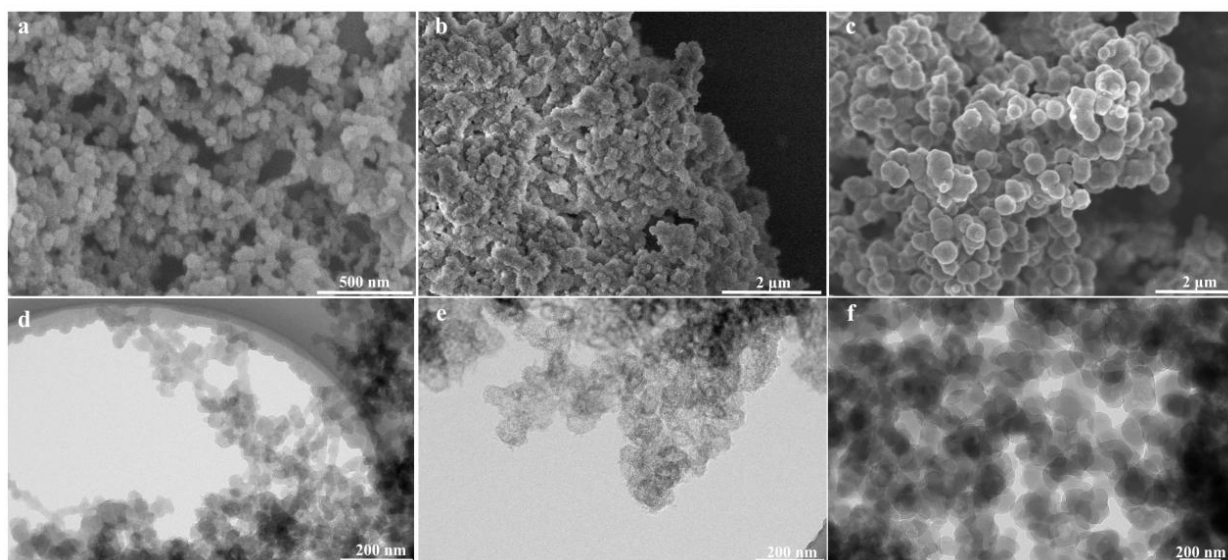
**Figure S13.** Synthesis (a) and  $^1\text{H}$  NMR spectrum (b) of tetrakis(4-(bromomethyl)phenyl)methane, ( $\text{CDCl}_3$ ,  $25^\circ\text{C}$ ).



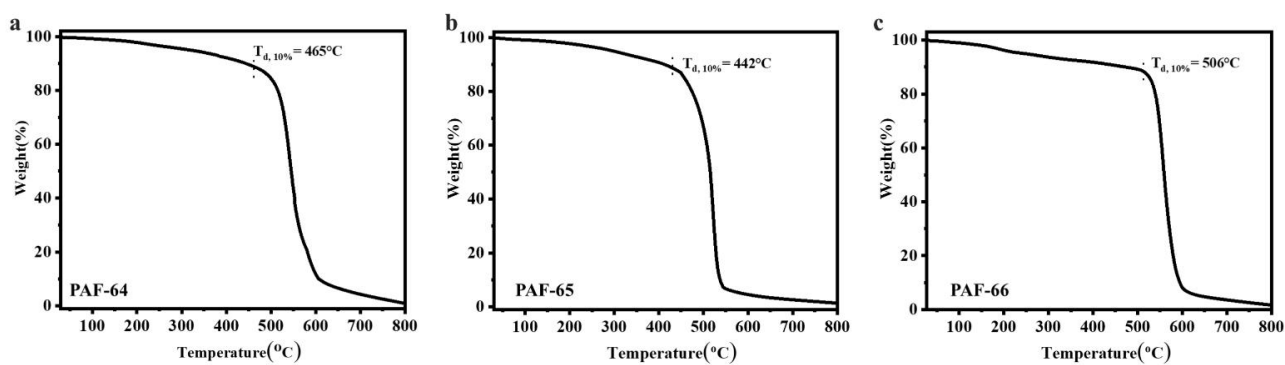
**Figure S14.** FTIR spectra of PAF-64 (a, red), PAF-65 (b, red), PAF-66 (c, red) and their monomers (black).



