Electronic Supplementary Information

Thienyltriazine based conjugated porous organic polymers: tuning of porosity and band gap, and CO_2 capture

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Experimental section

General instrumentation

^{1}H and ^{13}C NMR spectra of the monomers and precursors were recorded at room temperature on a Jeol JNM-ECS 400 spectrometer (400 MHz ^{1}H, 100 MHz ^{13}C) or Bruker Avance 500 (500 MHz ^{1}H, 125 MHz ^{13}C) spectrometer with tetramethylsilane as the internal reference; chemical shifts (δ) are given in parts per million (ppm). Spectra were processed using MestReNova v*5* and referenced to residual protonated solvent signals ($CDCl_3$: ^{1}H 7.26 ppm, ^{13}C 77.16 ppm). Fourier transform infrared spectroscopy (FTIR) spectra were recorded in the range of 4000-400 cm^{-1} using the KBr pellet technique on a Perkin-Elmer RX1 IR Spectrometer. The thermal properties of CPPs were measured bythermogravimeter analyzer (Mettler Toledo, TGA/SDTA 851) from 40 ºC to 800 ºC at a heating rate of 10 ºC min^{-1} under nitrogen atmosphere. A Rigaku (Mini Flex II, Japan) powder X-ray diffractometer having Cu Kα (λ = 1.54059 Å) radiation was used to record the X-ray diffraction (XRD) patterns. Solid-state UV-vis absorption spectra were recorded on a JASCO V-670 spectrophotometer.Elemental analysis was performed using Perkin Elmer CHN analyzer. A Carl Zeiss SUPRA 55VP microscope was used to obtain the field-emission scanning electron microscopy (FESEM) images after coating the sample with Au film. Transmission electron microscopy (TEM) images were recorded with a JEOL JEM-2100F microscope at the Department of Science and Technology, Fund for Improvement of S&T Infrastructure in Higher Educational Institutions (DST-FIST) facility of IISER Kolkata. The ^{1}H-^{13}C CP/MAS NMR spectra were recorded on a Bruker AVANCE 500-MHz type (^{1}H, 500 MHz; ^{13}C, 125 MHz) spectrometer at a spinning speed of 8 KHz and a relaxation delay of 10 seconds. UV−visible absorption spectra were recorded on an Agilent Cary60 UV−vis spectrophotometer.N_2 adsorption-desorption isotherms were obtained on a Micromeritics Gemini VII surface area analyzer at 77 K and reported by Barrett-Joyner-Halenda surface/volume pore analysis. Samples were degassed at 120 °C under a N_2 atmosphere for 12 h. The specific surface area was determined as per the Brunauer-Emmett-Teller (BET) method. CO_2 sorption data were recorded for pressures in the range 0–1.2 bar by the volumetric method using a BELSORP MAX instrument. Isosteric heats of adsorption (Q_{st}) were calculated using the Clausius-Clapeyron equation based on pure-component isotherms collected at three different temperatures of 273 K, 283 K and 298 K. Q_{st} is defined as: $Q_{st} = -R(\partial lnx/\partial(1/T))y$, where, x is the pressure, T is the

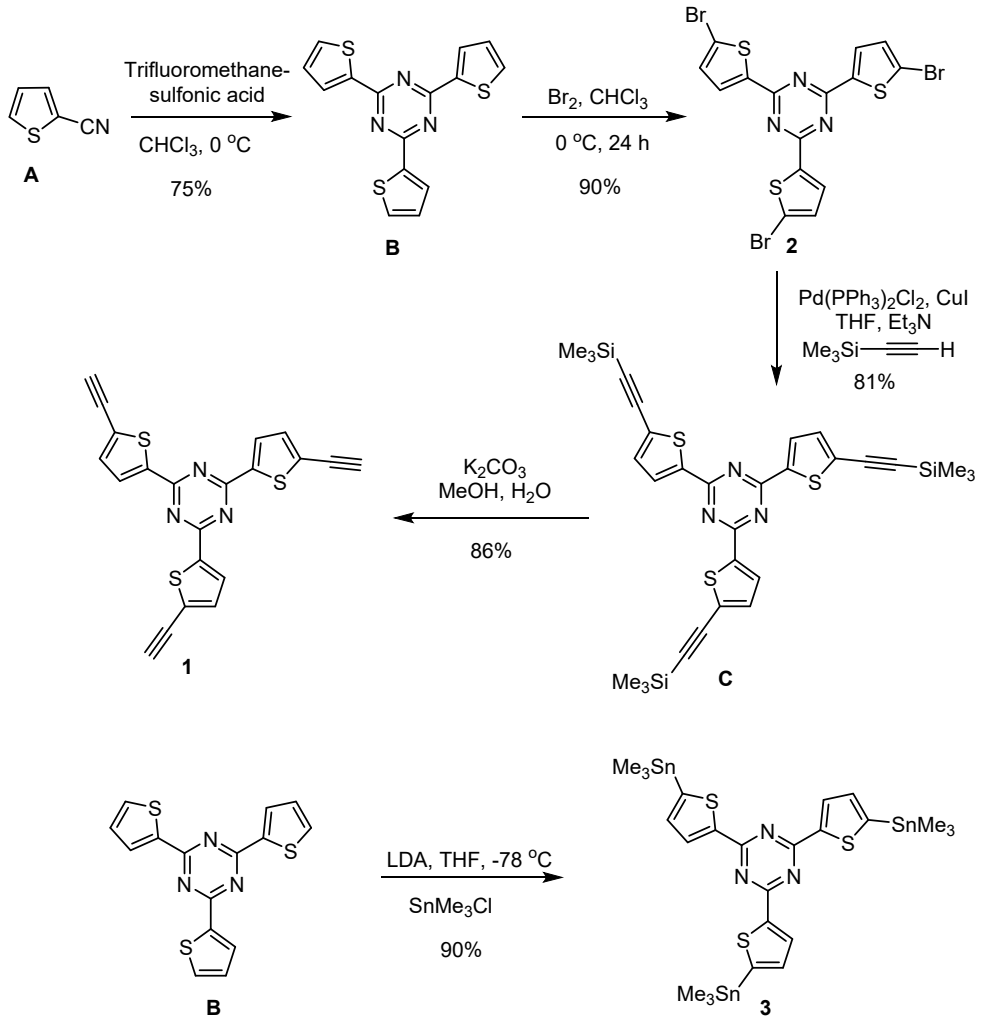
temperature, R is the gas constant and y is the adsorption amount.These calculations are done through the "Heat of Adsorption" function embedded in the Belsorp adsorption/desorption data analysis software version 6.3.1.0.

Configurational biasMonte Carlo (CBMC) molecular simulation[1]

The structures of **TT-CPC-1**,**2**,**3** was assumed to be hexagonal rigid in the crystallographic position, which is obtained from single-crystal XRD data. The simulation boxes representing **TT-CPC-1**,**2**,**3** adsorbents consist of (1 x 1 x 1) unit cells for CO_2. All the calculations were performed at different temperatures. Interatomic interactions were modelled with standard Lennard-Jones potential and Coulombic potentials. Lennard-Jones parameters between unlike atom types were computed using the Lorentz-Berthelot mixing rules. For the pairwise interactions between host-guest atoms of the particular force field, the nonbonding parameter has been utilized. The long-range part of electrostatic interactions was handled using the Ewald summation technique with a relative precision of 10^{-6}. Periodic boundary conditions were applied in all three dimensions. For each state point, the CBMC simulation consists of 1 x 10^7 steps to guarantee equilibration, followed by 1 x 10^7 steps to sample the desired thermodynamic properties.

