Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

An unprecedented 2D covalent organic framework with an htb net topology

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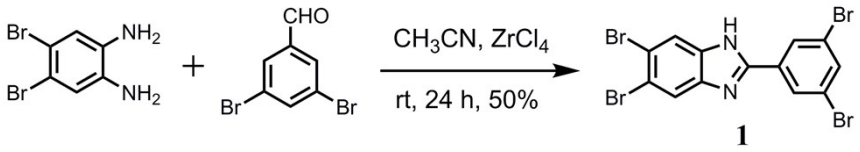
Section S1. *General information and synthetic procedures.*

General information: 5,6-dibromo-2-(3,5-dibromophenyl)-1*H*-benzoimidazole (compound **1**)[1] and the benzimidazole-based tetra-aldehyde (BITA) building block[2] were prepared according to the modified literature procedures. All the other chemicals were of analytical grade quality purchased from commercial sources and were used directly without further purification. Elemental analysis (C, H, and N) of the **htb** type BITA-DPA COF was carried out on a Perkin Elmer 2400 Series II elemental analyzer. Low-dose TEM image of the **htb** type BITA-DPA COF was acquired on the TEAM I FEI Titan-class microscope at 300 kV, equipped with both geometric aberrations corrected to third order and chromatic aberrations corrected to the first order. Imaging datum was collected in the Gatan K2 direct-detection camera operated in electron-counting mode (camera counting frame rate of 400 fps (frames per second) at 4 k × 4 k resolution) with a final image output rate of 40 fps at 4 k X 4 k resolution. High resolution transmission electron (HRTEM) image of the **htb** type BITA-DPA COF was measured on an FEI TitanX 60 300 microscope at 200 kV. The BITA-DPA COF sample was sonicated in toluene with a sonication probe for about 15 min and drop-casted onto a copper grid (Lacey C only, 300 mesh Cu). While the other instrument information were given separately in the following sections.

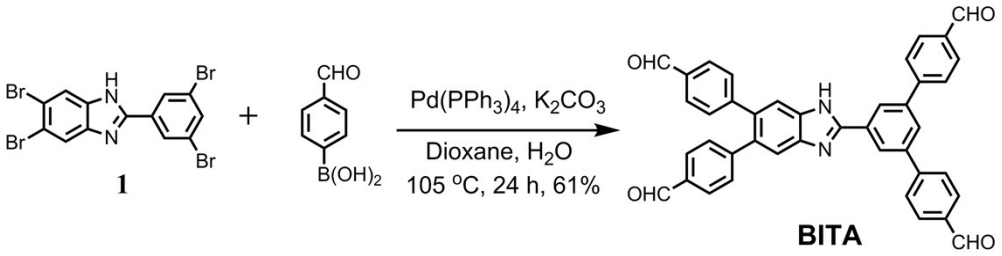
Synthesis of 5,6-dibromo-2-(3,5-dibromophenyl)-1*H*-benzoimidazole (1)



Scheme S1. Synthesis of compound **1**.

4,5-dibromobenzene-1,2-diamine (917 mg, 3.45 mmol) and 3,5-dibromobenzaldehyde (1093 mg, 4.14 mmol) were dissolved in acetonitrile (60 mL), and then zirconium tetrachloride (40 mg, 0.17 mmol) was added. The resulting mixture was stirred at room temperature for 24 h, during which a yellow precipitate was formed. The yellow solid was filtered and washed with cold acetonitrile several times. The crude product was further purified by recrystallization from DMSO to produce the desired compound **1** as brown prismatic crystals (880 mg, yield: 50%). ^{1}H NMR (DMSO-d_6, 298 K, 400 MHz): δ (ppm) = 8.35 (d, J = 1.7 Hz, 2H), 8.04 (s, 2H), 8.02 (t, J = 1.7 Hz, 1H). ^{13}C NMR (DMSO-d_6, 298 K, 100 MHz): δ (ppm) = 150.4, 134.8, 132.8, 128.3, 123.0, 116.9. MS (LC-MS) for $C_{13}H_6Br_4N_2$ (Calcd. 509.82): m/z = 510.64 $[M + H]^+$.

