Electronic Supplementary Information

A building block exchange strategy for rational fabrication of *de novo* unreachable amino-functionalized imine-linked covalent organic frameworks

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Supplementary Methods

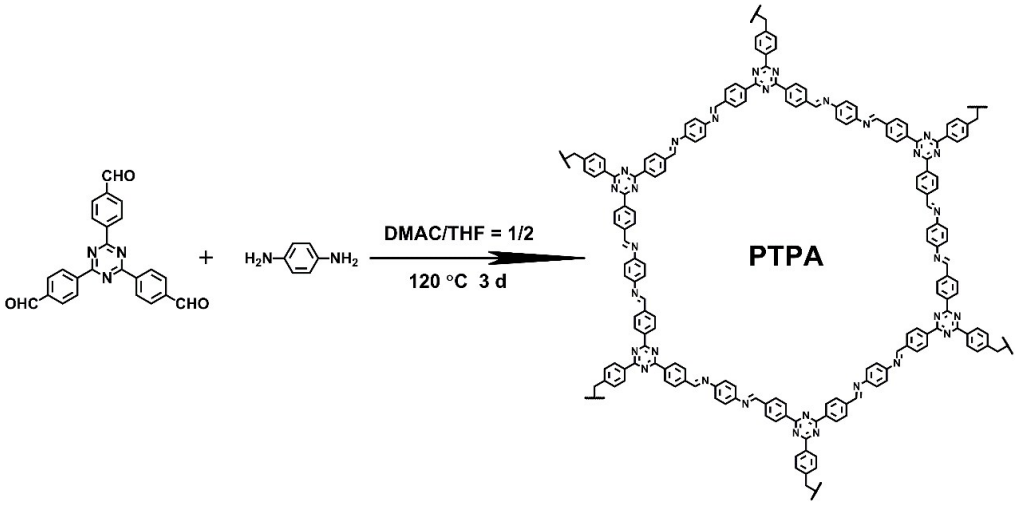
Reagents. All chemicals and reagents used were at least of analytical grade. 1, 3,5-tris(4-formyl-phenyl)triazine (PT) was obtained from Bide Pharmatech Ltd. (Shanghai, China). 1,2,4-Benzenetriamine dihydrochloride (PA-NH_2·2HCl) and 3,3'-Diaminobenzidine (BD-NH_2) were purchased from J&K scientific Co. Ltd. (Beijing, China). 1,4-phenelynediamine (PA), benzidine (BD), N,N-dimethylacetamide (DMAC) and tetrahydrofuran (THF) were purchased from Aladdin Chemistry Co. Ltd. (Shanghai, China). Analytical grade solvent of N,N-dimethylformamide (DMF), Acetone and acetic acid were obtained from Sinopharm Chemical Reagent Co., Ltd (Shanghai, China). Ultrapure water was obtained from Wahaha Foods Co. Ltd. (Shanghai, China).

Instrumentation. PXRD patterns were recorded on a D2 PHASER diffractometer (Bruker, German) using Cu Kα radiation (λ = 1.5418 Å) with a scanning speed of 8° min^{-1} and a step size of 0.02° in 2θ. Solid-state NMR experiments were performed on Infinityplus 400 (VARIAN, USA). SEM images were recorded on an S-3500N (Hitachi, Japan) scanning electron microscope. TEM images were obtained on a JEM-2100 transmission electron microscope (JEOL, Japan) with an accelerating voltage of 200 kV. FTIR spectra were measured on a Nicolet IR IS10 spectrometer (Nicolet, USA) with pure KBr pellets. N_2 adsorption experiments were performed on Autosorb-iQ (Quantachrome, USA) using N_2 adsorption at 77 K. The pore size distribution of prepared COFs was calculated using the density functional theory model. Elemental analysis was carried out on a vario EL CUBE analyzer (Elementary, Germany).

Dynamic light scattering experiments and zeta potential determination were carried out on a Malvern Nano-ZSE (Worcester shire, UK).

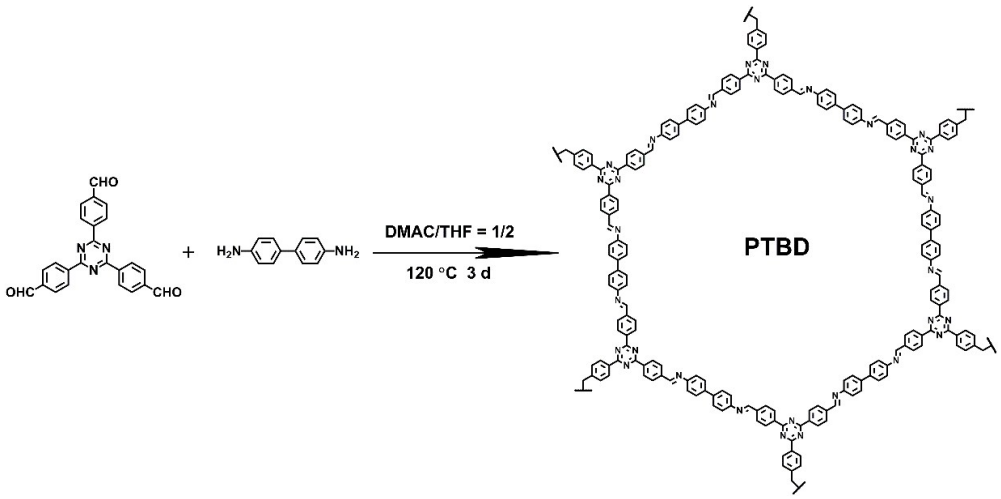
Synthetic Procedures

PTPA: A 35 mL Schlenk tube (OD 26 × L 125 mm) was charged with PT (39.9 mg, 0.1 mmol), PA (16.3 mg, 0.15 mmol), THF (2.0 mL), DMAC (1 mL) and aqueous acetic acid (0.3 mL, 6 M). The tube was sonicated for 10 min and then frozen by liquid nitrogen. After degassing with three freeze–pump–thaw cycles, the tube was sealed and left undisturbed at 120 °C for 3 d. The obtained dark yellow precipitate was centrifuged to remove the solvent. After rinsing with DMF and THF, The crude product was extracted with acetone followed by drying under vacuum at 80 °C for 12 h to obtain PTPA in ca. 81 % isolated yield. EA of sample: Anal. Calcd. for $(C_{11}H_7N_2)n$ (%): C 79.02; H 4.22; N 16.76. Found (mean ± *s*, *n* = 3; %): C 76.85 ± 1.98; H 4.70 ± 0.36; N 17.45 ± 1.05.



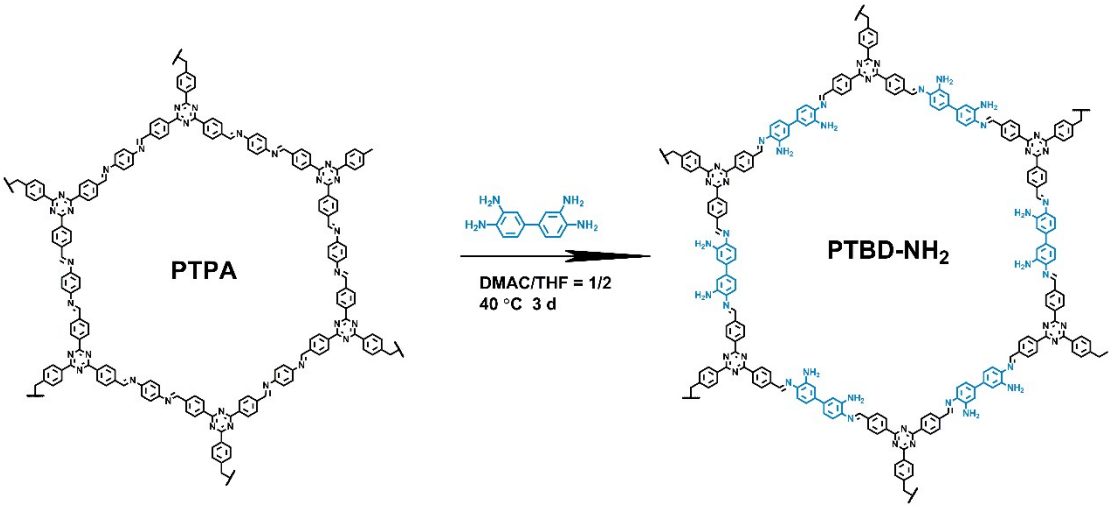
PTBD: A 35 mL Schlenk tube (OD 26 × L 125 mm) was charged with PT (39.93 mg, 0.1 mmol), BD (27.6 mg, 0.15 mmol), THF (2.0 mL), DMAC (1 mL) and aqueous acetic acid (0.3 mL, 6 M). The tube was sonicated for 10 min and then frozen by

liquid nitrogen. After degassing with three freeze–pump–thaw cycles, the tube was sealed and left undisturbed at 120 °C for 3 d. The obtained dark yellow precipitate was centrifuged to remove the solvent. After rinsing with DMF and THF, The crude product was extracted with acetone followed by drying under vacuum at 80 °C for 12 h to obtain PTBD in ca. 85 % isolated yield. EA of sample: Anal. Calcd. for $(C_{14}H_9N_2)n$ (%): C 81.93; H 4.42; N 13.65. Found (mean ± *s*, *n*=3; %): C 79.74 ± 2.25; H 4.54 ± 0.43; N 14.16 ± 0.84.