Materials

All reagents were obtained from commercial sources (Sigma Aldrich, Spectrochem, Merck and Alfa Aesar) and used as received without further purification unless otherwise specified. Toluene and Tetrahydrofuran (THF) were dried over sodium/benzophenone before use. Dry reactions were conducted in oven-dried glassware using a standard Schlenk line under an inert atmosphere of dry nitrogen. Dimethylformamide (DMF) for polymerization reaction was dried over calcium hydride followed by distillation under vacuum. Triethylamine was dried over potassium hydroxide (KOH) flakes. Dichloromethane (DCM) and chloroform ($CHCl_3$) were dried over calcium chloride. Solvents for Soxhlet extraction were used directly as obtained from commercial sources.



Scheme S1. Synthesis of the precursors used for polymerization.

2,4,6-tris(5-ethynylthiophen-2-yl)-1,3,5-triazine (**1**) was synthesized from 2-cyano thiophene (**A**) according to the procedure reported by Misra and the group.[2] ^{1}H data of all the compounds were consistent with the reported values. ^{1}H NMR of **1** (400 MHz, Jeol, $CDCl_3$): δ ppm 8.04 (d, 1H, J = 4 Hz); 7.30 (d, 1H, J = 4 Hz); 3.52 (s, 1H). Stannylation of compound **2** was carried out by using the method reported by Ogawa and the group.[3] ^{1}H data of the compound matched with the reported data.^{1}H NMR of **3** (400 MHz, Jeol, $CDCl_3$): δ ppm 8.33 (d, 3H, J = 4 Hz); 7.27 (d, 3H, J = 8 Hz), 0.45 (s, 27H).

Procedure for the synthesis ofTT-CPP1 [by the cyclotrimerisation reaction using $Co_2(CO)_8$ catalyst]

A 50 mL oven-dried three-neck round bottom flask fitted with a reflux condenser and a nitrogen purger on the top was charged with a small magnetic stirring bar. The reaction vessel was degassed and purged with nitrogen several times. The flask was then charged with 2,4,6-tris(5-ethynylthiophen-2-yl)-1,3,5-triazine (**1**) (1 g, 1 equiv) and 10 mL deoxygenated dioxane and the mixture was purged with nitrogen at room temperature for 20 minutes. In a separate single neck round-bottomed flask 10 mol % of dicobalt octacarbonyl, $Co_2(CO)_8$ was placed, followed by the addition of 5 mL of deoxygenated dioxane. The mixture was purged with nitrogen for 10 minutes. Meanwhile, the temperature of the flask containing the acetylene precursor **1**was set to 110 ^{o}C. After completion of purging, the solution of cobalt catalyst was added dropwise to the reaction mixture, and the refluxing was continued for 1.5 h. The reaction mixture was then cooled, and the crude reaction mixture was suspended in conc. HCl(aq) toremove metal residues and was purified with a successiveSoxhlet extraction with water, methanol and ethanol. The polymer was further dried under vacuum for 3 h. Yield: 98%.

Procedure for the synthesis of TT-CPP2 (by the Sonogashira-Hagihara coupling reaction)

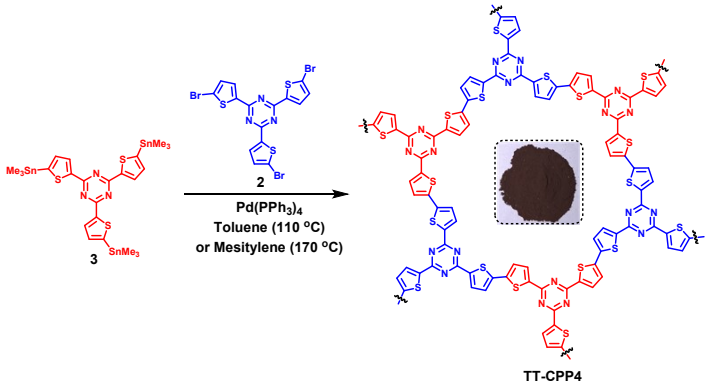
A 50 mL oven-dried three-neck round bottom flask fitted with a reflux condenser and a nitrogen purger on the top was charged with a small magnetic stirring bar. The reaction vessel was degassed and purged with nitrogen several times. Then the flask was charged with tribromo precursor (**2**, 0.67 equiv) and 2,4,6-tris(5-ethynylthiophen-2-yl)-1,3,5-triazine (**1**, 1 equiv). 7 mL anhydrous dimethylformamide (DMF) and 7 mL anhydrous triethylamine (Et_3N) were added to the flask under nitrogen and then $Pd(PPh_3)_4$ (5 mol%) and copper(I)iodide (CuI), (5 mol%). The reaction mixture was stirred at 130 ºC for 72 hours under a nitrogen atmosphere. The mixture was cooled to room temperature, and the precipitated polymer was filtered and washed three times with dichloromethane, water, methanol and acetone (100 mL each) to remove any unreacted monomers or catalyst residues. Further purification of the polymer was done by Soxhlet extraction with methanol and then $CHCl_3$ for 24 hours each. The product was then dried under vacuum for 5 hours at 100 ºC. Yield: 90%.

Procedure for the synthesis of TT-CPP3 (by the Glaser coupling reaction)

A 50 mL oven-dried three-neck round bottom flask fitted with a reflux condenser under atmospheric condition was charged with a small magnetic stirring bar. The flask was then charged with 2,4,6-tris(5-ethynylthiophen-2-yl)-1,3,5-triazine (**1**) (0.45 g, 1 equiv) and 10 mL of Et_3N and THF (1:1)mixture. This was followed by the addition of 5 mol% of $Pd(PPh_3)_2Cl_2$ and 5 mol% CuI. The mixture is then heated to 60 ºC, and stirring continued as such for 72 hours. The mixture was cooled to room temperature, and the precipitated polymer was filtered and washed three times with dichloromethane, water, methanol and acetone (100 mL each) to remove any unreacted monomers or catalyst residues. Further purification of the polymer was done by Soxhlet extraction with methanol and then $CHCl_3$ for 24 hours each. The product was then dried under vacuum for 5 hours at 100 ºC. Yield: 94%.

Procedure for the synthesis of TT-CPP4 (by the Stille coupling reaction)

2,4,6-tris(5-(trimethylstannyl)thiophen-2-yl)-1,3,5-triazine (**3**)(0.5 g, 0.6 mmol, 1 equiv) and 2,4,6-tris(5-bromothiophen-2-yl)-1,3,5-triazine (**2**) (0.226 g, 0.4 mmol, 0.67 equiv), tetrakis(triphenylphosphine)palladium(0) (5 mol% with respect to**3**) and 5 mL of mesitylene were added to a two-neck flask fitted with a reflux condenser under an inert atmosphere. The solution was further purged with nitrogen for around 15 minutes, and then the solution was heated at 170 °C for 3 days with stirring. After the reaction, the solution was poured into methanol, and a red precipitate was collected by filtration. Then, the red powder was purified by Soxhlet extraction with methanol, dichloromethane, tetrahydrofuran, and acetone for 24 h each. Finally, the purified red powder was vacuum-dried for 3 h. Yield: 92%.



Scheme S2. Synthesis of TT-CPP4.

