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

Supporting Information

Ionic liquid as a green solvent for high potency synthesis of 2D covalent organic frameworks

Limin Zhao[1*], Huimin Liu[1], Yue Du[1], Xiang Liang[1], Wenju Wang[2], Hui Zhao[1], Wenzhi Li[1]

1. College of Materials Science and Engineering, Liaocheng University, Liaocheng 252059, PR China

2. School of Energy and Power Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

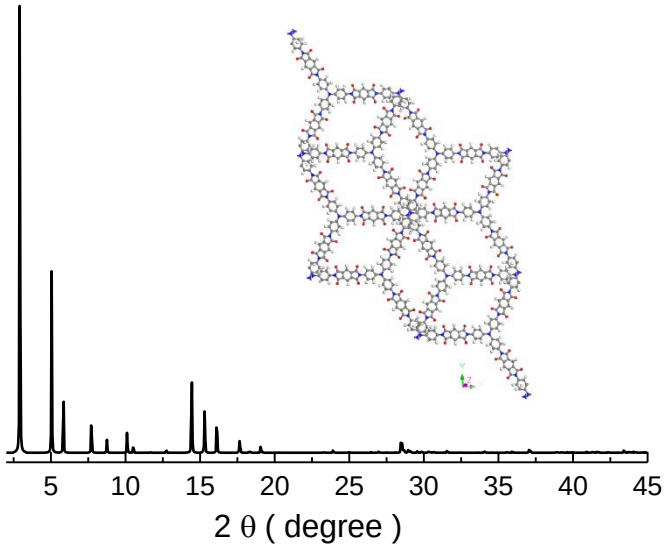

Fig. S1 Calculated PXRD pattern of PI-COF-1 based on the space group of $P6_3$ /mmc

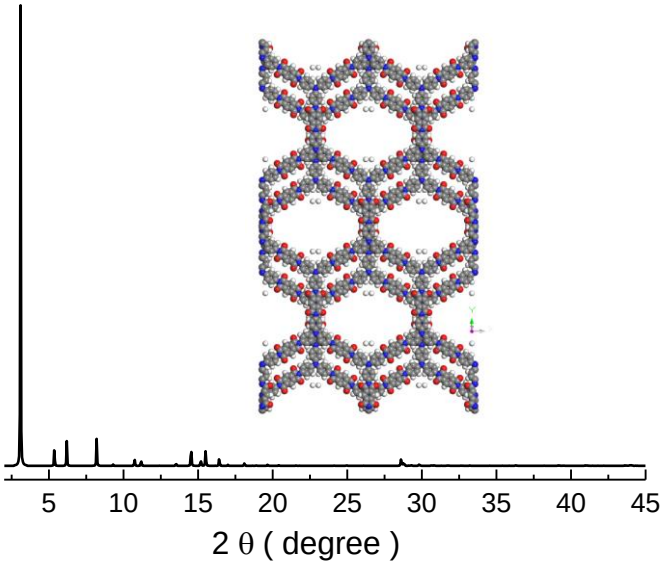

Fig. S2 Calculated PXRD pattern of PI-COF-1 based on the space group of Cmcm

Table S1 Unit cell parameters and fractional atomic coordinates for PI-COF-1 calculated based on the space group of P6/mmm

Space group	P6/mmm		
Calculated unit cell	a = b = 32.9283 Å, c = 3.4305 Å, α = β = 90 º, γ = 120 º		
atom	x	y	z
C1	0.36094	0.63906	0.50000
C2	0.41416	0.58584	0.50000
C3	0.41118	0.65863	0.50000
C4	0.43632	0.63435	0.50000
C5	0.42126	0.51178	0.50000
C6	0.45736	0.49876	0.50000
C7	0.45531	0.45531	0.50000
O1	0.37965	0.48294	0.50000
N1	0.43997	0.56003	0.50000
N2	0.33333	0.66667	0.50000
H1	0.34478	0.52599	0.50000
H2	0.30817	0.56182	0.50000
H3	0.57754	0.57754	0.50000

Table S2 Unit cell parameters and fractional atomic coordinates for PI-COF-1 calculated based on the space group of $P6_3/mmc$.