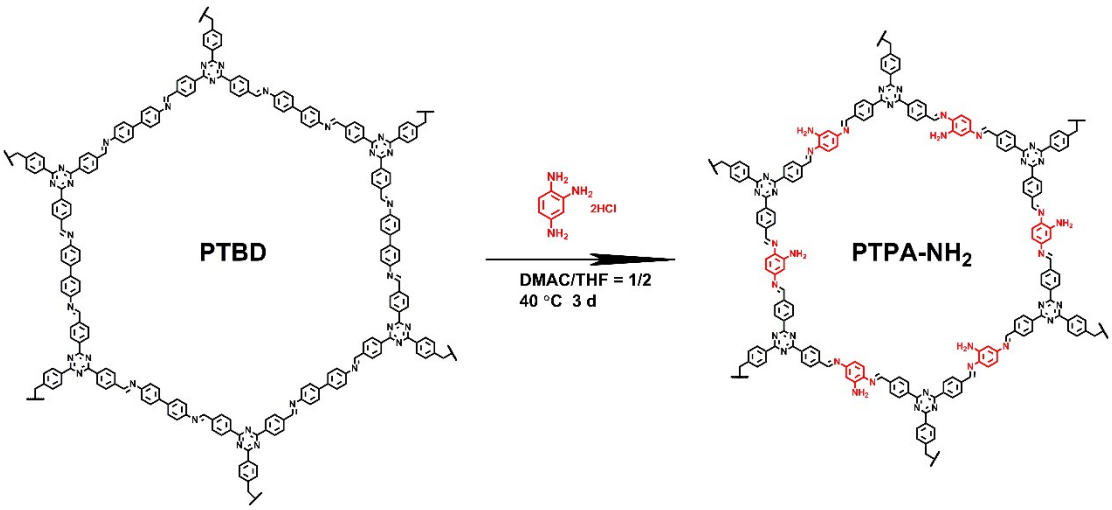
PTBD-NH_2 via BBE: A 35 mL Schlenk tube (OD 26 × L 125 mm) was filled with PT (39.9 mg, 0.1 mmol), PA (16.3 mg, 0.15 mmol), aqueous acetic acid (0.3 mL, 6 M), THF (2.0 mL) and DMAC (1 mL). The tube was sonicated for 10 min and then frozen by liquid nitrogen. After degassing with three freeze–pump–thaw cycles, the tube was sealed and left undisturbed at 120 °C for 3 d. After the Schlenk tube containing PTPA was cooled to room temperature (RT), BD-NH_2 (321.4 mg, 1.5 mmol, 10 equiv), aqueous acetic acid (150 μL, 6 M), tetrahydrofuran (THF) (1.0 mL) and N,N-dimethylacetamide (DMAC) (0.5 mL) were added in sequence. The tube was sonicated for 10 min and then frozen by liquid nitrogen. After degassing with

three freeze–pump–thaw cycles, the tube was sealed and left undisturbed with a 40 °C water bath for 3 d. The obtained dark red precipitate was centrifuged to remove the solvent. After rinsing with N,N-dimethylformamide (DMF) and THF, The crude product was extracted with acetone followed by drying under vacuum at 80 °C for 12 h to obtain PTBD-NH_2 in ca.79 % isolated yield. EA of sample: Anal. Calcd. for $(C_{84}H_{60}N_{18})n$ (%): C 76.35; H 4.58; N 19.08. Found (mean ± *s*, *n* = 3; %): C 73.51 ± 2.39; H 4.78 ± 0.44; N 20.15 ± 1.21.



PTPA-NH_2 via BBE: A 35 mL Schlenk tube (OD 26 × L 125 mm) was filled with PT (39.93 mg, 0.1 mmol), BD (27.6 mg, 0.15 mmol), aqueous acetic acid (0.3 mL, 6 M), THF (2.0 mL) and DMAC (1 mL). The tube was sonicated for 10 min and then frozen by liquid nitrogen. After degassing with three freeze–pump–thaw cycles, the tube was sealed and left undisturbed at 120 °C for 3 d. After the Schlenk tube containing PTBD was cooled to RT, PA-NH_2·2HCl (29.4 mg, 0.15 mmol, 1 equiv), THF (1.0 mL), DMAC (0.5 mL) aqueous acetic acid (150 μL, 6 M) and 12 M NaOH (24 μL) were added in sequence. The tube was then sonicated for 10 min and frozen by liquid

nitrogen. After degassing with three freeze–pump–thaw cycles, the tube was sealed and left undisturbed with a 40 °C water bath for 3 d. The obtained tangerine precipitate was centrifuged to remove the solvent. After rinsing with DMF and THF, the crude product was extracted with acetone followed by drying under vacuum at 80 °C for 12 h to obtain PTPA-NH_2 in ca.73 % isolated yield. EA of sample: Anal. Calcd. for $(C_{66}H_{45}N_{15})n$ (%): C 75.63; H 4.33; N 20.04. Found (mean ± *s*, *n*=3; %): C 73.73 ± 1.94; H 4.67 ± 0.40; N 20.26 ± 1.16.



Charaterization

Structural simulation and PXRD analysis. Structure modeling of the PTPA, PTBD, PTPA-NH_2 and PTBD-NH_2 were conducted with Material Studio suite of programs by Accelrys according to the previous work[1-3].

The initial lattice was generated with the space group P6/m (a = b = 36.2000 Å, c = 3.4000 Å), and the unit cell was defined by two PT molecules bond to PA via six hydrazine linkages. After geometry optimization using MS Forcite molecular module (Universal force fields, Ewald summations), the crude structure modeling of the

PTPA was obtained. Subsequently, pawley refinement was applied to obtain the refined PXRD profile with the lattice parameters of a = b = 35.58449 Å, c = 3.504939 Å, Rwp = 5.36%, Rp = 3.93%. Moreover, a staggered arrangement for PTPA as an alternative structure was also performed wherein the initial lattice was generated with the space group P63/m, a = b = 37.242832 Å, c = 6.944807 Å.

Molecular modeling of PTBD, PTPA-NH_2 and PTBD-NH_2 was performed in the same way as for PTPA. The results imply that the structure of PTBD, PTPA-NH_2 and PTBD-NH_2 adopts the AA stacking mode of a space group P6/m with a = b = 43.918247 Å, c = 3.554862 Å, $\alpha = \beta = 90°$ and $\gamma = 120°$, P1 with a = b = 37.09307 Å, c = 3.478291 Å, $\alpha = \beta = 90°$ and $\gamma = 120°$ and P1 with a = b = 41.870403 Å, c = 3.76792 Å, $\alpha = \beta = 90°$ and $\gamma = 120°$, respectivly. The alternative structure of staggered arrangement for PTBD, PTPA-NH_2 and PTBD-NH_2 were generated by P63/m with a = b = 44.86391 Å, c = 6.934825 Å, P1 with a = b = 37.242832 Å, c = 6.944807 Å and P1 with a = b = 44.639395 Å, c = 6.927715 Å respectivly.