Characterization of the synthesized polymers and monomers

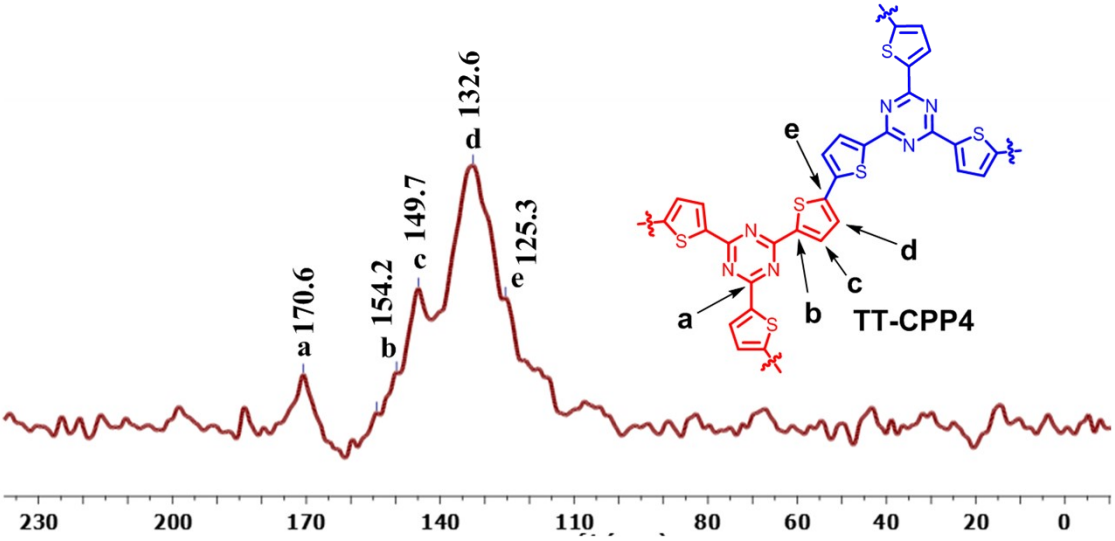


Fig. S1 Solid state CP-MAS^{13}C NMR spectrum of **TT-CPP4**.

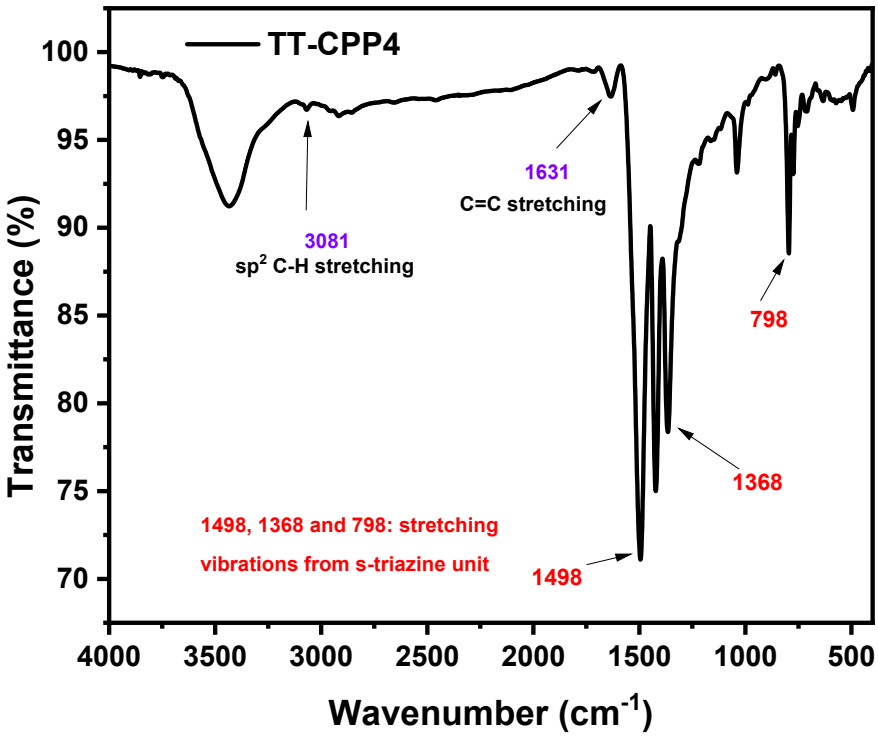


Fig. S2 FTIR spectrum of **TT-CPP4**.

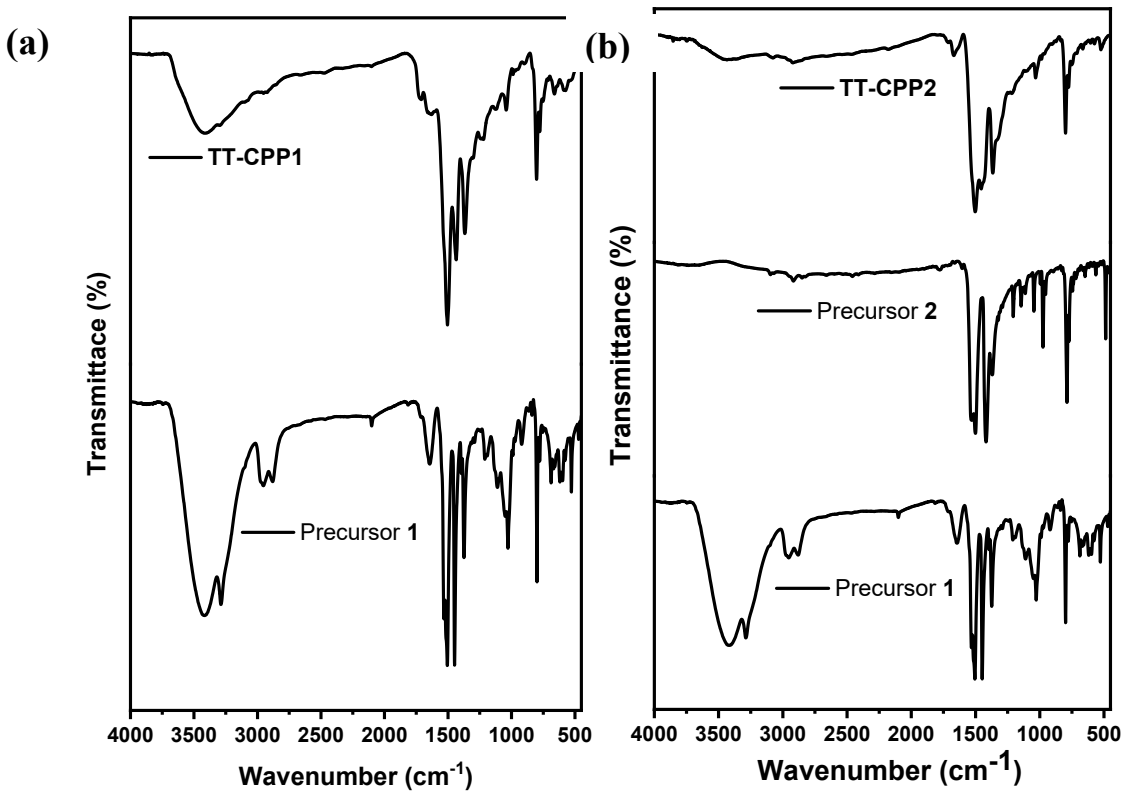


Fig. S3(a) FTIR spectra of Precursor **1**and **TT-CPP1** and **(b)** FTIR spectra of Precursor **1, 2** and **TT-CPP2**.