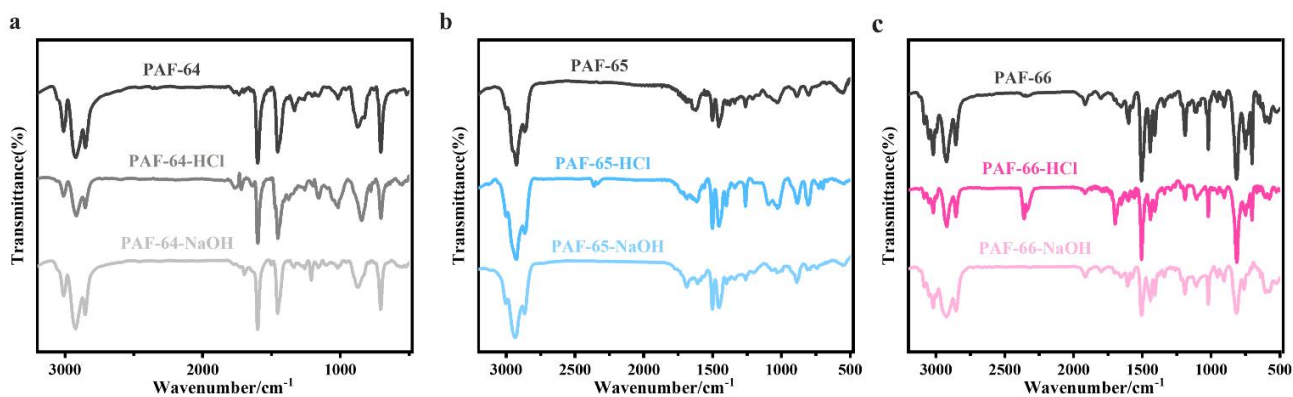
**Figure S15.** XRD patterns for PAF-66 (pink), PAF-65 (blue), PAF-64 (gray).



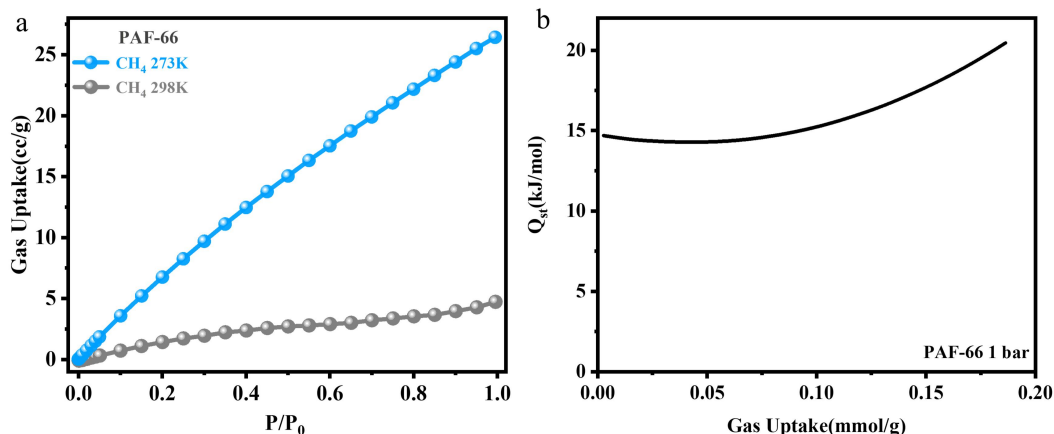
**Figure S16.** SEM images and TEM images for PAF-64 (a,d), PAF-65 (b,e) and PAF-66 (c,f).