Space group	$P6_3/mmc$		
Calculated unit cell	a = b = 34.9980 Å, c = 6.2645 Å, α = β = 90 º, γ = 120 º		
atom	x	y	z
C1	0.38855	0.69428	0.25
C2	0.4949	0.74745	0.25
C3	0.83858	0.91929	0.25
C4	0.94482	0.97241	0.25
C5	0.41923	0.6747	0.25
C6	0.46863	0.69898	0.25
C7	0.57625	0.8213	0.25
C8	0.62517	0.83347	0.25
C9	0.66678	0.78983	0.25
C10	0.70839	0.83331	0.25
C11	0.7573	0.84546	0.25
C12	0.86481	0.89708	0.25
C13	0.91418	0.92221	0.25
O1	0.56388	0.85044	0.25
O2	0.76968	0.81633	0.25
N1	0.54646	0.77323	0.25
N2	0.78707	0.89354	0.25
N3	0.33333	0.66667	0.25
N4	1	1	0.75
H1	0.41302	0.64149	0.25
H2	0.48558	0.67823	0.25
H3	0.66679	0.75699	0.25
H4	0.84791	0.85938	0.25
H5	0.92035	0.89519	0.25

Table S3 Unit cell parameters and fractional atomic coordinates for PI-COF-1 calculated based on the space group of Cmcm

Space group	Cmcm		
Calculated unit cell	a = 32.9466 Å, b = 57.0651 Å, c = 6.2388 Å, α = β = γ = 90 º		
atom	x	y	z
C1	-0.54142	-0.23619	0.75
C2	-0.62118	-0.2096	0.75
C3	-0.87894	-0.12368	0.75
C4	-0.95861	-0.09712	0.75
C5	-0.54696	-0.21106	0.75
C6	-0.58381	-0.1985	0.75
C7	-0.69878	-0.20585	0.75

C8	-0.72932	-0.18747	0.75
C9	-0.7283	-0.14485	0.75
C10	-0.77085	-0.14578	0.75
C11	-0.80138	-0.12741	0.75
C12	-0.88094	-0.09946	0.75
C13	-0.91819	-0.08734	0.75
C14	-0.53491	-0.29294	0.75
C15	-0.53533	-0.31764	0.75
C16	-0.46683	-0.37145	0.75
C17	-0.47912	-0.39591	0.75
C18	-0.54356	-0.41672	0.75
C19	-0.52089	-0.43752	0.75
C20	-0.53318	-0.46197	0.75
C21	-0.53533	-0.51573	0.75
C22	-0.53488	-0.54041	0.75
C23	-0.41812	-0.24597	0.75
C24	-0.38086	-0.23383	0.75
C25	-0.3344	-0.17267	0.75
C26	-0.29156	-0.16659	0.75
C27	-0.22813	-0.18841	0.75
C28	-0.20826	-0.16667	0.75
C29	-0.16544	-0.16059	0.75
C30	-0.08373	-0.13479	0.75
C31	-0.04693	-0.12222	0.75
C32	-0.5	-0.2776	0.75
C33	-0.5	-0.33078	0.75
C34	-0.5	-0.50262	0.75
C35	-0.5	-0.55573	0.75
O1	-0.70716	-0.22661	0.75
O2	-0.793	-0.10665	0.75
O3	-0.4315	-0.36526	0.75
O4	-0.56851	-0.46817	0.75
O5	-0.36134	-0.1581	0.75
O6	-0.13848	-0.17516	0.75
N1	-0.65984	-0.19671	0.75
N2	-0.8403	-0.13656	0.75
N3	-0.5	-0.35655	0.75
N4	-0.5	-0.47686	0.75
N5	-0.5	-0.24999	0.75
N6	0	0.08332	1.25
H1	-0.52726	-0.19756	0.75
H2	-0.5819	-0.17965	0.75
H3	-0.71189	-0.12843	0.75