Supplementary Figures

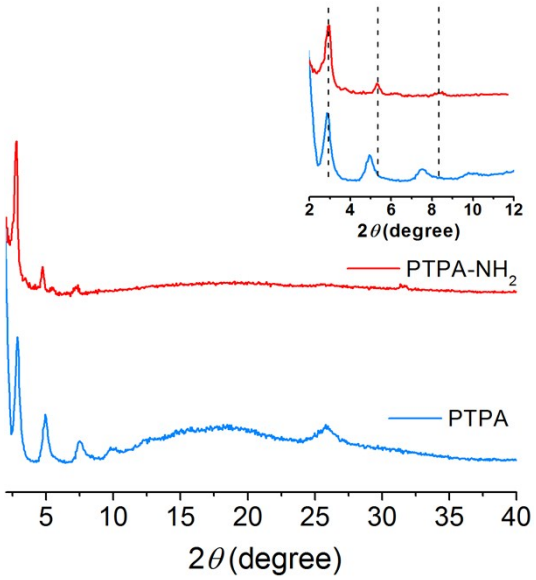


Fig. S1 Comparison of PXRD patterns of PTPA and PTPA-NH_2 via BBE.

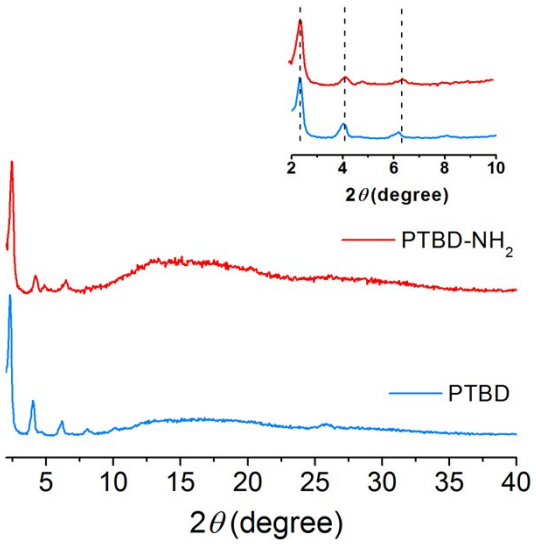


Fig. S2 Comparison of PXRD patterns of PTBD and PTBD-NH_2 via BBE.

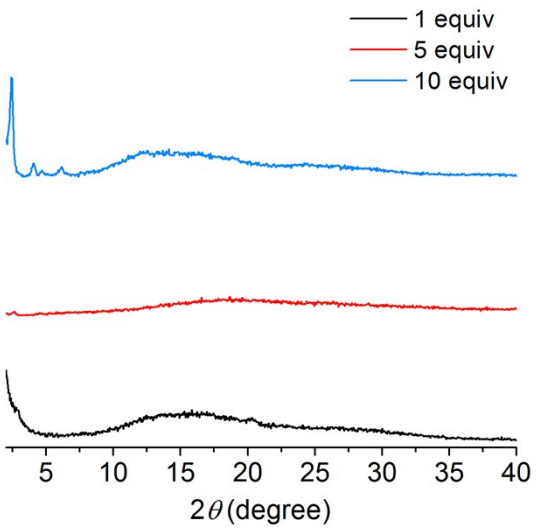


Fig. S3 Effect of BD-NH_2 content on the PXRD pattern of the PTBD-NH_2.

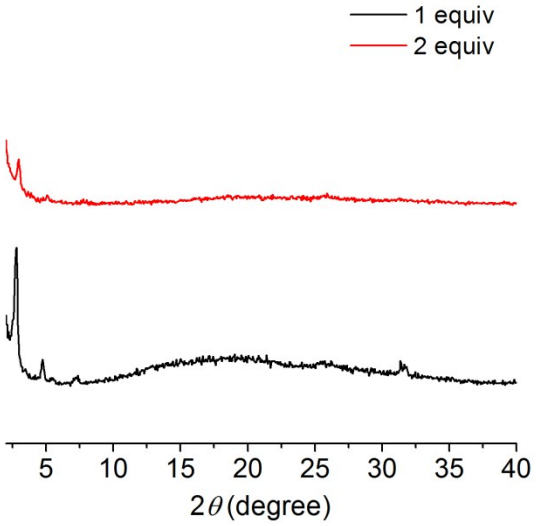


Fig. S4 Effect of PA-NH_2 content on the PXRD pattern of the PTPA-NH_2.

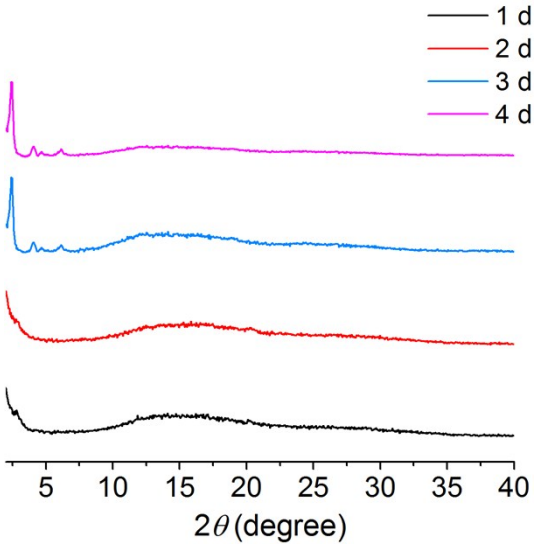


Fig. S5 Effect of reaction time on the PXRD pattern of the PTBD-NH_2.

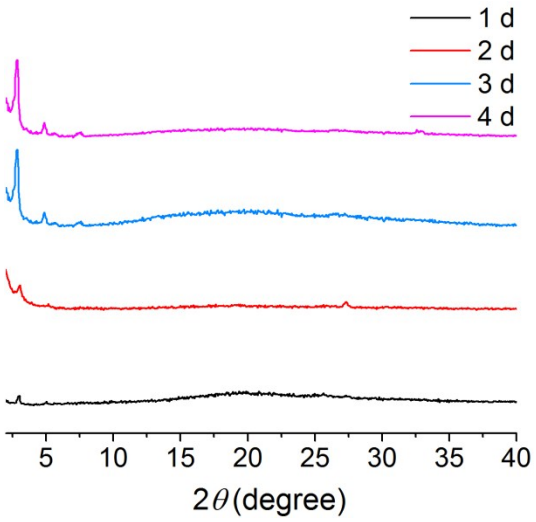


Fig. S6 Effect of reaction time on the PXRD pattern of the PTPA-NH_2.

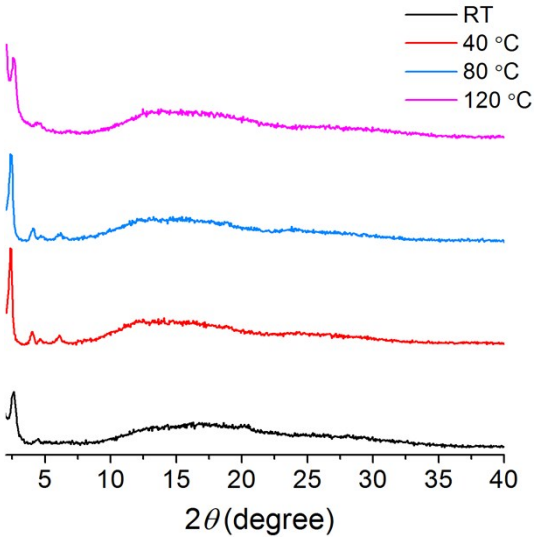


Fig. S7 Effect of reaction temperature on the PXRD pattern of the PTBD-NH_2.

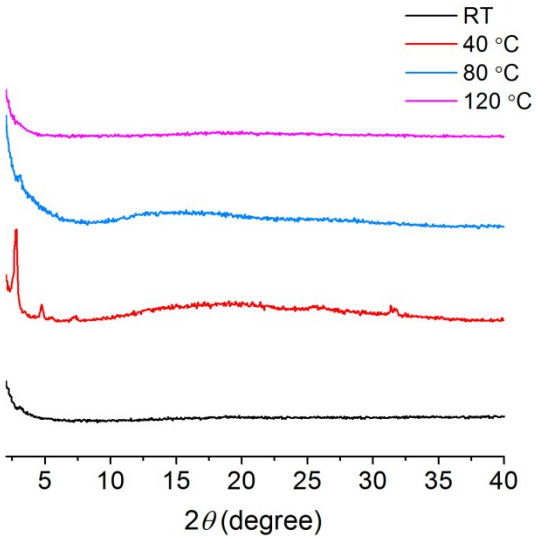


Fig. S8 Effect of reaction temperature on the PXRD pattern of the PTPA-NH_2.