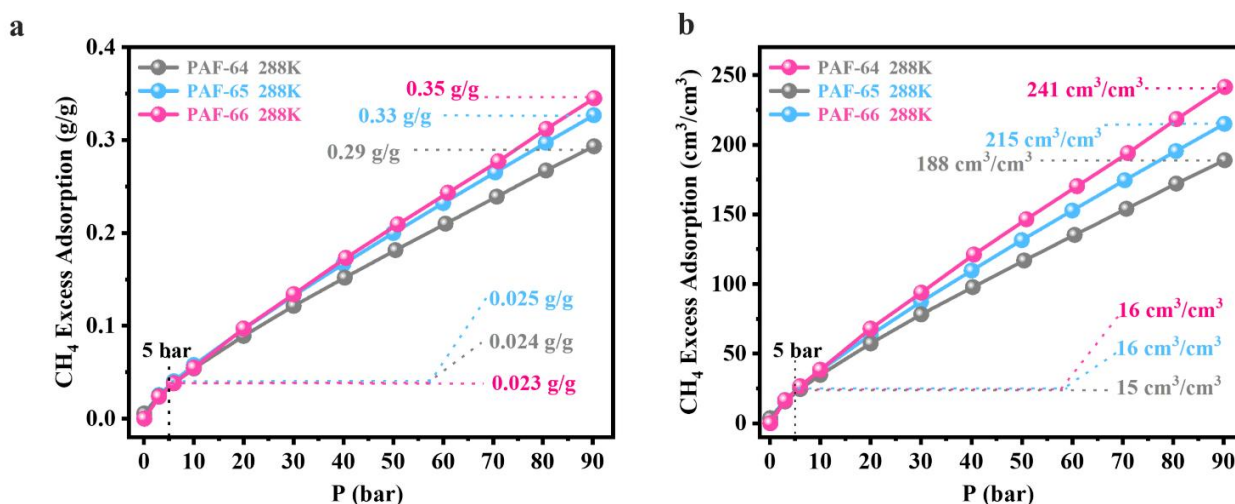
**Figure S17.** TGA curves of PAF-64 (a), PAF-65 (b), PAF-66 (c) under N<sub>2</sub>.



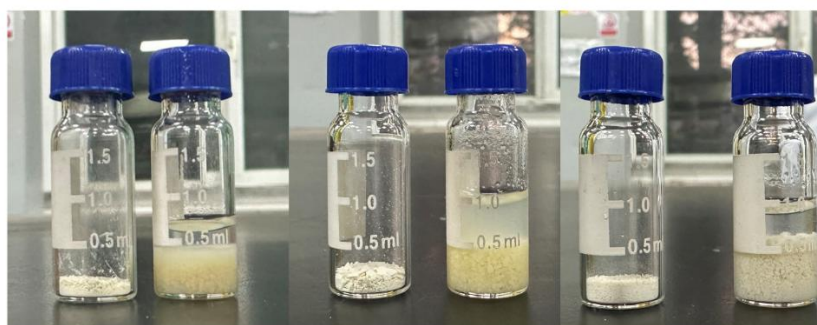
**Figure S18.** (a) FTIR spectra of PAF-64, PAF-64-HCl that soaked in HCl solution ( $5 \text{ mol L}^{-1}$ ) for 5 days and PAF-64-NaOH that soaked in NaOH solution ( $10 \text{ mol L}^{-1}$ ) for 5 days. (b) FTIR spectra of PAF-65, PAF-65-HCl that soaked in HCl solution ( $5 \text{ mol L}^{-1}$ ) for 5 days and PAF-65-NaOH that soaked in NaOH solution ( $10 \text{ mol L}^{-1}$ ) for 5 days. (c) FTIR spectra of PAF-66, PAF-66-HCl that soaked in HCl solution ( $5 \text{ mol L}^{-1}$ ) for 5 days and PAF-66-NaOH that soaked in NaOH solution ( $10 \text{ mol L}^{-1}$ ) for 5 days.