H4	-0.85364	-0.08906	0.75
H5	-0.90777	-0.07075	0.75
H6	-0.56502	-0.28984	0.75
H7	-0.56456	-0.32612	0.75
H8	-0.57641	-0.41672	0.75
H9	-0.56458	-0.50728	0.75
H10	-0.06498	-0.0435	0.75
H11	-0.40772	-0.26258	0.75
H12	-0.35353	-0.24421	0.75
H13	-0.21171	-0.20483	0.75
H14	-0.08178	-0.15364	0.75
H15	-0.52724	0.36427	0.75

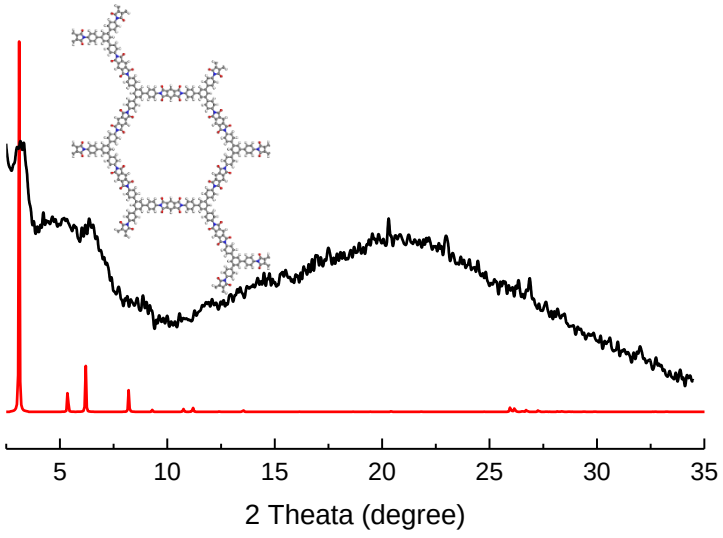

Fig. S3 Calculated and experimental PXRD pattern of PMDA-TAPB

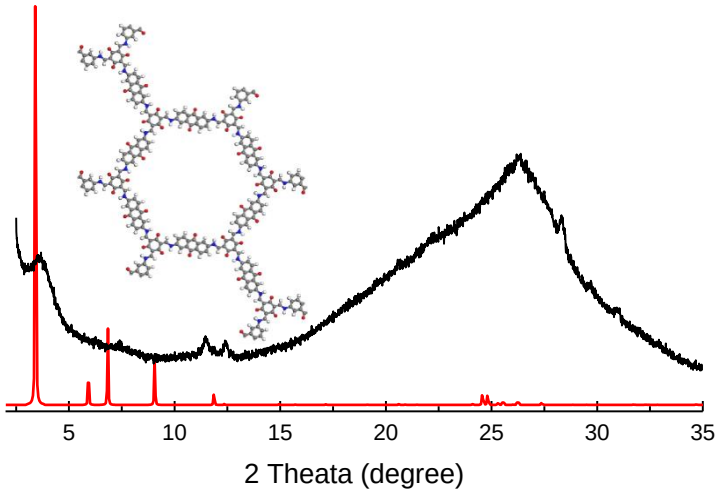

Fig. S4 Calculated and experimental PXRD pattern of TFP-DAAQ

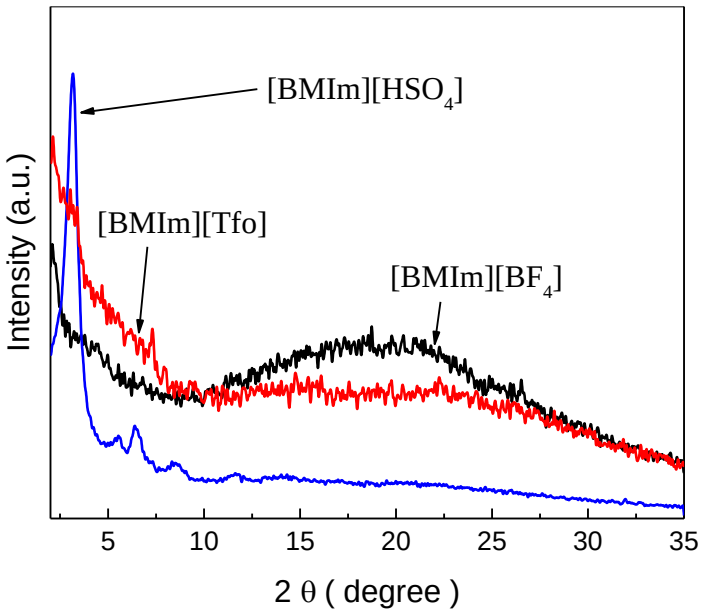

Fig. S5 PXRD pattern of PMDA-TAPA prepared with different ILs