Fig. S9 Photos for the prepared PTBD-NH_2 (right) from PTPA (left) via the BBE strategy.

Fig. S10 Photos for the prepared PTPA-NH_2 (right) from PTBD (left) via the BBE strategy.

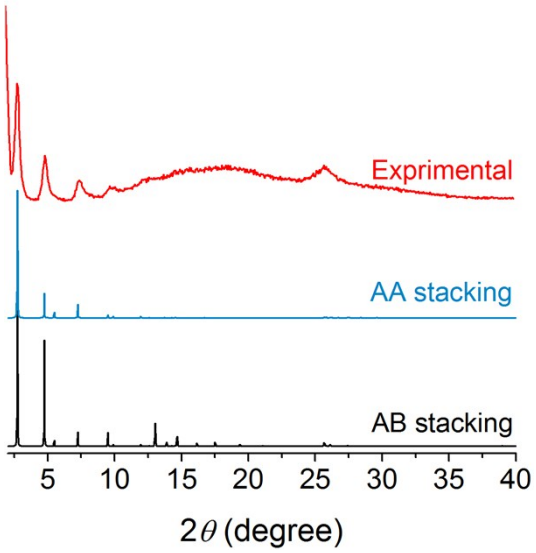


Fig. S11 PXRD patterns of PTPA: experimental (red), simulated for the AA eclipsed model (blue), and AB staggered model (black).

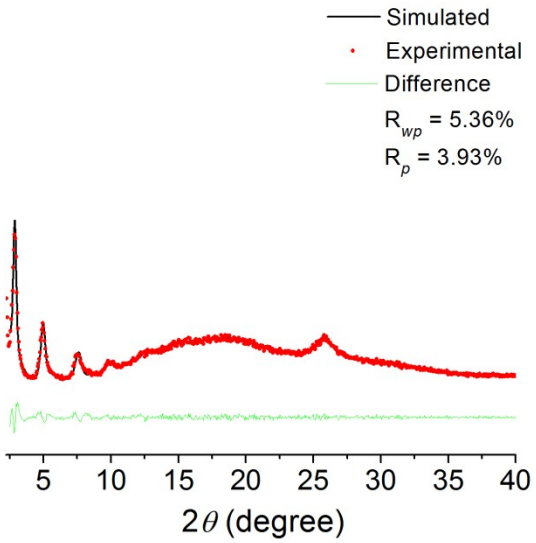


Fig. S12 Pawley refinement of PTPA

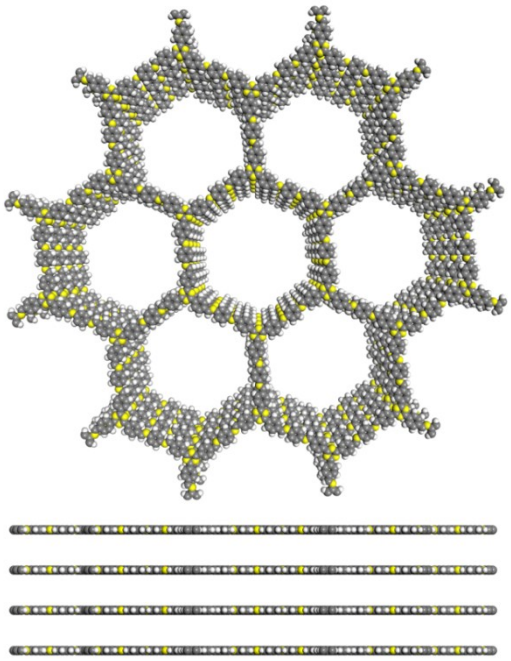


Fig. S13 AA Staggered unit cell of PTPA.

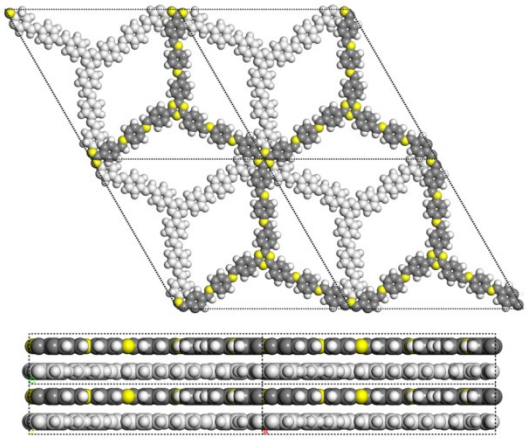


Fig. S14 AB Staggered unit cell of PTPA.

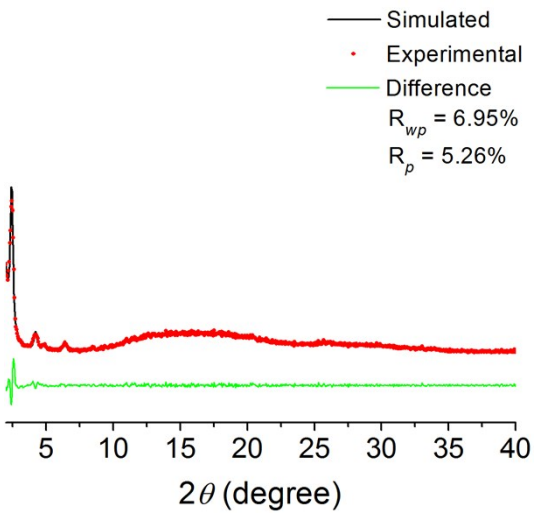


Fig. S15 Pawley refinement of PTBD-NH_2.

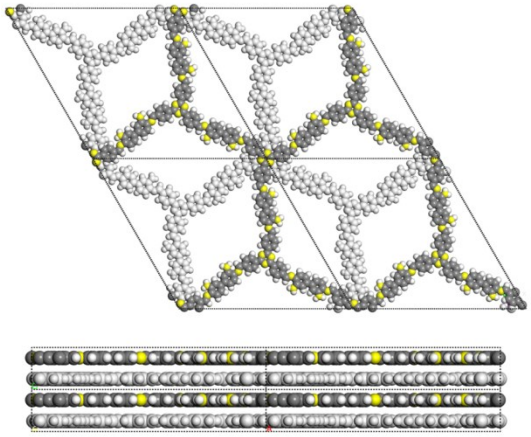


Fig. S16 AB Staggered unit cell of PTBD-NH_2.

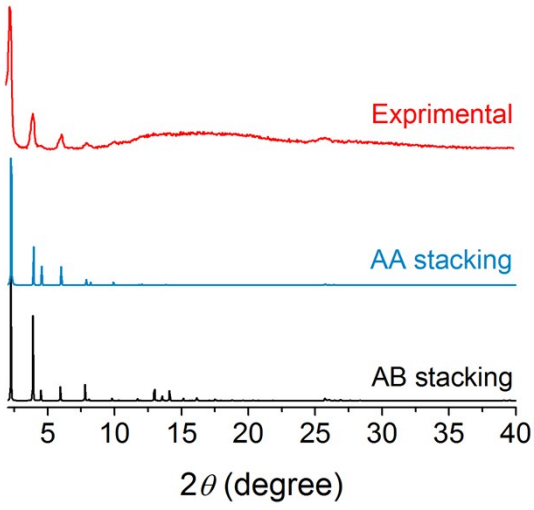


Fig. S17 Experimental pattern, simulated pattern for the AA eclipsed model and AB

staggered model of PTBD.

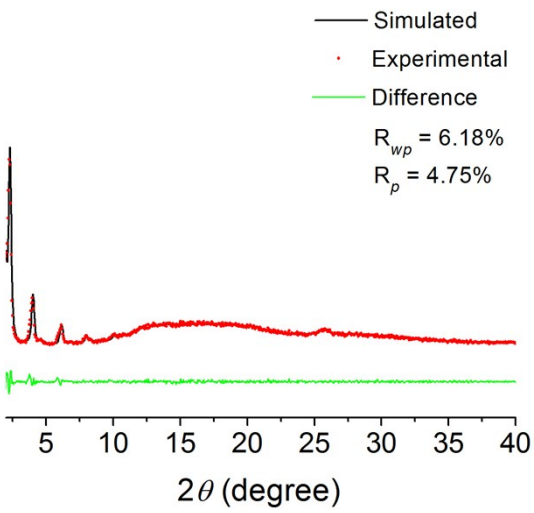


Fig. S18 Pawley refinement of PTBD.