**Figure S19.** (a) Adsorption isotherms and (b) isosteric heat of adsorption of PAF-66 at 273K/298K and 1 bar.

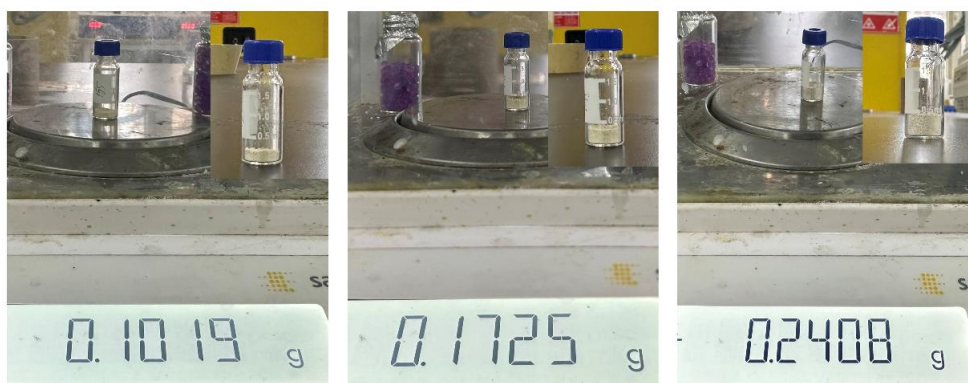


**Figure S20.** (a) Gravimetric methane adsorption isotherms and (b) volumetric methane adsorption of PAF-64, PAF-65 and PAF-66 at 288K



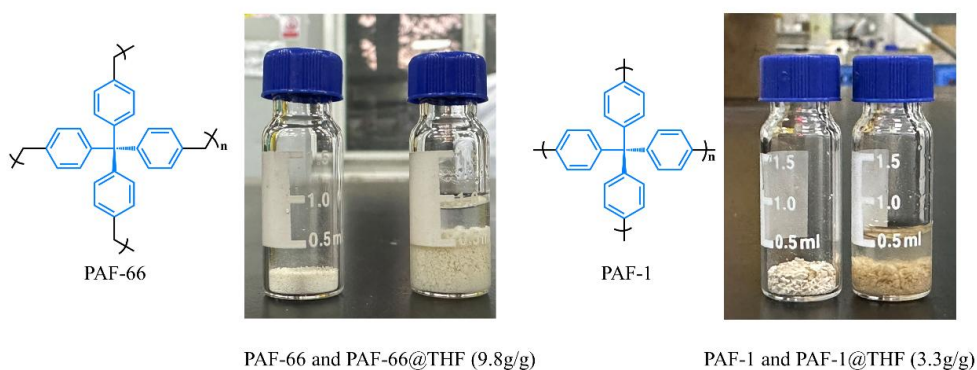
PAF-64 and PAF-64@THF PAF-65 and PAF-65@THF PAF-66 and PAF-66@THF

**Figure S21.** Absorption capacities of all PAFs for organic solvent with a volume swelling behavior owing to their flexible structure<sup>6-7</sup>.



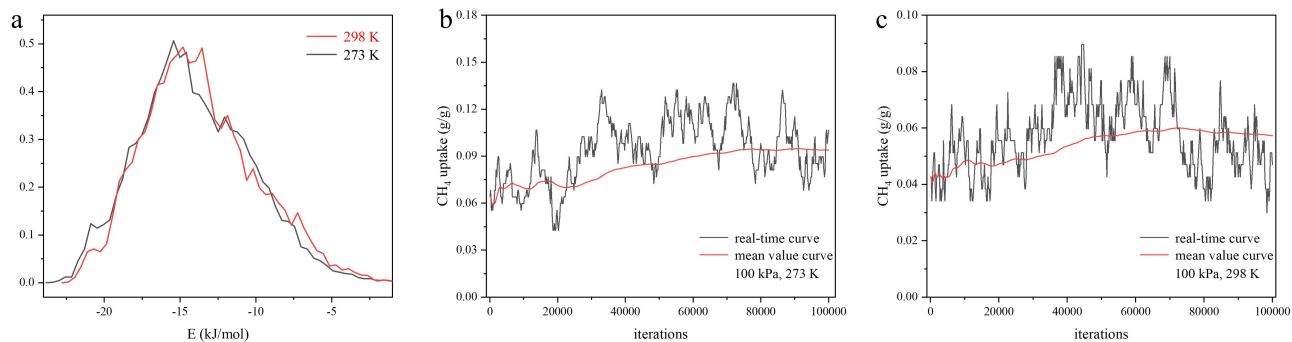
$\rho_{(\text{PAF-64})} = 0.1019 \text{ g} / 0.22 \text{ cc} = 0.46 \text{ g/cc}$      $\rho_{(\text{PAF-65})} = 0.1725 \text{ g} / 0.37 \text{ cc} = 0.47 \text{ g/cc}$      $\rho_{(\text{PAF-66})} = 0.2408 \text{ g} / 0.48 \text{ cc} = 0.50 \text{ g/cc}$