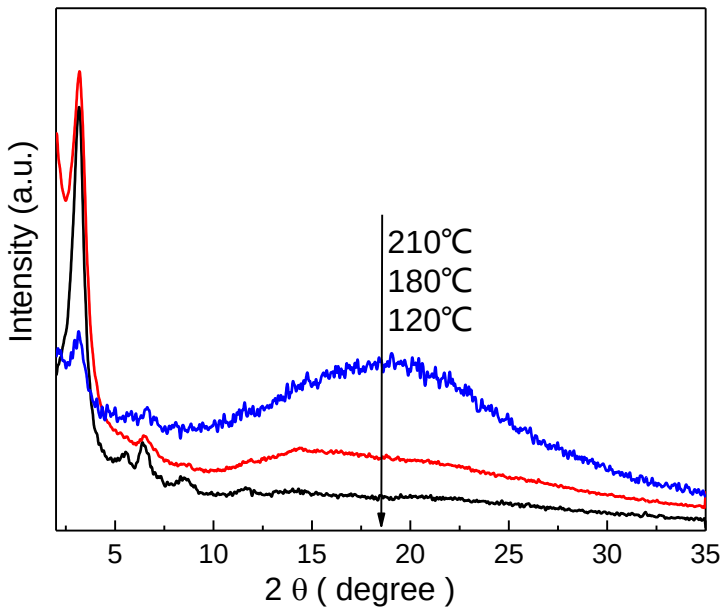

Fig. S6 PXRD pattern of PMDA-TAPA prepared with different temperature

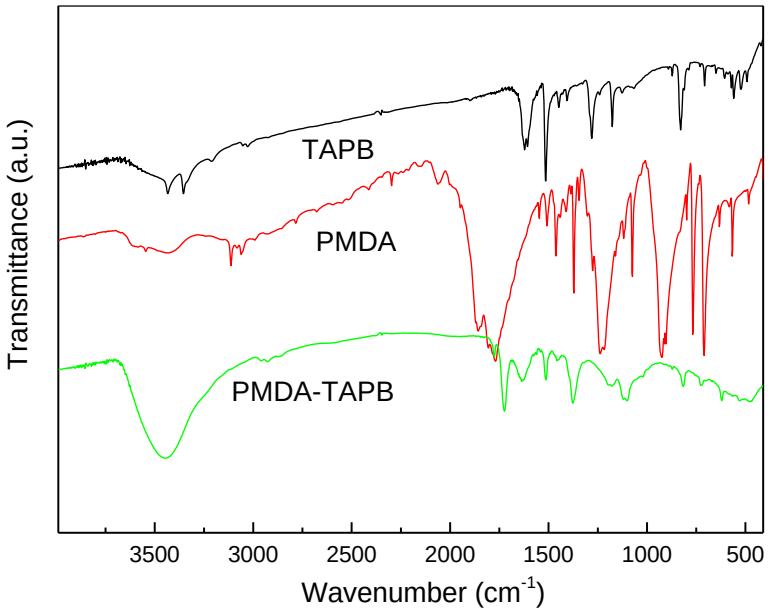

Fig. S7 FT-IR of TAPB, PDMA and PMDA-TAPB

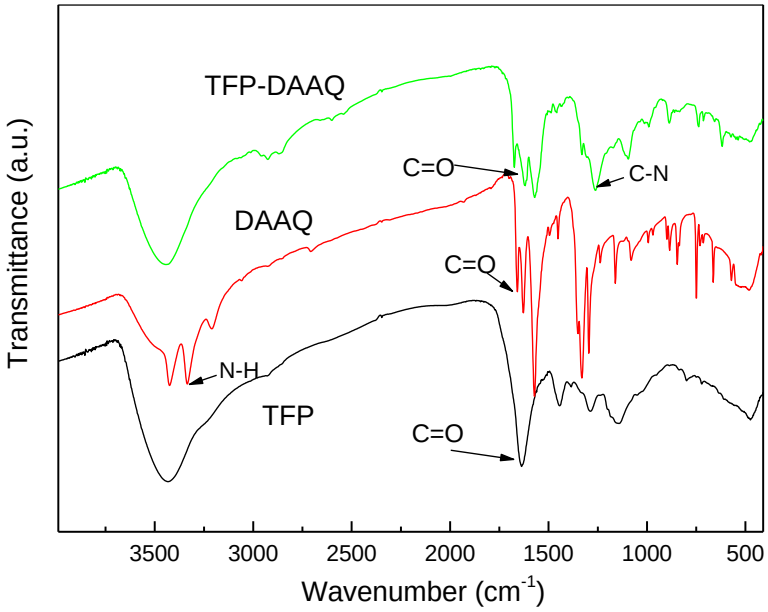

Fig. S8 FT-IR of TFP, DAAQ and TFP-DAAQ