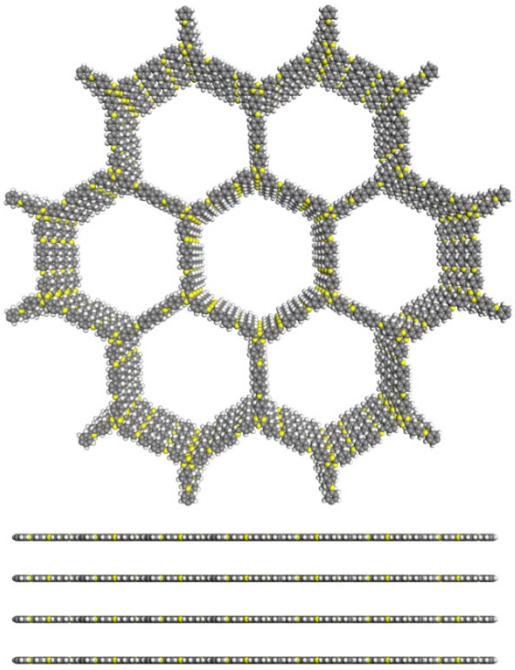


Fig. S19 AA Staggered unit cell of PTBD.

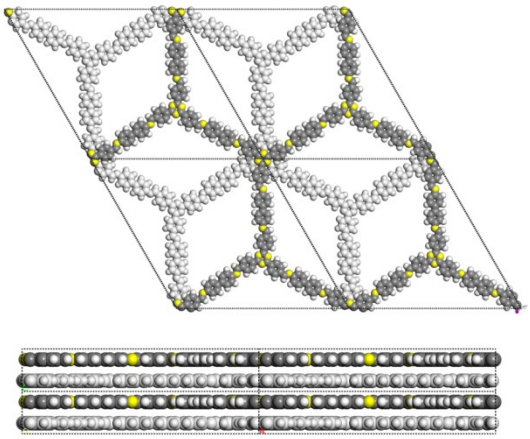


Fig. S20 AB Staggered unit cell of PTBD.

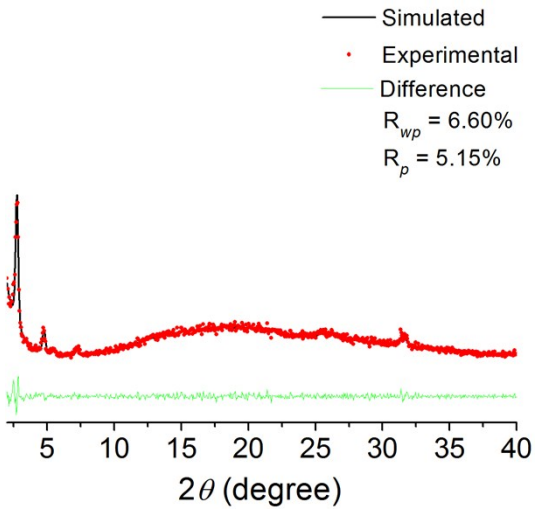


Fig. S21 Pawley refinement of PTPA-NH_2.

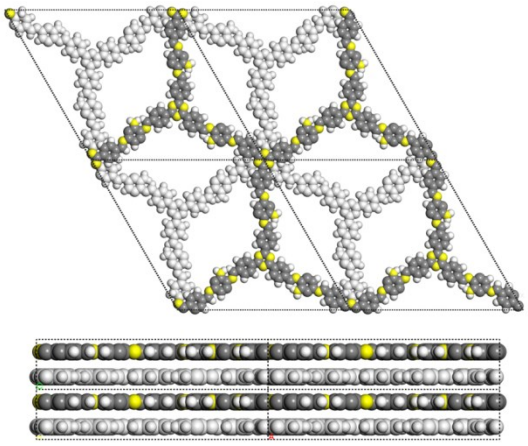


Fig. S22 AB Staggered unit cell of PTPA-NH_2.

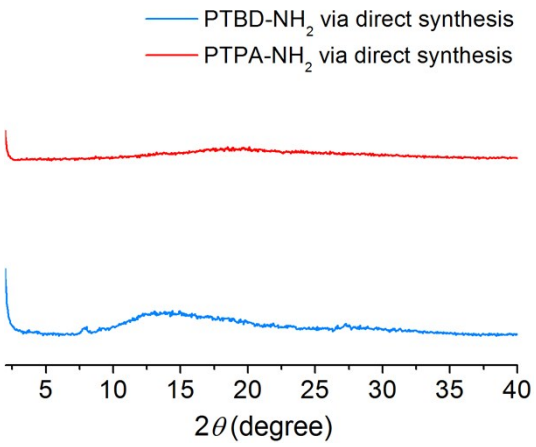


Fig. S23 PXRD patterns of the polymers prepared from the direct condensation of PT with PA-NH_2 and BD-NH_2.

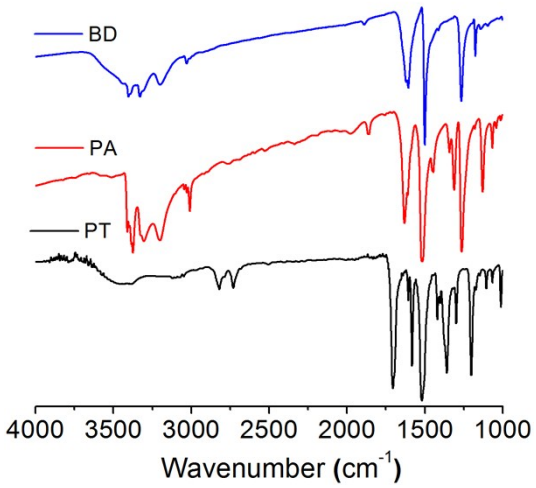


Fig. S24 FTIR spectra of PT, BD and PA.

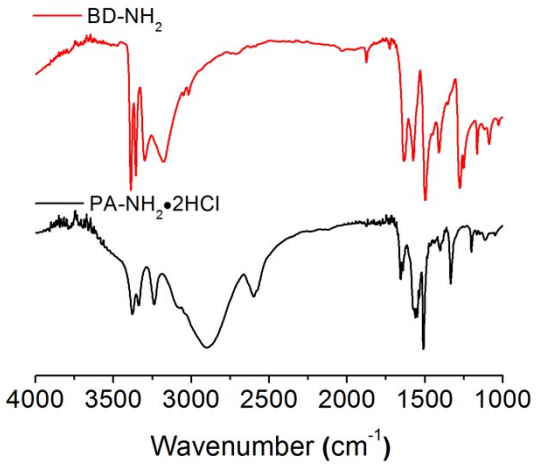


Fig. S25 FTIR spectra of BD-NH_2 and PA-NH_2.

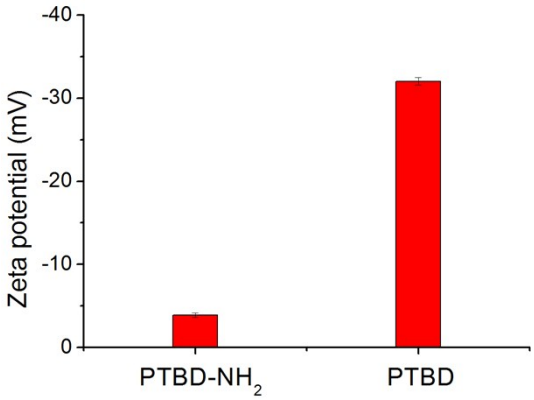


Fig. S26 Zeta potential of PTBD and PTBD-NH_2.