**Figure S22.** The packing density measurements of PAF-64, PAF-65 and PAF-66.

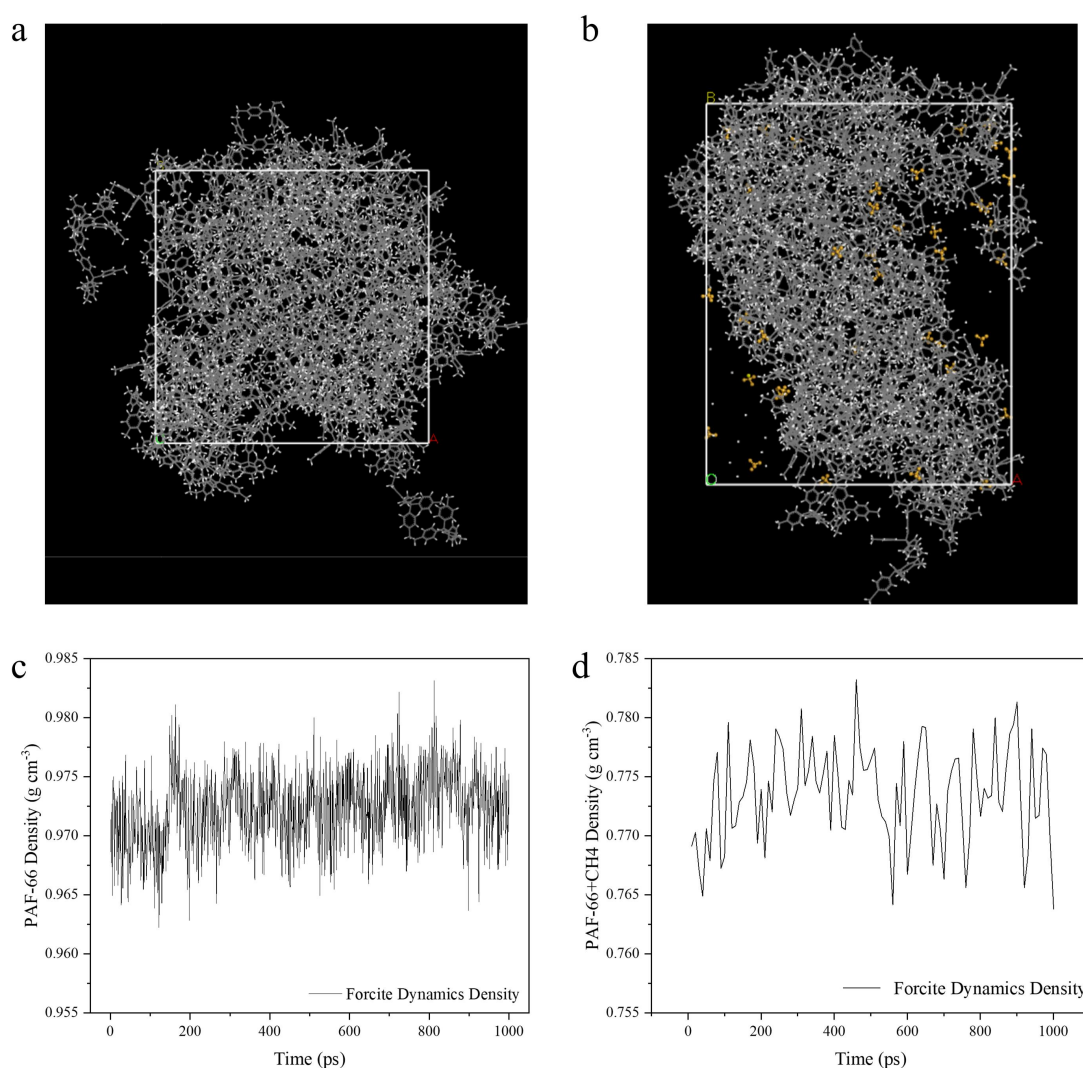


**Figure S23.** Structures and absorption capacities of PAF-66 and PAF-1<sup>8</sup> for organic solvent with a volume swelling behavior owing to their different flexible structure.





**Figure S24.** Simulated distribution of CH<sub>4</sub>-PAF-66 interaction energies is centered around at 273 K and 298 K (a) and