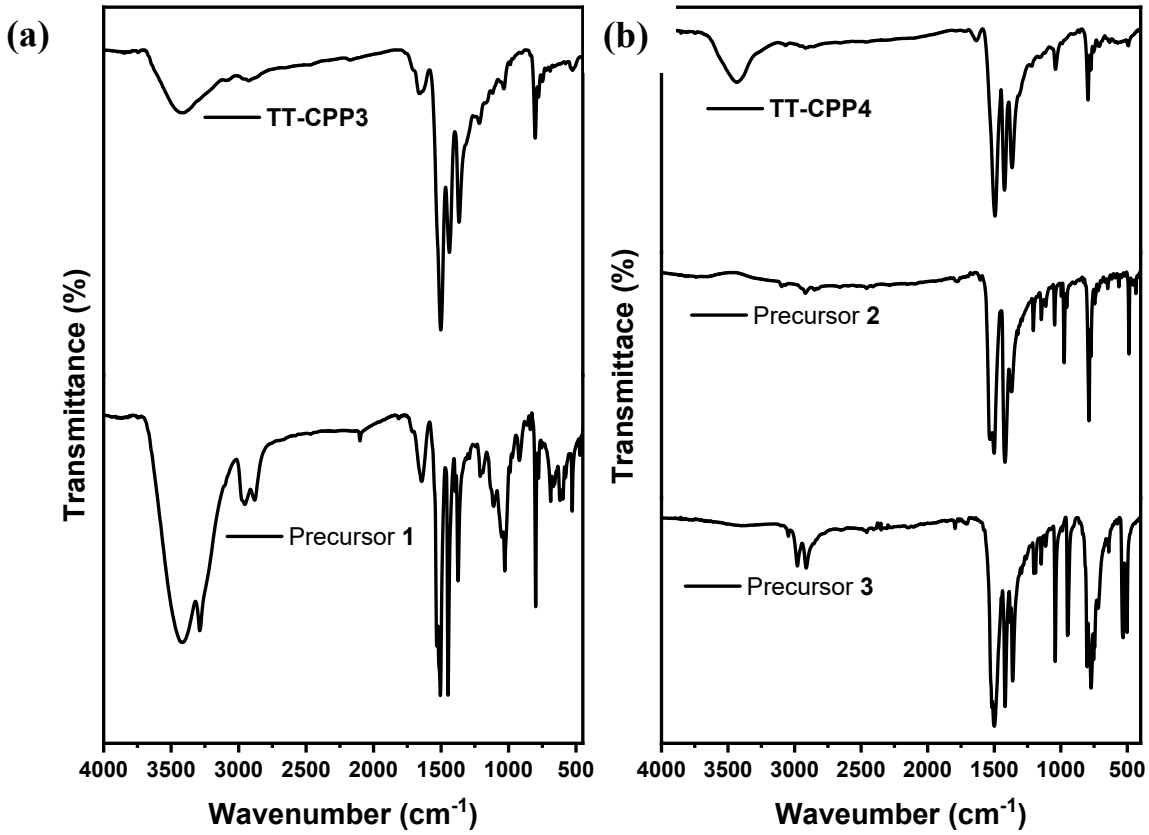


Fig. S4 (a) FTIR spectra of Precursor **1** and **TT-CPP3** and **(b)** FTIR spectra of Precursor **3, 2** and **TT-CPP4**.

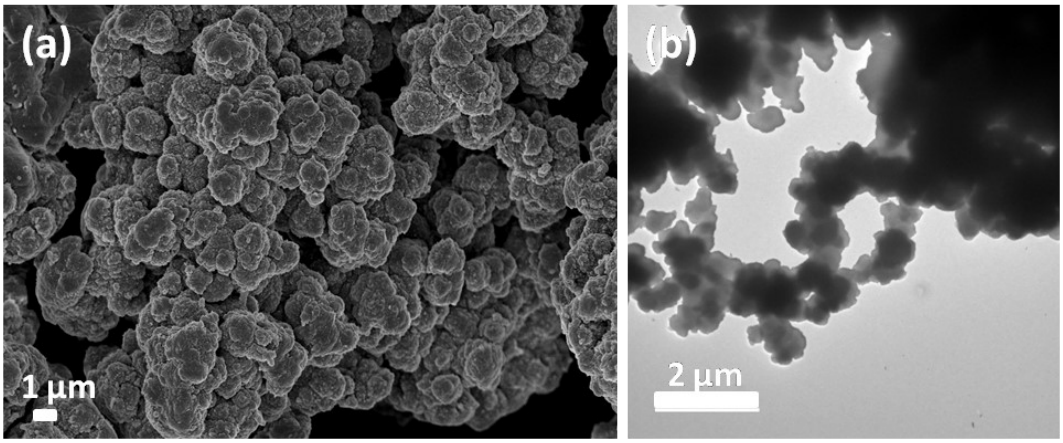


Fig. S5 (a) SEM image of **TT-CPP4** at 1 µm scale and **(b)** TEM image of **TT-CPP4** at 2 µm scale.

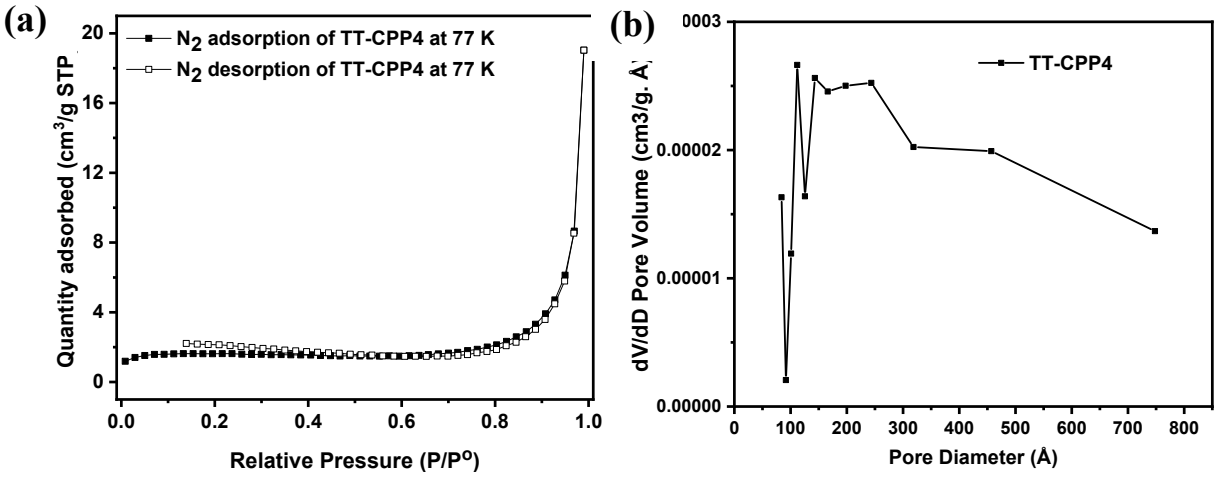


Fig. S6 (a) N_2 adsorption-desorption isotherm of **TT-CPP4** at 77Kand **(b)** Pore size distribution of **TT-CPP4**.

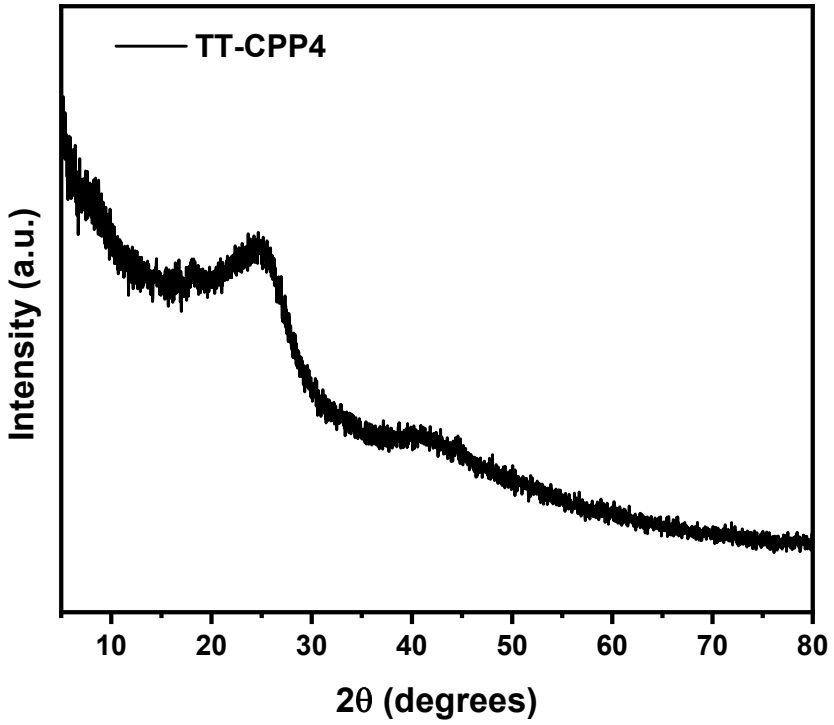


Fig. S7 Powder X-ray diffraction pattern of **TT-CPP4**.