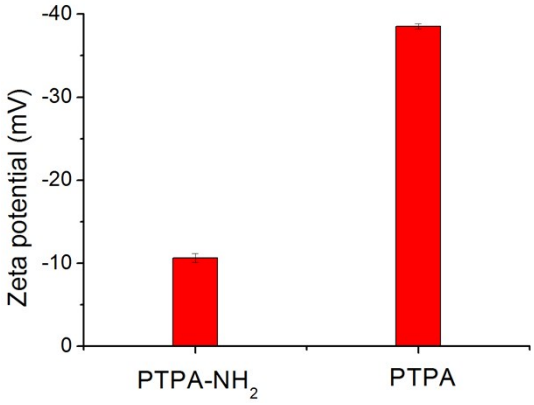


Fig. S27 Zeta potential of PTPA and PTPA-NH_2.

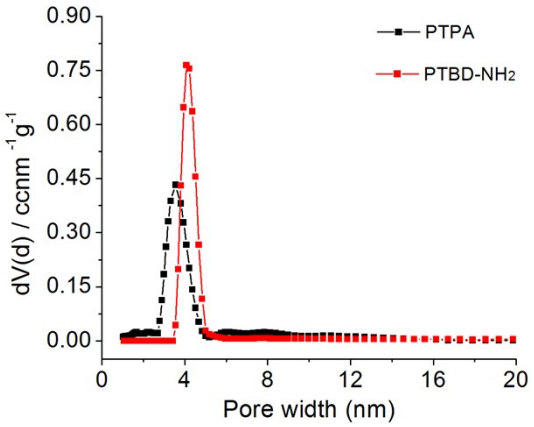


Fig. S28 Pore size distribution curves of PTPA and PTBD-NH_2.

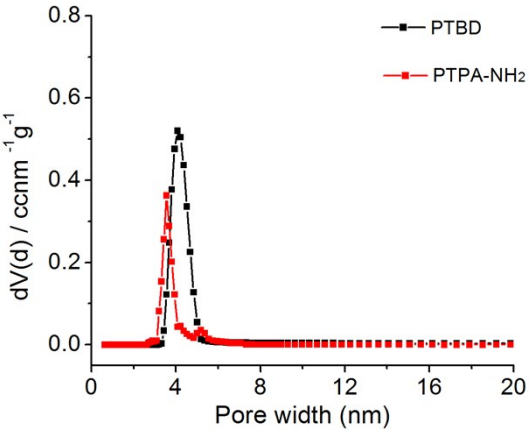


Fig. S29 Pore size distribution curves of PTBD and PTPA-NH_2.

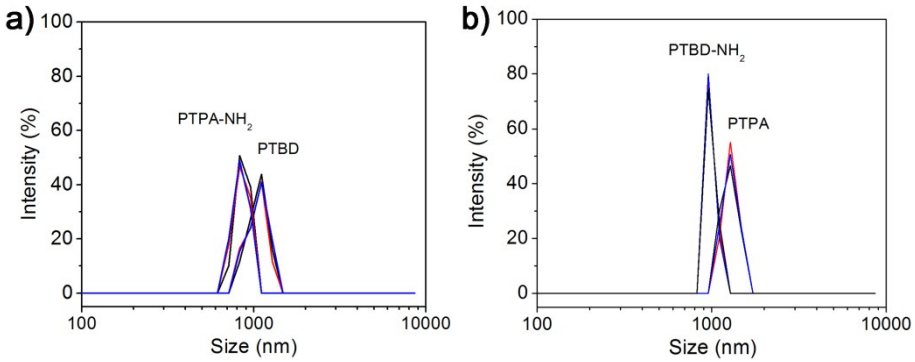


Fig. S30 The dynamic light scattering spectra of (a) PTBD and PTPA-NH_2, and (b) PTPA and PTPA-NH_2.

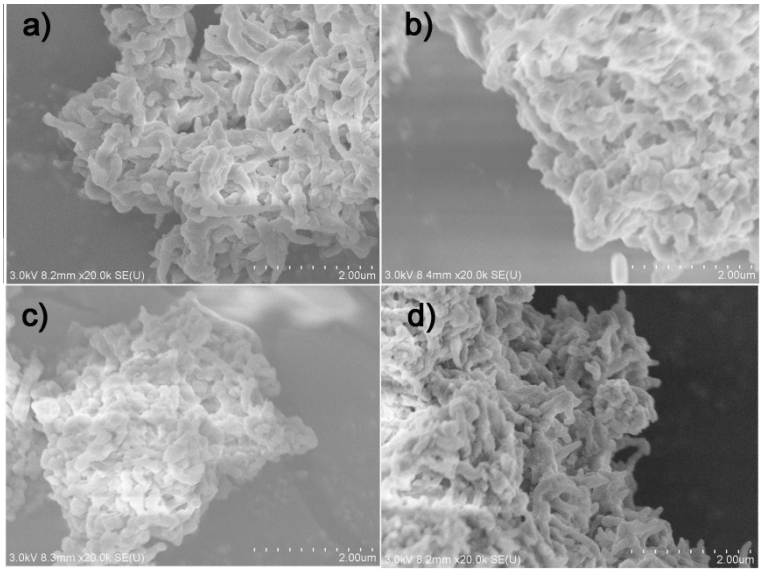


Fig. S31 SEM images of the as-prepared COFs. (a,b) SEM images of mother ICOFs PTPA and PTBD. (c,d) SEM images of daughter ICOFs-NH_2 PTBD-NH_2 and PTPA-NH_2.

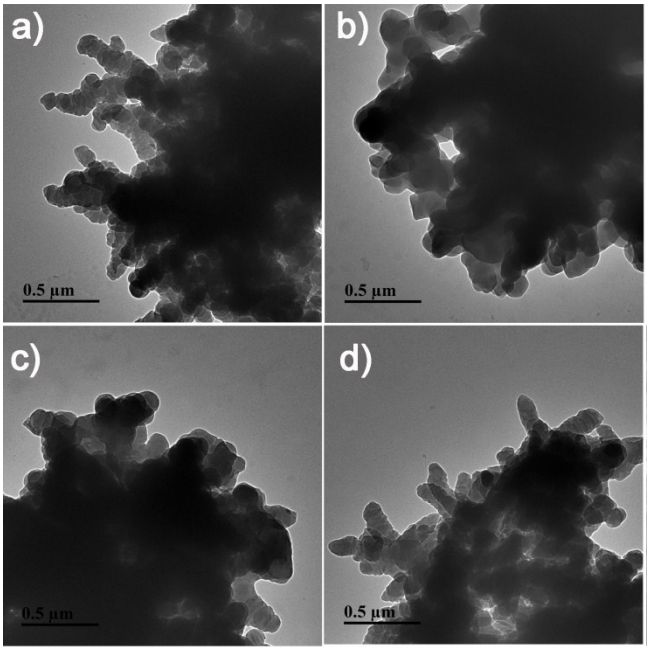


Fig. S32 TEM images of the as-prepared COFs. (a,b) TEM images of mother ICOFs PTPA and PTBD. (c,d) TEM images of daughter ICOFs-NH_2 PTBD-NH_2 and PTPA-NH_2.

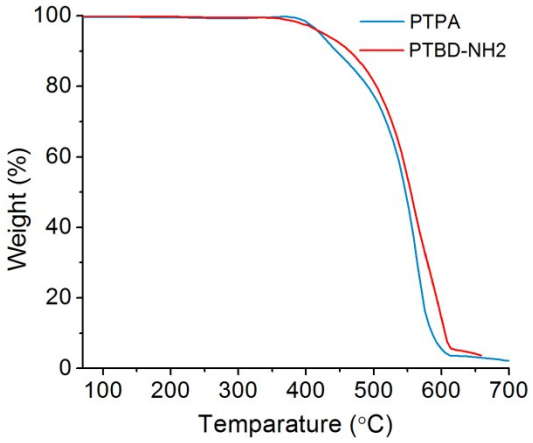


Fig. S33 Thermogravimetric curves for PTPA and PTBD-NH_2.

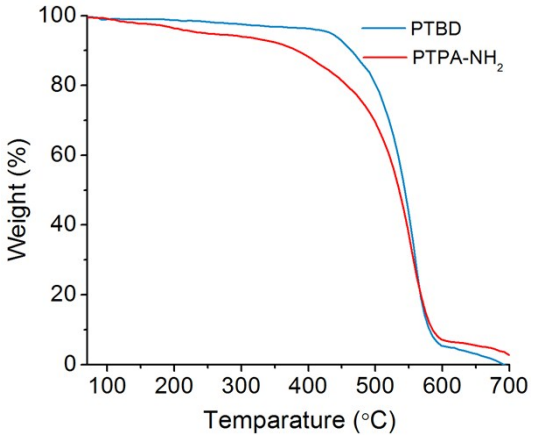


Fig. S34 Thermogravimetric curves for PTBD and PTPA-NH_2.