simulated CH<sub>4</sub> sorption isotherms at 273 K(b) and 298 K(c).



**Figure S25.** Visualization of enlarged cell in PAF-66 before (a) and after (b) adsorption of CH<sub>4</sub> and the Forcite Dynamics Density of PAF-66 before (c) and after (d) adsorption of CH<sub>4</sub>.

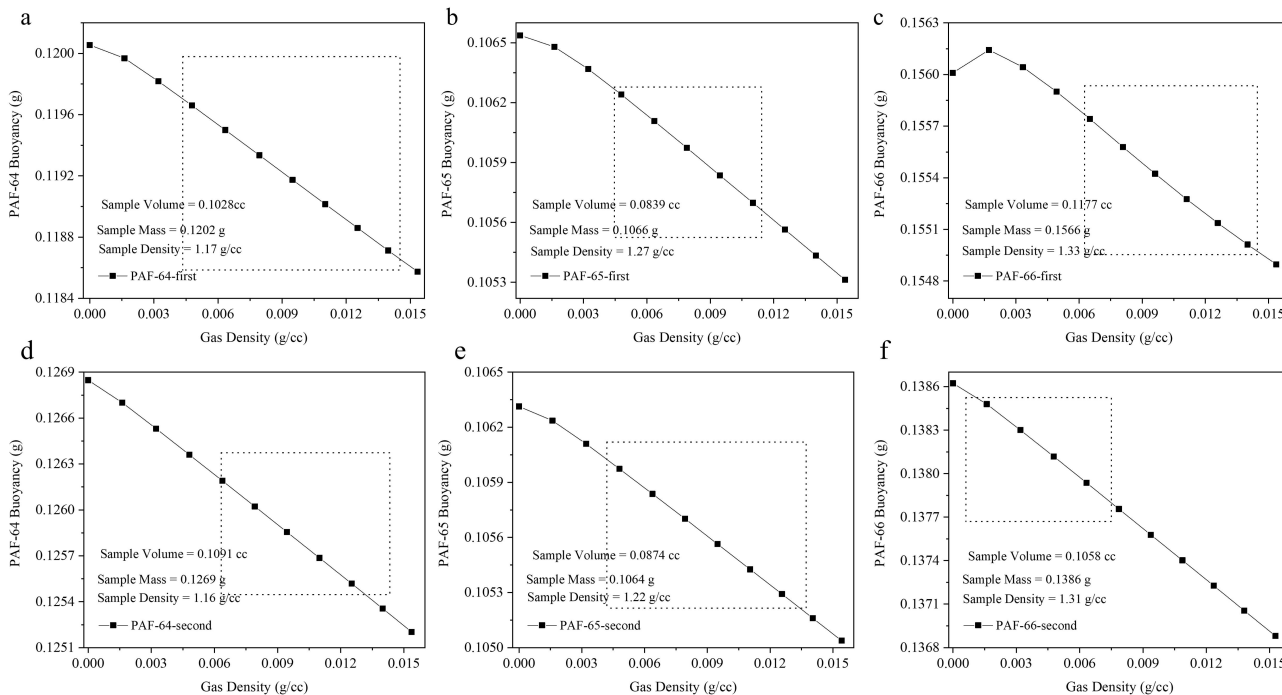


Figure S26. The sample densities of PAF-64 (a,d), PAF-65 (b,e), PAF-65 (c,f) basing on helium buoyancy test.