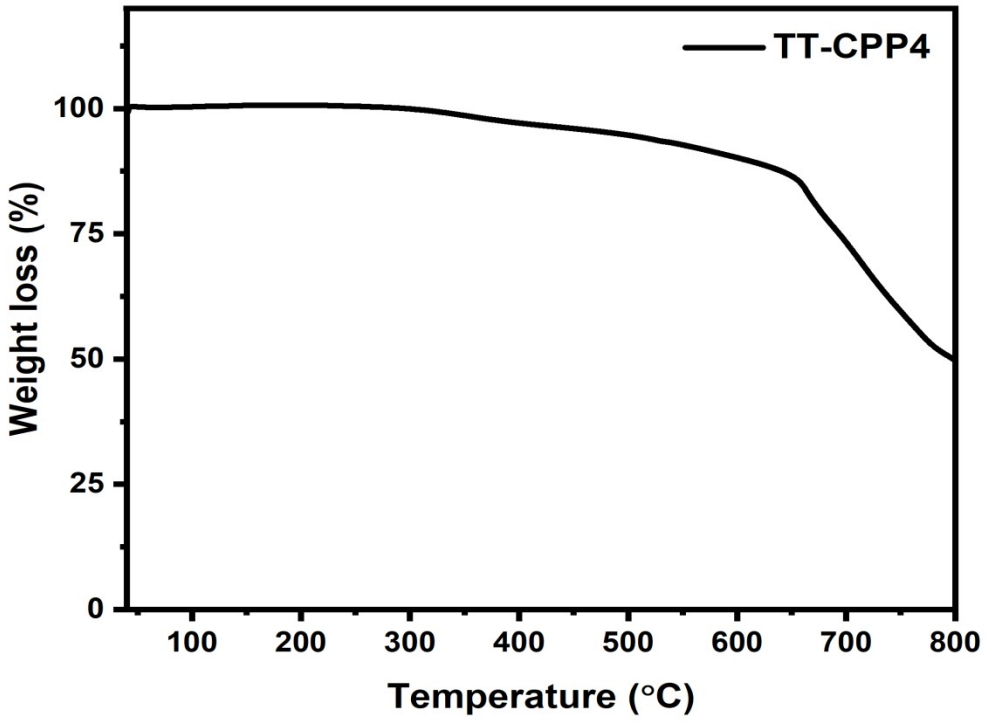


Fig. S8 TGA profile of **TT-CPP4**.

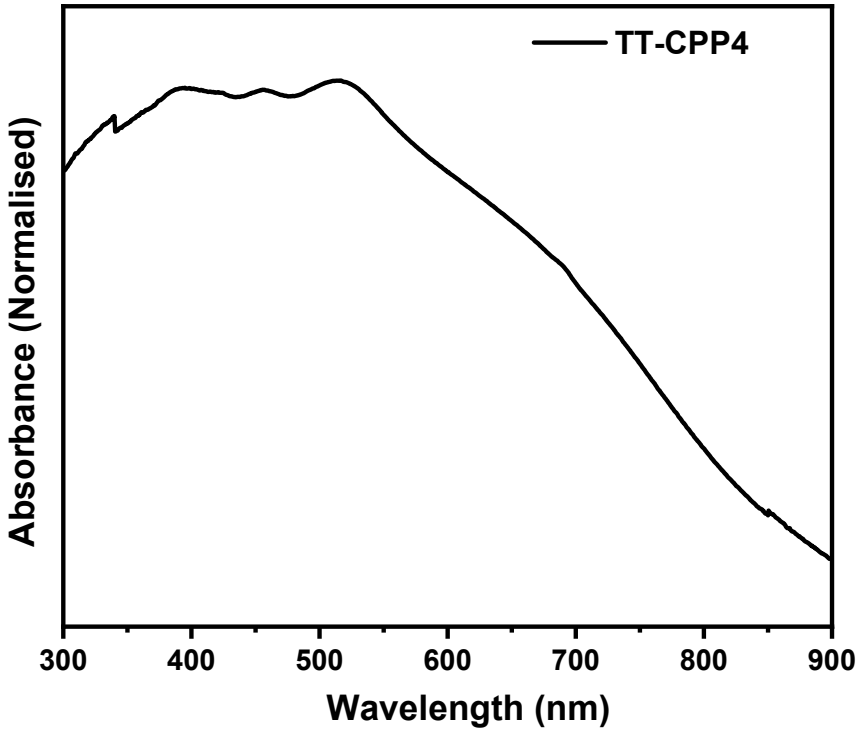


Fig. S9 Solid State UV-visible spectrum of **TT-CPP4**.

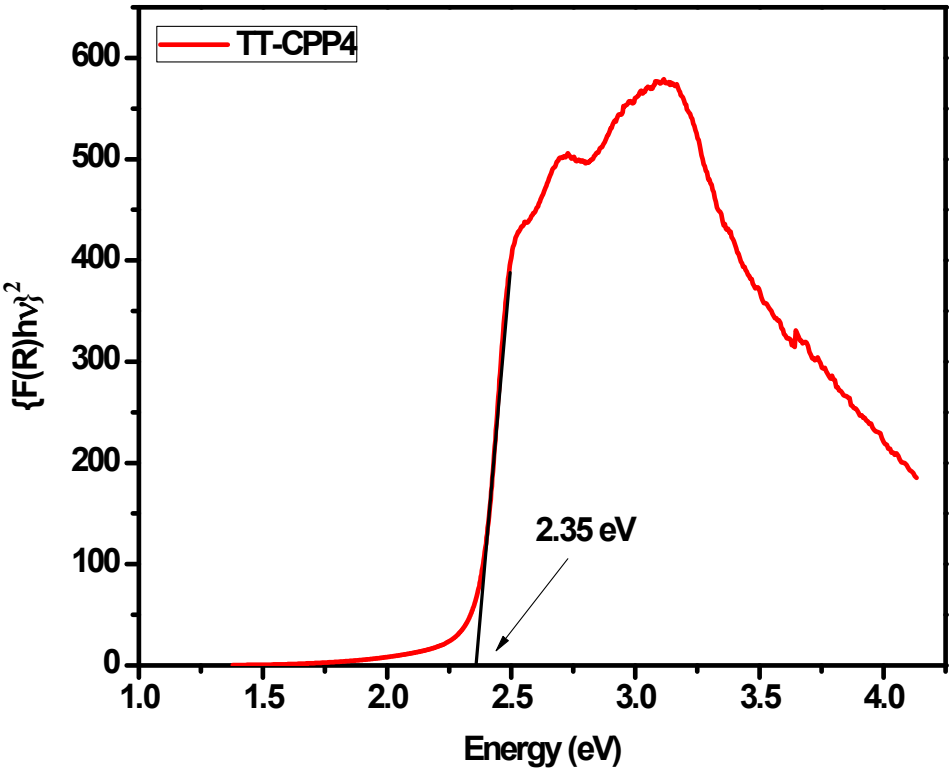


Fig. S10 Kubelka-Munk plot for band gap calculation of**TT-CPP4**.