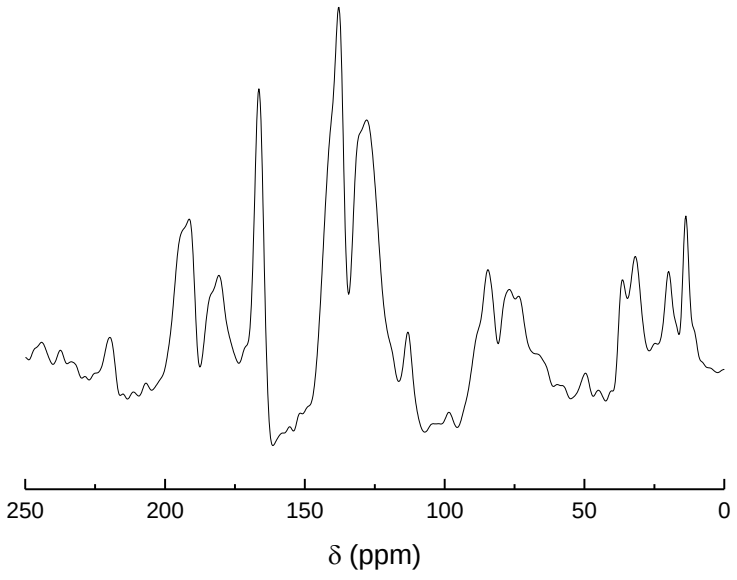

Fig. S9 The ^{13}C NMR spectra of PMDA-TAPA

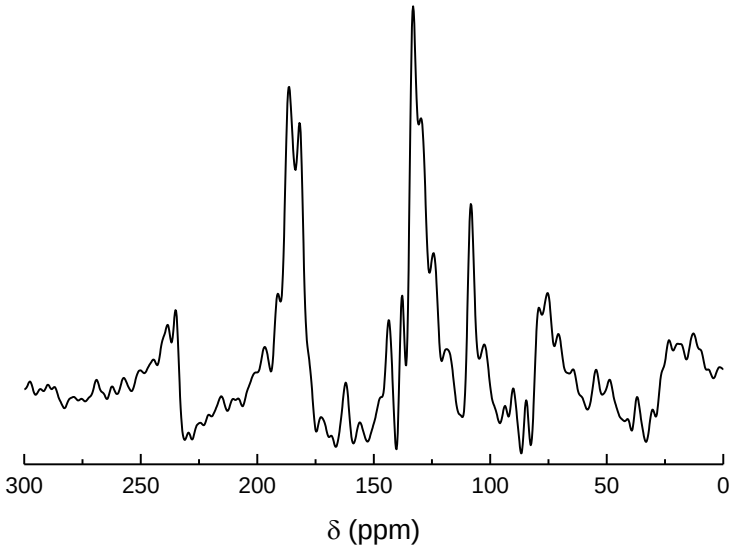

Fig. S10 The ^{13}C NMR spectra ofTFP-DAAQ

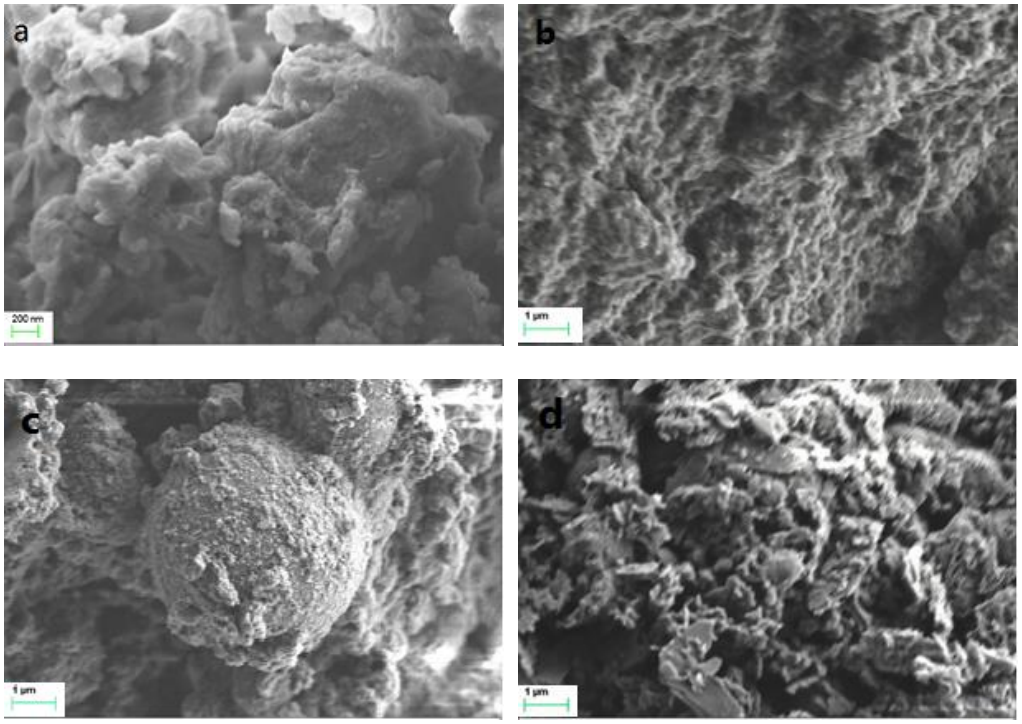

Fig. S11 SEM image of COFs (a. PMDA-TAPA, b. PMDA-TAPB, c. TFP-EB, d. TFP-DAAQ)