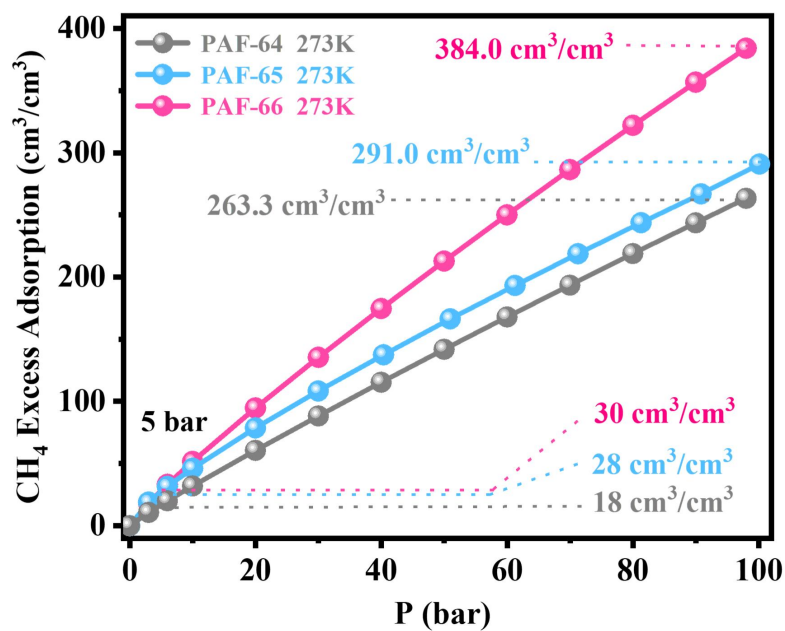
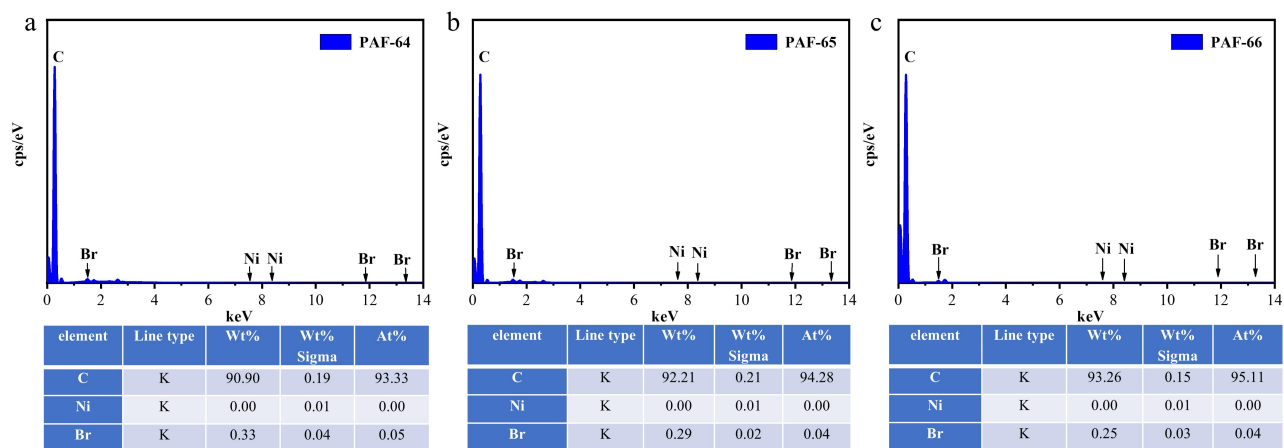


Figure S27. Volumetric methane adsorption of PAF-64, PAF-65 and PAF-66 at 273K on the base of the density measurement by helium-buoyancy.