Table S1. Elemental Analysis of **TT-CPP1**, **TT-CPP2**, **TT-CPP3** and **TT-CPP4**.

Polymer	Theoretically calculated value	Experimental value
TT-CPP1 (C21H9N3S3)	C = 63.13, H = 2.27, N = 10.52	C = 58.91, H = 1.62, N = 8.41
TT-CPP2 (C40H12N6S6)	C = 62.48, H = 1.57, N = 10.93	C = 56.15, H = 1.21, N = 8.12
TT-CPP3 (C42H12N6S6)	C = 63.62, H = 1.53, N = 10.60	C = 60.08, H = 1.25, N = 8.01
TT-CPP4 (C30H12N6S6)	C = 55.53, H = 1.86, N = 12.95	C = 52.23, H = 1.31, N = 10.21

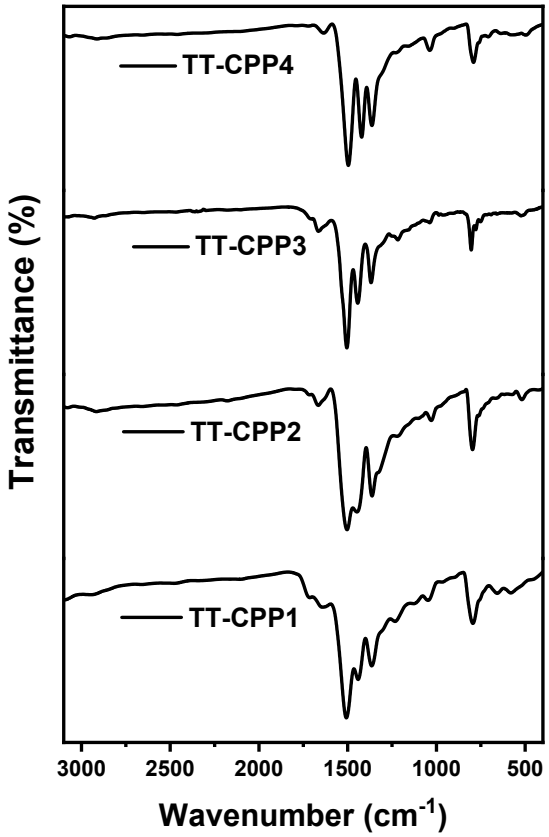


Fig. S11 FTIR spectra of **TT-CPP (1-4)** after treatment with the organic solvent,acid, and base for 3 days.

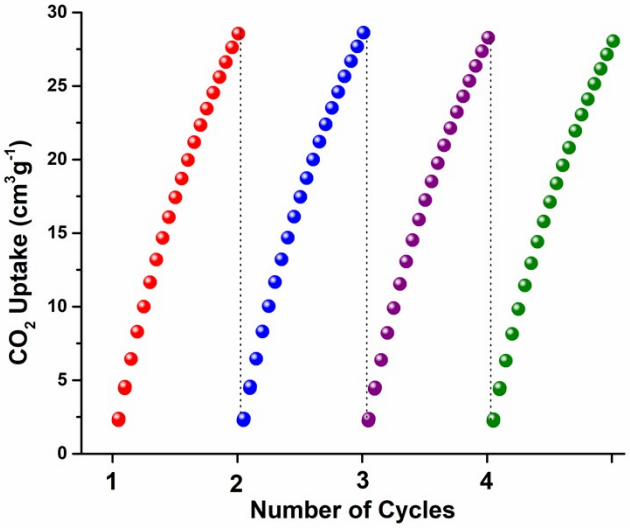


Fig. S12 Recycling efficiency of **TT-CPP1** for CO_2 uptake.

Table S2. Summary of the CO_2 adsorption capacity data of various CPPs.

Entry	Material	SA_{BET} (m^2 g^{-1})	Temperature (K)	Pressure (bar)	Adsorption capacity (mmol g^{-1})	Reference
1	**TT-CPP1**	545	263	1	2.62	*This work*
			273		2.18	
			298		1.27	
	TT-CPP2	511	263		1.75	
			273		1.63	
			298		1.08	
	TT-CPP3	491	263		1.42	
			273		1.22	
			298		0.76	
2	**Py-azo-COP**	700	273	1	1.93	*ACS Omega*, **2017**, *2*, 3572–3582.
				15.5	4.14	
3	**Zn-CMP**	791	298	1.01	1.33	*ChemSusChem*, **2014**, *7*, 2110–2114.
4	**CMP1**	258	298	1	0.46	*Polymer*, **2016**, *90*, 187–192.
	CMP2	567			0.67	
5	**NWPTPE**	508	298	1	0.68	*J. Polym. Sci., Part A: Polym. Chem.*, **2017**, *55*, 3862–3867.
	NWPPYR	824			0.93	
6	**HCTPP**	582	273	1	2.79	*New J. Chem.*, **2017**, *41*, 3915–3919.
	HCTPA	921			2.27	
	HCTPM	670			2.14	
7	**TCMP-0**	963	273	1	2.38	*Polym. Chem.*, **2012**, *3*, 928–934.
			298		1.34	
	CMP-0	1018	273		2.1	
			298		1.21	
	TNCMP-2	995	273		2.62	
			298		1.45	
	TCMP-3	691	273		2.25	
			298		1.26	
	TCMP-5	494	273		1.22	
			298		0.68	
8	**TPB-BD-CMP**	657	273	1	2.5	*Mater. Chem. Front.*, **2017**, *1*, 867–872.
	TPA-BD-CMP	543			2.94	
	TPM-BD-CMP	1008			3.78	
	SPF-BD-CMP	833			3.25	
9	**P1**	914	273	1	3.01	*Chem. Eur. J.*, **2016**, *22*, 7179–7183.
	P2	834			2.53	
	P3	873			2.12	
10	**ACMP-C**	629	195	1.06	11.14	*Macromolecules*, **2010**, *43*, 5508–5511.
			273		1.56	
			298		1.08	
	ACMP-C6	380	195		9.97	
			273		0.79	
			298		0.54	
	ACMP-N	46	195		11.5	
			273		1.16	
			298		0.79	
11	**CMP1**	767	273	1	2.94	*Macromolecules*, **2019**, *52*, 3935–3941.
	CMP2	624			2.7	
	CMP3	780			2.37	