Supplementary Tables

Table S1 Fractional main atomic coordinates for the unit cell of PTPA after Pawley refinement.

PTPA: Space group symmetry P6/m **a = b = 35.5845 Å, c = 3.5049 Å, α = β = 90° and γ = 120°**			
Atom	x	y	z
N1	0.31743	-0.30775	0.50000
C2	0.29153	-0.34936	0.50000
C3	0.38725	-0.24591	0.50000
C4	0.43054	-0.22891	0.50000
C5	0.45703	-0.18595	0.50000
C6	0.44085	-0.1591	0.50000
C7	0.39766	-0.17592	0.50000
C8	0.37113	-0.21887	0.50000
C9	0.46937	-0.11382	0.50000
N10	0.4566	-0.45506	0.50000
C11	0.47757	-0.47863	0.50000
C12	0.45663	-0.52227	0.50000
C13	0.47908	-0.54321	0.50000
H14	0.44386	-0.24893	0.50000
H15	0.49023	-0.17366	0.50000
H16	0.38455	-0.15571	0.50000
H17	0.33795	-0.23101	0.50000
H18	0.50227	-0.10269	0.50000
H19	0.42328	-0.5405	0.50000
H20	0.46281	-0.57674	0.50000
N1	0.31743	-0.30775	0.50000

Table S2 Fractional main atomic coordinates for the unit cell of PTBD-NH_2 after Pawley refinement.

PTBD-NH2: Space group symmetry P1 **a = b = 41.8704 Å, c = 3.7679 Å, α = β = 90° and γ = 120°**							
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	
N1	0.32022	0.68798	0.50000	N82	0.67978	0.31202	0.50000
C2	0.35481	0.70135	0.50000	C83	0.64519	0.29865	0.50000
C3	0.37825	0.73921	0.50000	C84	0.62175	0.26079	0.50000
C4	0.36496	0.76174	0.50000	C85	0.63504	0.23826	0.50000
C5	0.38706	0.79738	0.50000	C86	0.61294	0.20262	0.50000
C6	0.4229	0.81125	0.50000	C87	0.5771	0.18875	0.50000
C7	0.43624	0.78887	0.50000	C88	0.56376	0.21113	0.50000
C8	0.41417	0.75323	0.50000	C89	0.58583	0.24677	0.50000
C9	0.44667	0.84881	0.50000	C90	0.55333	0.15119	0.50000
N10	0.43488	0.87005	0.50000	N91	0.56512	0.12995	0.50000
C11	0.45454	0.90703	0.50000	C92	0.54546	0.09297	0.50000
C12	0.49064	0.92578	0.50000	C93	0.50936	0.07422	0.50000
C13	0.50825	0.96178	0.50000	C94	0.49175	0.03822	0.50000
C14	0.49047	0.98047	0.50000	C95	0.50953	0.01953	0.50000
C15	0.45404	0.96092	0.50000	C96	0.54596	0.03908	0.50000
C16	0.43663	0.92496	0.50000	C97	0.56337	0.07504	0.50000
H17	0.3359	0.7507	0.50000	H98	0.6641	0.2493	0.50000
H18	0.37602	0.8154	0.50000	H99	0.62398	0.1846	0.50000
H19	0.46528	0.79972	0.50000	H100	0.53472	0.20028	0.50000
H20	0.42524	0.73523	0.50000	H101	0.57476	0.26477	0.50000
H21	0.47567	0.85947	0.50000	H102	0.52433	0.14053	0.50000
H22	0.50568	0.91311	0.50000	N103	0.49432	0.08689	0.50000
H23	0.53759	0.97677	0.50000	H104	0.46241	0.02323	0.50000
H24	0.43831	0.97451	0.50000	H105	0.56169	0.02549	0.50000
N25	0.40879	0.91071	0.50000	H106	0.59121	0.08929	0.50000
H26	0.39478	0.88572	0.50000	H107	0.50388	0.11173	0.50000
H27	0.39423	0.9211	0.50000	H108	0.46928	0.0751	0.50000
N28	0.31202	0.63224	0.50000	N109	0.68798	0.36776	0.50000
C29	0.29865	0.65346	0.50000	C110	0.70135	0.34654	0.50000
C30	0.26079	0.63904	0.50000	C111	0.73921	0.36096	0.50000
C31	0.23826	0.60322	0.50000	C112	0.76174	0.39678	0.50000
C32	0.20262	0.58969	0.50000	C113	0.79738	0.41031	0.50000
C33	0.18875	0.61166	0.50000	C114	0.81125	0.38834	0.50000
C34	0.21113	0.64737	0.50000	C115	0.78887	0.35263	0.50000
C35	0.24677	0.66094	0.50000	C116	0.75323	0.33906	0.50000
C36	0.15119	0.59786	0.50000	C117	0.84881	0.40214	0.50000
N37	0.12995	0.56483	0.50000	N118	0.87005	0.43517	0.50000
C38	0.09297	0.54751	0.50000	C119	0.90703	0.45249	0.50000
C39	0.07422	0.56486	0.50000	C120	0.92578	0.43514	0.50000
C40	0.03822	0.54647	0.50000	C121	0.96178	0.45353	0.50000
C41	0.01953	0.51	0.50000	C122	0.98047	0.49	0.50000
C42	0.03908	0.49312	0.50000	C123	0.96092	0.50688	0.50000
C43	0.07504	0.51168	0.50000	C124	0.92496	0.48832	0.50000
H44	0.2493	0.5852	0.50000	H125	0.7507	0.4148	0.50000
H45	0.1846	0.56062	0.50000	H126	0.8154	0.43938	0.50000
H46	0.20028	0.66556	0.50000	H127	0.79972	0.33444	0.50000

H47	0.26477	0.69001	0.50000	H128	0.73523	0.30999	0.50000
H48	0.14053	0.6162	0.50000	H129	0.85947	0.3838	0.50000
H49	0.08689	0.59257	0.50000	N130	0.91311	0.40743	0.50000
H50	0.02323	0.56082	0.50000	H131	0.97677	0.43918	0.50000
H51	0.02549	0.4638	0.50000	H132	0.97451	0.5362	0.50000
N52	0.08929	0.49807	0.50000	H133	0.91071	0.50193	0.50000
H53	0.11428	0.50906	0.50000	H134	0.88827	0.39215	0.50000
H54	0.0789	0.47313	0.50000	H135	0.9249	0.39418	0.50000
N55	0.36776	0.67978	0.50000	N136	0.63224	0.32022	0.50000
C56	0.34654	0.64519	0.50000	C137	0.65346	0.35481	0.50000
C57	0.36096	0.62175	0.50000	C138	0.63904	0.37825	0.50000
C58	0.39678	0.63504	0.50000	C139	0.60322	0.36496	0.50000
C59	0.41031	0.61294	0.50000	C140	0.58969	0.38706	0.50000
C60	0.38834	0.5771	0.50000	C141	0.61166	0.4229	0.50000
C61	0.35263	0.56376	0.50000	C142	0.64737	0.43624	0.50000
C62	0.33906	0.58583	0.50000	C143	0.66094	0.41417	0.50000
C63	0.40214	0.55333	0.50000	C144	0.59786	0.44667	0.50000
N64	0.43517	0.56512	0.50000	N145	0.56483	0.43488	0.50000
C65	0.45249	0.54546	0.50000	C146	0.54751	0.45454	0.50000
C66	0.43514	0.50936	0.50000	C147	0.56486	0.49064	0.50000
C67	0.45353	0.49175	0.50000	C148	0.54647	0.50825	0.50000
C68	0.49	0.50953	0.50000	C149	0.51	0.49047	0.50000
C69	0.50688	0.54596	0.50000	C150	0.49312	0.45404	0.50000
C70	0.48832	0.56337	0.50000	C151	0.51168	0.43663	0.50000
H71	0.4148	0.6641	0.50000	H152	0.5852	0.3359	0.50000
H72	0.43938	0.62398	0.50000	H153	0.56062	0.37602	0.50000
H73	0.33444	0.53472	0.50000	H154	0.66556	0.46528	0.50000
H74	0.30999	0.57476	0.50000	H155	0.69001	0.42524	0.50000
H75	0.3838	0.52433	0.50000	H156	0.6162	0.47567	0.50000
H76	0.40743	0.49432	0.50000	N157	0.59257	0.50568	0.50000
H77	0.43918	0.46241	0.50000	H158	0.56082	0.53759	0.50000
H78	0.5362	0.56169	0.50000	H159	0.4638	0.43831	0.50000
N79	0.50193	0.59121	0.50000	H160	0.49807	0.40879	0.50000
H80	0.49094	0.60522	0.50000	H161	0.60785	0.49612	0.50000
H81	0.52687	0.60577	0.50000	H162	0.60582	0.53072	0.50000

Table S3 Fractional main atomic coordinates for the unit cell of PTBD after Pawley refinement.