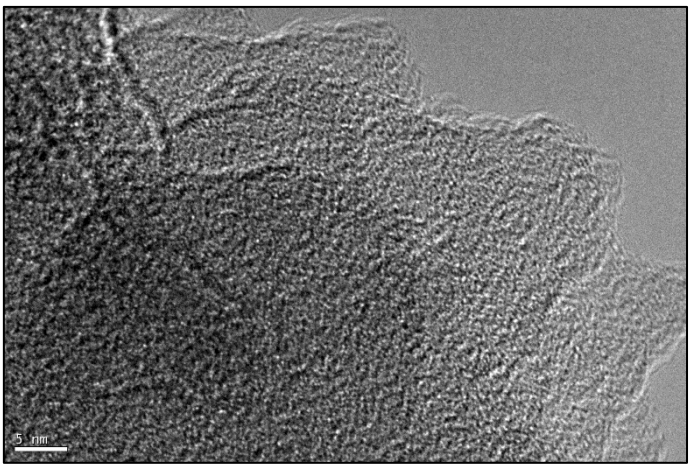

Fig. S12 TEM image of PMDA-TAPA

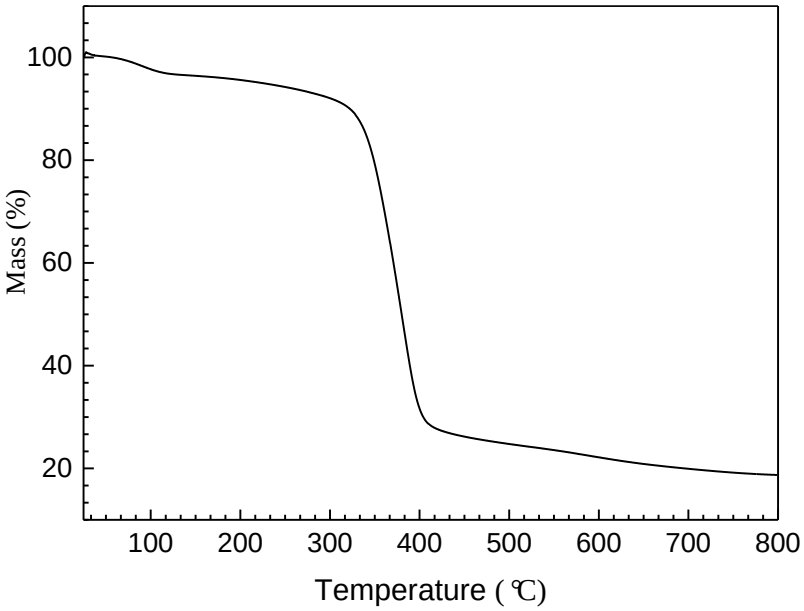

Fig. S13 TGA profile of PMDA-TAPB

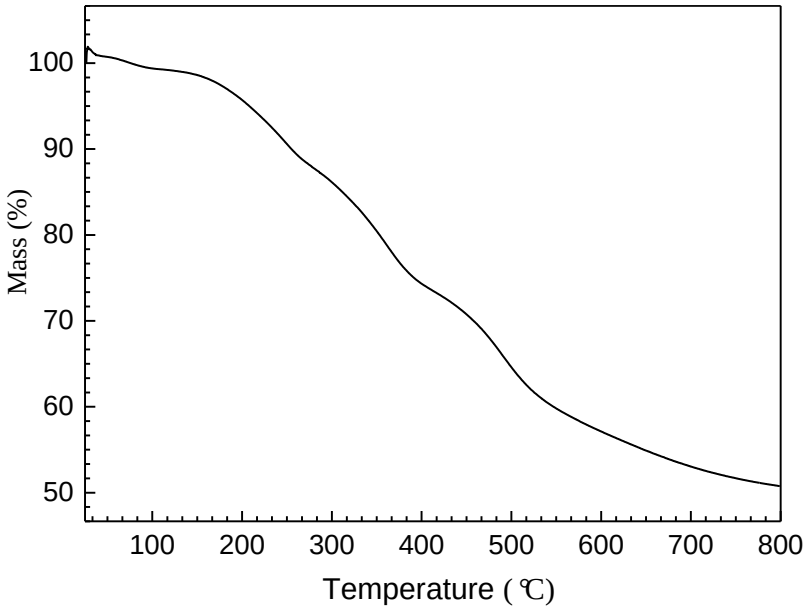

Fig. 14 TGA profile of TFP-DAAQ