12	**CMP-1-NH_2** **CMP-1-AMD1** **CMP-1-AMD2** **CMP-1-AMD3** **CMP-1-AMD4** **CMP-1-AMD5** **CMP-1-AMD9**	656 316 264 119 59 37 68	273 298 273 298 273 298 273 298 273 298 273 298 273 298	1	1.65 0.96 1.51 0.96 1.46 0.92 1.31 0.83 1.13 0.71 1.1 0.64 0.87 0.54	*Polymer*, **2014**, *55*, 321–325.
13	**PP_CMP@mmm** **PP_CMP@omp** **PP_CMP@omom**	1928 43 81	273 298 273 298 273 298	1	2.52 1.36 0.82 0.43 1.05 0.66	*Chem. Commun.*, **2014**, *50*, 2781–2783.
14	**Py-BF-CMP** **TPE-BF-CMP** **TPA-BF-CMP**	1306 777 590	273 273 273	1	3.21 2.1 1.83	*Macromolecules*, **2018**, *51*, 3443–3449.
15	**HP_E-CMP**	662	273 298	1	3.58 1.7	*RSC Adv.*, **2014**, *4*, 6447–6453.
16	**CMP** **Co-CMP** **Al-CMP**	772 965 798	298	1.01	1.61 1.8 1.74	*Nat. Commun.*, **2013**, *4*, 1960.
17	**Cr-CMP**	738	298	1.01	1.63	*J. Energy Chem.*, **2014**, *23*, 22–28.
18	**Al-CMP**	839	273 298	1.01	0.98 0.62	*RSC Adv.*,**2015**, *5*, 31664–31669.
19	**NCMP-I** **NCMP-III**	945 593	273 298 273 298	1	1.93 1.43 0.95 0.5	*Macromol. Mater. Eng.*, **2016**, *301*, 451–456.
20	**BQCMP-1** **DQCMP-1**	422 123	273 298 273 298	1	1.55 1.06 1.09 0.86	*Macromol. Mater. Eng.*, **2016**, *301*, 1104–1110.
21	**HCMP-1** **HCMP-2** **HCMP-3** **HCMP-4**	308 58 50 28	273 273 273 273	1	1.7 1.23 1.16 0.98	*Macromolecules*, **2016**, *49*, 6322–6333.
22	**PTEB aerogel**	1701	273	1	3.47	*Adv. Mater.*, **2014**, *26*, 8053–8058.
23	**CMP-PM** **CMP-PM-Me**	416 241	273 273	1.01	1.99 1.42	*Chem. Eur. J.*, **2018**, *24*, 7480–7488.
24	**BO-CMP-1** **BO-CMP-2** **oBO-CMP-1** **oBO-CMP-2**	440 1030 390 540	273	1	1.8 2.41 1.16 1.7	*Macromolecules*, **2018**, *51*, 947–953.

25	**CMP-1** **CMP-1-$(CH_3)_2$** **CMP-1-$(OH)_2$**	837 899 1043	298	1	1.18 0.94 1.07	*Chem. Sci*., **2011**, *2*, 1173–1177.
26	**BFCMP-1** **BFCMP-2**	1316 1470	273 298 273 298	1.13	2.45 1.39 2.77 1.64	*Polymer*, **2015**, *61*, 36–41
27	**PPTBC** **PMTBC** **PPETBC** **PMETBC**	917 704 702 540	273 298 273 298 273 298 273 298	1.13	2.93 1.71 2.86 1.79 2.23 1.25 1.96 1.09	*Macromol. Chem. Phys*., **2015**, *216*, 504–510.
28	**MFCMP-1**	840	273	1	3.69	*J. Mater. Chem. A*, **2014**, *2*, 13422–13430.
29	**CMP-YA** **CMP-SO-1B2** **CMP-SO-1B3**	1410 1085 1080	273 298 273 298 273 298	1	1.25 1.9 1.19 1.92 1.22 1.89	*Macromolecules*, **2017**, *50*, 4993–5003.
30	**CK-COP-1** **CK-COP-2**	54 615	273	1	0.65 2.21	*J. Polym. Sci., Part A: Polym. Chem*., **2017**, *55*, 2383–2389.
31	**ThPOP-1** **ThPOP-2**	1050 160	273	1	3.41 0.91	*Polym. Chem*., **2016**, *7*, 5031–5038.
32	**Porp-TPE** **Porp-Py-CMP**	547 31	273 273	1.05 1.05	2.09 1.29	*Polym. Chem*., **2019**, *10*, 819–822.
33	**Por-Py-CMP**	1014	273 298	1	3 1.86	*RSC Adv*., **2016**, *6*, 75478–75481.
34	**DA-CMP1** **DA-CMP2** **Azo-CMP1** **Azo-CMP2**	662 603 1146 898	273 298 273 298 273 298 272 298	1.13	2.28 1.35 1.64 0.95 3.72 2.15 3.17 1.96	*J. Mater. Chem. A*, **2015**, *3*, 21185–21193.
35	**SCMP-COOH@1** **SCMP-COOH@2** **SCMP-COOH@3**	911 622 820	298	1	1.39 1.07 1.25	*Polym. Chem*., **2016**, *7*, 4599–4602.
36	**ZnP-5N3-CMPs** **ZnP-25N3-CMPs** **ZnP-50N3-CMPs** **ZnP-75N3-CMPs** **ZnP-100N3-CMPs**	711 685 654 565 477	273 298 273 298 273 298 273 298 273 298	1	1 0.59 1.23 0.7 1.98 1.11 1.64 0.98 1.57 0.91	*Chem. Commun*., **2017**, *53*, 11422–11425.

	ZnP-5F-CMPs	430	273 298		1.32 0.77	
	ZnP-25F-CMPs	352	273 298		1.91 1.18	
	ZnP-50F-CMPs	240	273 298		2.95 2.04	
37	**PCZN-1** **PCZN-2** **PCZN-3** **PCZN-4** **PCZN-5** **PCZN-6** **PCZN-7** **PCZN-8** **PCZN-9** **PCZN-10**	1003 607 714 374 707 718 1058 1126 690 391	273	1	2.57 2.36 2.54 2.02 2.29 2.82 2.91 3.18 2.93 1.7	*Polym. Chem.*, **2017**, *8*, 7240–7247.
38	**PCTF-8**	625	273 293	1	2.47 1.41	*J. Mater. Chem. A*, **2016**, *4*, 13450–13457.
39	**BCMP3**	950	273 298	1	2.41 1.61	*Chem. Eur. J.*, **2015**, *21*, 17355–17362.
40	**LKK-CMP-1**	467	273 298	1	2.22 1.38	*Ind. Eng. Chem. Res.*, **2018**, *57*, 9254–9260.
41	**PCTF-1** **PCTF-2**	2235 784	273 298 273 298	1	3.22 1.84 1.82 0.99	*Chem. Commun.*, **2013**, *49*, 3961–3963.
42	**CPOP-8** **CPOP-9** **CPOP-10**	1610 2440 1110	273	1	3.75 4.13 3.36	*Macromolecules*, **2014**, *47*, 5926–5931.
43	**PTA-1** **PTA-2** **PTA-3**	52 62 450	273 273 303 273 303	1	0.84 1.25 0.59 1.48 0.77	*Chem. Commun.*, **2014**, *50*, 8002–8005.
44	**BILP-101**	536	298	1	2.43	*Chem. Commun.*, **2015**, *51*, 13393–13396.
45	**PAF-33** **PAF-33-NH$_2$** **PAF-33-COOH** **PAF-34** **PAF-34-OH** **PAF-35**	821 370 445 953 771 567	273 298 273 298 273 298 273 298 273 298 273 298	1	2.16 1.25 1.19 0.75 1.94 1.21 2.5 1.39 2.21 1.25 1.77 1.01	*Polym. Chem.*, **2014**, *5*, 2266–2272.
46	**Cu/BF$_4$/BIPLPL-1**	380	273	1	2.57	*J. Phys. Chem. C*, **2015**, *119*, 8174–8182.
47	**BILP-15** **BILP-16** **BILP-15(AC)**	448 435 862	273 298 273 298 273	1	2.68 1.82 2.7 1.83 3.43	*Environ. Sci. Technol.*, **2015**, *49*, 4715–4723.

	BILP-16(AC)	843	298 273 298		2.29 3.46 2.32	
48	**TBILP-1**	117	273 298	1	2.91 1.98	*Macromolecules*, **2014**, *47*, 8328–8334.
49	**BILP-10** **BILP-11** **BILP-13**	787 658 677	273 298 273 298 273 298	1	4.02 2.52 3.09 2 2.57 1.8	*J. Mater. Chem. A*, **2014**, *2*, 12492–12500.
50	**NPOF-1** **NPOF-1-NO_2** **NPOF-1-NO_2(xs)** **NPOF-1-NH_2** **NPOF-1-NH_2(xs)**	2062 1295 749 1535 1074	298	1	1.52 2.52 2 3.77 2.93	*J. Phys. Chem. C*, **2016**, *120*, 2592–2599.
51	**ALP-5** **ALP-6** **ALP-7** **ALP-8**	801 698 412 517	273 298 273 298 273 298 273 298	1	4.46 2.94 3.42 2.17 2.5 1.55 3.05 1.97	*J. Mater. Chem. A*, **2015**, *3*, 20586–20594.