PTBD: Space group symmetry P6/m **a = b = 43.9182 Å, c = 3.5549 Å, α = β = 90° and γ = 120°**			
Atom	**x**	**y**	**z**
N1	0.32022	0.68798	0.50000
C2	0.35481	0.70135	0.50000
C3	0.37825	0.73921	0.50000
C4	0.36496	0.76174	0.50000
C5	0.38706	0.79738	0.50000
C6	0.4229	0.81125	0.50000
C7	0.43624	0.78887	0.50000
C8	0.41417	0.75323	0.50000
C9	0.44667	0.84881	0.50000
N10	0.43488	0.87005	0.50000
C11	0.45454	0.90703	0.50000
C12	0.49064	0.92578	0.50000
C13	0.50825	0.96178	0.50000
C14	0.49047	0.98047	0.50000
C15	0.45404	0.96092	0.50000
C16	0.43663	0.92496	0.50000
H17	0.33743	0.75173	0.50000
H18	0.37624	0.81421	0.50000
H19	0.46379	0.79901	0.50000
H20	0.42517	0.73655	0.50000
H21	0.47396	0.85798	0.50000
H22	0.50568	0.91311	0.50000
H23	0.53586	0.97417	0.50000
H24	0.43812	0.97255	0.50000
H25	0.40879	0.91071	0.50000

Table S4 Fractional main atomic coordinates for the unit cell of PTPA-NH_2 after Pawley refinement.

PTPA-NH2: Space group symmetry P1 **a = b = 37.0931 Å, c = 3.4783 Å, α = β = 90° and γ = 120°**							
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
N1	0.31743	0.69225	0.50000	C64	0.56946	0.22891	0.50000
C2	0.29153	0.65064	0.50000	C65	0.54297	0.18595	0.50000
C3	0.38725	0.75409	0.50000	C66	0.55915	0.1591	0.50000
C4	0.43054	0.77109	0.50000	C67	0.60234	0.17592	0.50000
C5	0.45703	0.81405	0.50000	C68	0.62887	0.21887	0.50000
C6	0.44085	0.8409	0.50000	C69	0.53063	0.11382	0.50000
C7	0.39766	0.82408	0.50000	N70	0.5434	0.45506	0.50000
C8	0.37113	0.78113	0.50000	C71	0.52243	0.47863	0.50000
C9	0.46937	0.88618	0.50000	C72	0.54337	0.52227	0.50000
N10	0.4566	0.54494	0.50000	C73	0.52092	0.54321	0.50000
C11	0.47757	0.52137	0.50000	H74	0.55569	0.25022	0.50000
C12	0.45663	0.47773	0.50000	H75	0.50794	0.17253	0.50000
C13	0.47908	0.45679	0.50000	H76	0.61599	0.15451	0.50000
H14	0.44431	0.74978	0.50000	H77	0.6639	0.23225	0.50000
H15	0.49206	0.82747	0.50000	H78	0.49567	0.10089	0.50000
H16	0.38401	0.84549	0.50000	H79	0.57871	0.54065	0.50000
H17	0.3361	0.76775	0.50000	N80	0.53719	0.57674	0.50000
H18	0.50433	0.89911	0.50000	H81	0.52385	0.59352	0.50000
H19	0.42129	0.45935	0.50000	H82	0.56722	0.59437	0.50000
H20	0.46281	0.42326	0.50000	N83	0.69225	0.37482	0.50000
N21	0.30775	0.62518	0.50000	C84	0.65064	0.35911	0.50000
C22	0.34936	0.64089	0.50000	C85	0.75409	0.36684	0.50000
C23	0.24591	0.63316	0.50000	C86	0.77109	0.34055	0.50000
C24	0.22891	0.65945	0.50000	C87	0.81405	0.35701	0.50000
C25	0.18595	0.64299	0.50000	C88	0.8409	0.40005	0.50000
C26	0.1591	0.59995	0.50000	C89	0.82408	0.42642	0.50000
C27	0.17592	0.57358	0.50000	C90	0.78113	0.41001	0.50000
C28	0.21887	0.58999	0.50000	C91	0.88618	0.4168	0.50000
C29	0.11382	0.5832	0.50000	N92	0.54494	0.08834	0.50000
N30	0.45506	0.91166	0.50000	C93	0.52137	0.0438	0.50000
C31	0.47863	0.9562	0.50000	C94	0.47773	0.0211	0.50000
C32	0.52227	0.9789	0.50000	C95	0.45679	0.97771	0.50000
C33	0.54321	0.02229	0.50000	H96	0.74978	0.30547	0.50000
H34	0.25022	0.69453	0.50000	H97	0.82747	0.33541	0.50000
H35	0.17253	0.66459	0.50000	H98	0.84549	0.46148	0.50000
H36	0.15451	0.53852	0.50000	H99	0.76775	0.43164	0.50000
H37	0.23225	0.56836	0.50000	H100	0.89911	0.39478	0.50000
H38	0.10089	0.60522	0.50000	H101	0.45935	0.03806	0.50000
H39	0.54065	0.96194	0.50000	N102	0.42326	0.96045	0.50000
H40	0.57674	0.03955	0.50000	H103	0.40648	0.93033	0.50000
N41	0.37482	0.68257	0.50000	H104	0.40563	0.97285	0.50000
C42	0.35911	0.70847	0.50000	N105	0.62518	0.31743	0.50000
C43	0.36684	0.61275	0.50000	C106	0.64089	0.29153	0.50000
C44	0.34055	0.56946	0.50000	C107	0.63316	0.38725	0.50000
C45	0.35701	0.54297	0.50000	C108	0.65945	0.43054	0.50000
C46	0.40005	0.55915	0.50000	C109	0.64299	0.45703	0.50000

C47	0.42642	0.60234	0.50000	C110	0.59995	0.44085	0.50000
C48	0.41001	0.62887	0.50000	C111	0.57358	0.39766	0.50000
C49	0.4168	0.53063	0.50000	C112	0.58999	0.37113	0.50000
N50	0.08834	0.5434	0.50000	C113	0.5832	0.46937	0.50000
C51	0.0438	0.52243	0.50000	N114	0.91166	0.4566	0.50000
C52	0.0211	0.54337	0.50000	C115	0.9562	0.47757	0.50000
C53	0.97771	0.52092	0.50000	C116	0.9789	0.45663	0.50000
H54	0.30547	0.55569	0.50000	C117	0.02229	0.47908	0.50000
H55	0.33541	0.50794	0.50000	H118	0.69453	0.44431	0.50000
H56	0.46148	0.61599	0.50000	H119	0.66459	0.49206	0.50000
H57	0.43164	0.6639	0.50000	H120	0.53852	0.38401	0.50000
H58	0.39478	0.49567	0.50000	H121	0.56836	0.3361	0.50000
H59	0.03806	0.57871	0.50000	H122	0.60522	0.50433	0.50000
H60	0.96045	0.53719	0.50000	H123	0.96194	0.42129	0.50000
N61	0.68257	0.30775	0.50000	N124	0.03955	0.46281	0.50000
C62	0.70847	0.34936	0.50000	H125	0.06967	0.47615	0.50000
C63	0.61275	0.24591	0.50000	H126	0.02715	0.43278	0.50000

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