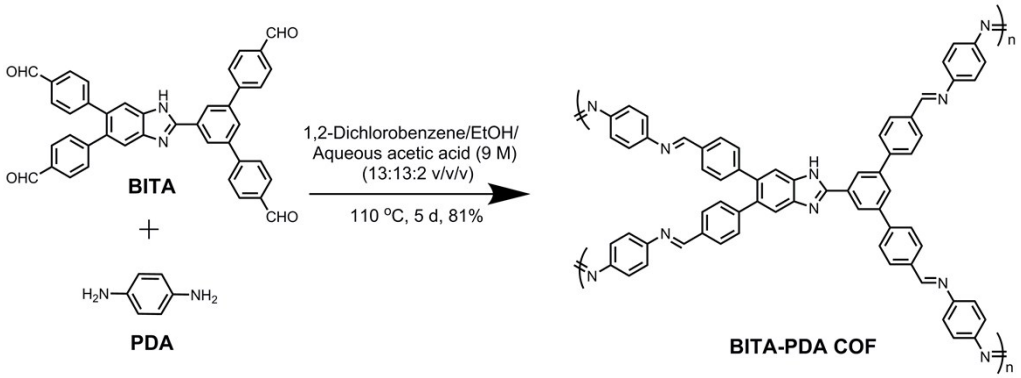
Synthesis of the building block BITA



Scheme S2. Synthesis of the building block BITA.

A mixture of compound **1** (510 mg, 1.0 mmol), 4-formylphenylboronic acid (900 mg, 6.0 mmol), K_2CO_3 (1382 mg, 10 mmol), dioxane (20 mL) and water (5 mL) was degassed with argon. Then tetrakis(triphenylphosphine)palladium (150 mg, catalyst) was added, and the reaction mixture was heated at 105 °C for 24 h under stirring. After cooling to room temperature, the mixture was evaporated to dryness under reduced pressure. The residue was dissolved in DMF and then filtered through a pad of Celatom, and the resulting filtrate was finally poured into methanol under stirring. The precipitation that formed was collected by vacuum filtration, washed with water, dioxane, and methanol, respectively, offering the building block BITA as a light green solid (373 mg, 61% yield based on compound **1**). ^{1}H NMR (DMSO-d_6, 298 K, 400 MHz): δ (ppm) = 13.40 (s, 1H), 10.10 (s, 2H), 9.97 (s, 2H), 8.64 (s, 2H), 8.24 (s, 1H), 8.16 (d, J = 8.0 Hz, 4H), 8.08 (d, J = 8.1 Hz, 4H), 7.80 (dd, J = 12.8, 5.8 Hz, 5H), 7.63 (s, 1H), 7.38 (t, J = 6.5 Hz, 4H). ^{13}C NMR (DMSO-d_6, 298 K, 100 MHz): δ (ppm) = 192.7, 152.5, 147.8, 144.8, 140.2, 135.5, 134.1, 133.9, 131.2, 130.7, 130.1, 129.2, 127.7, 127.2, 125.1. MS (LC-MS) for $C_{41}H_{26}N_2O_4$ (Calcd. 610.67): *m/z* =609.04 $[M - H]^-$.

Synthesis of the htb type BITA-PDA COF



Scheme S3. Synthesis of the **htb** type BITA-PDA COF.

A mixture of the building block BITA (15.3 mg, 0.025 mmol), PDA (10.8 mg, 0.10 mmol), 1,2-dichlorobenzene (0.65 mL), and ethanol (0.65 mL) was placed in a 10 mL vial, firstly sonicated for 2 minutes and then bubbled with argon for 5 minutes, after which degassed 9 M acetic acid (0.1 mL) was added. The reaction mixture was bubbled again with argon for 15 minutes and the vial was sealed quickly, heated to 110 ^{o}C for 5 days under autogenously pressure. After naturally cooling to room temperature, the green precipitate was collected by filtration, washed with anhydrous THF several times and anhydrous acetone once, and finally dried under vacuum overnight, producing a green solid of the target **htb** type BITA-PDA COF (15.3 mg, 81% yield based on BITA). Elemental analysis: Calcd. for $C_{53}H_{34}N_6$: C, 84.33; H, 4.54; N, 11.13%. Found: C, 76.35; H, 4.93; N, 10.62%.

Section S2. Powder X-ray diffraction (PXRD) measurements.

Powder X-ray diffraction (PXRD) patterns were collected on a Bruker D8 Advance diffractometer at 40 kV, 40 mA utilizing Cu-*K*α radiation (λ = 1.5418 Å) at ambient temperature. Samples were mounted on zero-background quartz sample holders and flattened with a glass microscope slide. No sample grinding or sieving was done prior to the measurements.