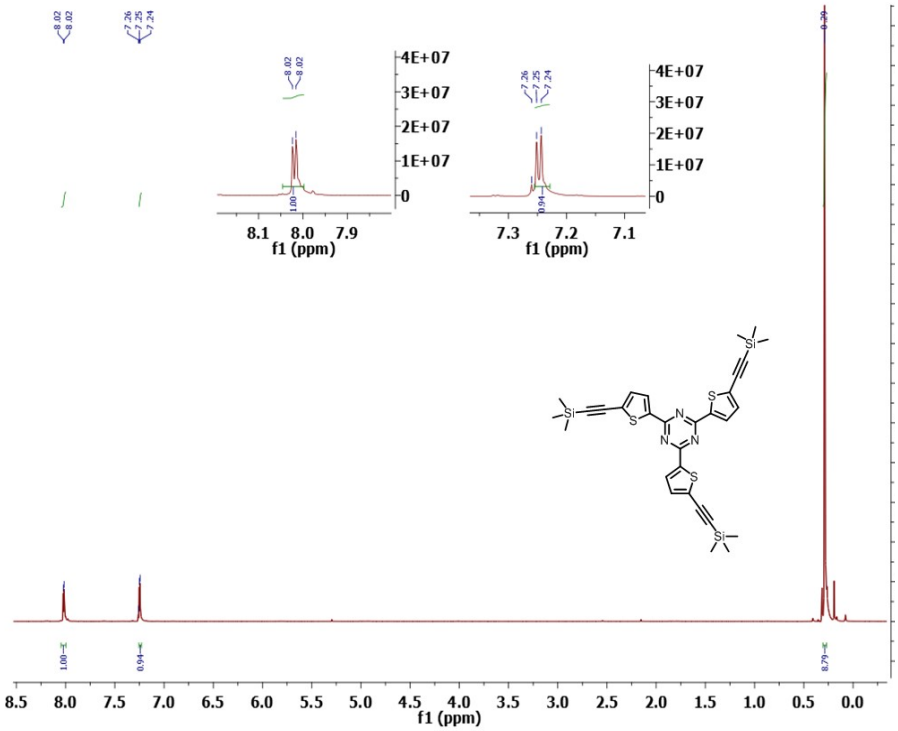


Fig. S13 ^{1}H NMR spectrum of **C** (400 MHz, $CDCl_3$).

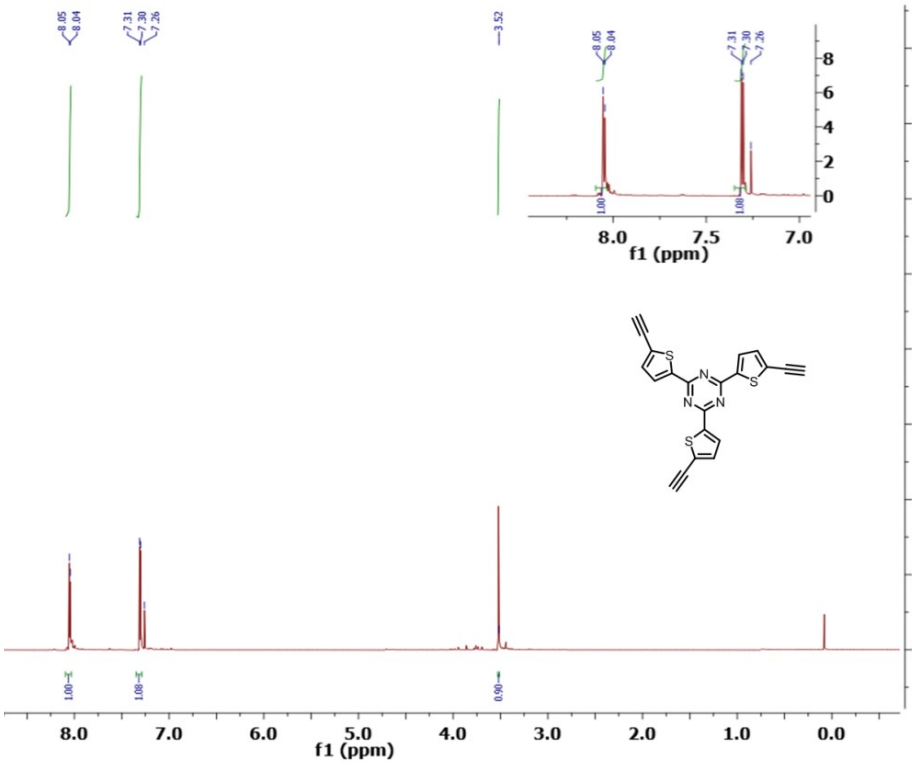


Fig. S14 ^{1}H NMR spectrum of **1**(400 MHz, $CDCl_3$).

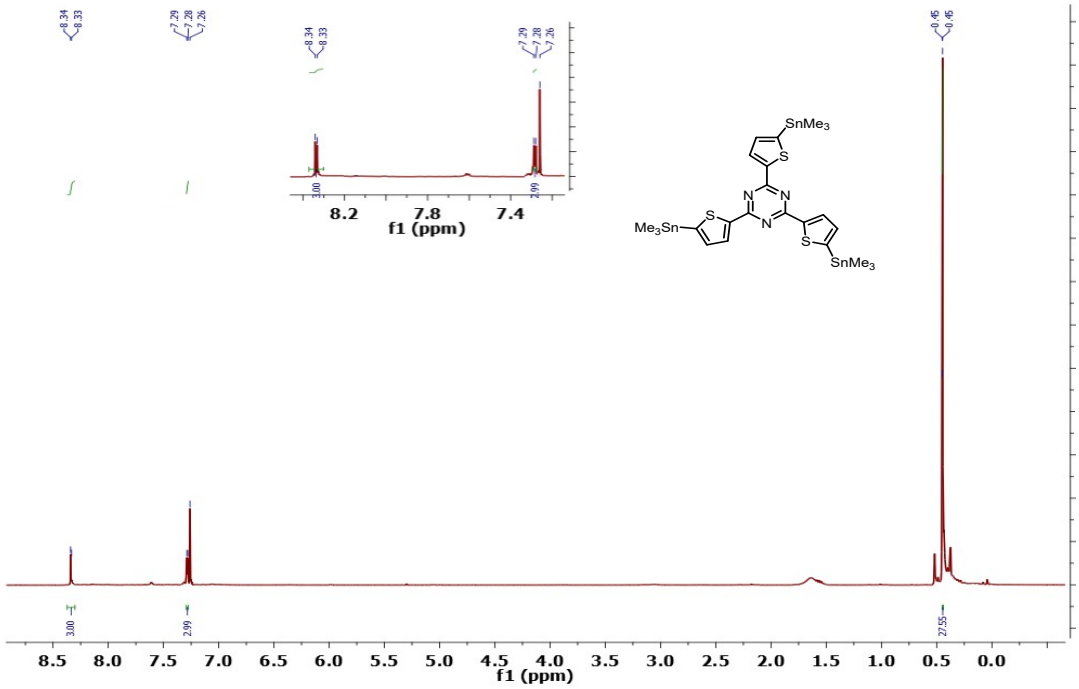


Fig. S15 ^{1}H NMR spectrum of**3** (400 MHz, $CDCl_3$).

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