**Figure S28.** SEM-EDS element analysis of PAF-64 (a), PAF-65 (b) and PAF-66 (c).

**Table S1.** Comparisons for the preparation of P2 with different catalytic systems (1-4), P3 with different catalytic systems (5-8), PAF-64 with different catalytic systems (9-12), PAF-65 with different catalytic systems (13-16).

entry	monomer	catalyst	ligand	time (h)	conv. (%)
1	1,3-Bis(bromomethyl)benzene	CuI/Sm	—	48h	6%
2	1,3-Bis(bromomethyl)benzene	NiCl <sub>2</sub> /Sm	HMPA	48h	10%
3	1,3-Bis(bromomethyl)benzene	NiCl <sub>2</sub> /Zn	Tpy	48h	18%
4	1,3-Bis(bromomethyl)benzene	Ni(COD) <sub>2</sub>	Bpy	5h	93%
5	1,4-Bis(bromomethyl)benzene	CuI/Sm	—	48h	trace
6	1,4-Bis(bromomethyl)benzene	NiCl <sub>2</sub> /Sm	HMPA	48h	2%
7	1,4-Bis(bromomethyl)benzene	NiCl <sub>2</sub> /Zn	Tpy	48h	4%
8	1,4-Bis(bromomethyl)benzene	Ni(COD) <sub>2</sub>	Bpy	5h	95%
9	1,3,5-Tris(bromomethyl)benzene	CuI/Sm	—	48h	trace
10	1,3,5-Tris(bromomethyl)benzene	NiCl <sub>2</sub> /Sm	HMPA	48h	trace
11	1,3,5-Tris(bromomethyl)benzene	NiCl <sub>2</sub> /Zn	Tpy	48h	trace
12	1,3,5-Tris(bromomethyl)benzene	Ni(COD) <sub>2</sub>	Bpy	5h	97%
13	1,2,4,5-Tetrakis (bromomethyl)benzene	CuI/Sm	—	48h	trace
14	1,2,4,5-Tetrakis (bromomethyl)benzene	NiCl <sub>2</sub> /Sm	HMPA	48h	trace
15	1,2,4,5-Tetrakis (bromomethyl)benzene	NiCl <sub>2</sub> /Zn	Tpy	48h	trace
16	1,2,4,5-Tetrakis (bromomethyl)benzene	Ni(COD) <sub>2</sub>	Bpy	5h	98%

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**Crystal data of 1,2-diphenyl ethane**

**Table S2.** Crystal data and structure refinement for 1,2-diphenyl ethane (2)

Identification code	2	$\rho_{\text{calc}}/\text{cm}^3$	1.202
Empirical formula	CH	$\mu/\text{mm}^{-1}$	0.503
Formula weight	13.02	F(000)	357.0
Temperature/K	294.85	Crystal size/ $\text{mm}^3$	$0.2 \times 0.16 \times 0.12$
Crystal system	monoclinic	Radiation	? ( $\lambda = 1.54178$ )
Space group	$P2_1/c$	$2\Theta$ range for data collection/ $^\circ$	8.806 to 128.128
a/ $\text{\AA}$	5.8945(12)	Index ranges	$-6 \leq h \leq 6, -8 \leq k \leq 9, -23 \leq l \leq 22$
b/ $\text{\AA}$	7.7498(14)	Reflections collected	6909
c/ $\text{\AA}$	20.085(4)	Independent reflections	1513 [ $R_{\text{int}} = 0.0818, R_{\text{sigma}} = 0.0694$ ]
$\alpha/^\circ$	90	Data/restraints/parameters	1513/0/118
$\beta/^\circ$	91.072(15)	Goodness-of-fit on $F^2$	1.135
$\gamma/^\circ$	90	Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.1492, wR_2 = 0.4509$
Volume/ $\text{\AA}^3$	917.3(3)	Final R indexes [all data]	$R_1 = 0.1949, wR_2 = 0.4744$
Z	51	Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.42/-0.42