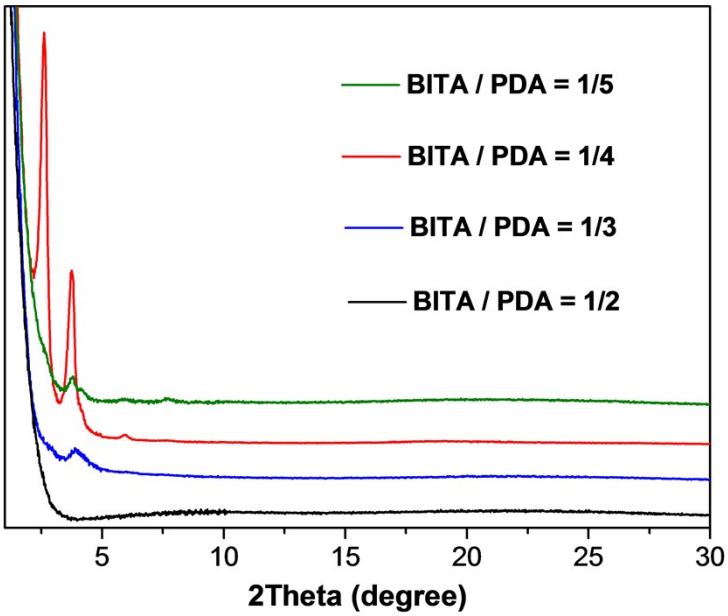


Figure S1. PXRD patterns for the BITA-PDA COF materials prepared from the reactions of BITA and PDA in different mole ratios using 1,2-dichlorobenzene/ethanol (1:1 v/v) as the cosolvents.

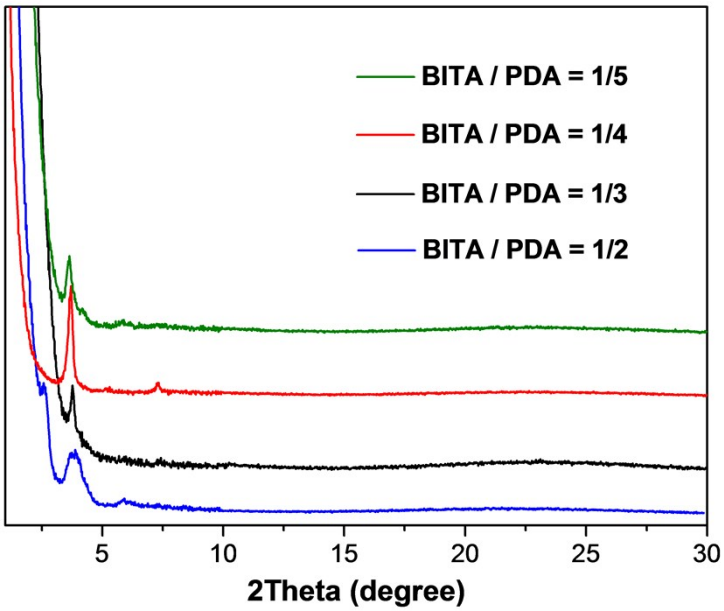


Figure S2. PXRD patterns for the BITA-PDA COF materials prepared from the reactions of BITA and PDA in different mole ratios using 1,2-dichlorobenzene/tert-butanol (1:1 v/v) as the cosolvents.

Section 3. *Crystal structure modeling*.

The crystal structure modeling for **htb** type BITA-DPA COF, including the unit cell parameters and the atomic positions were simulated by utilizing the Crystal Building module in Accelrys Materials Studio 5.0 software[3] (Biovia, San Diego, CA). In the very first place, the AA packing model of BITA-DPA COF was constructed based on a 2D layered **htb** topology obtained from the Reticular Chemistry Structure Resource (RCSR)[4] by replacing the relevant vertex and edge with the BITA and PDA subunits, in which the symmetry of lattice was slightly degraded to *P*6/*m*. All hydrogen atoms were also added in the structure and the resulting lattice model was then geometrically optimized by employing the MS Forcite module (universal force fields, Ewald summations), thus generating a hexagonal unit cell with the optimized parameters of $a = b = 70.26$ Å, $c = 3.44$ Å, $\alpha = \beta = 90°$ and $\gamma = 120°$. Last but not least, the Pawley PXRD refinement was carried out using the MS Reflex module, in which a Pseudo-Voigt profile function was employed for whole profile fitting (peak asymmetry, peak broadening, and zero shift error were all taken into consideration) and Berrar–Baldinozzi function was utilized for asymmetry correction during the refinement process. Unit cell parameters were refined at same time, yielding the final unit cell parameters of $a = b = 72.87$ Å, $c = 3.24$ Å, $\alpha = \beta = 90°$ and $\gamma = 120°$, and the final R_p and R_{wp} of 3.17% and 4.48%, respectively. Moreover, the AB packing structure model for BITA-DPA COF was built as well, in which alternating stacked units were offset by a/2 and b/2. Atomic coordinates of the **htb** type BITA-DPA COF with AA packing and AB packing structures are provided in Tables S1-S2.

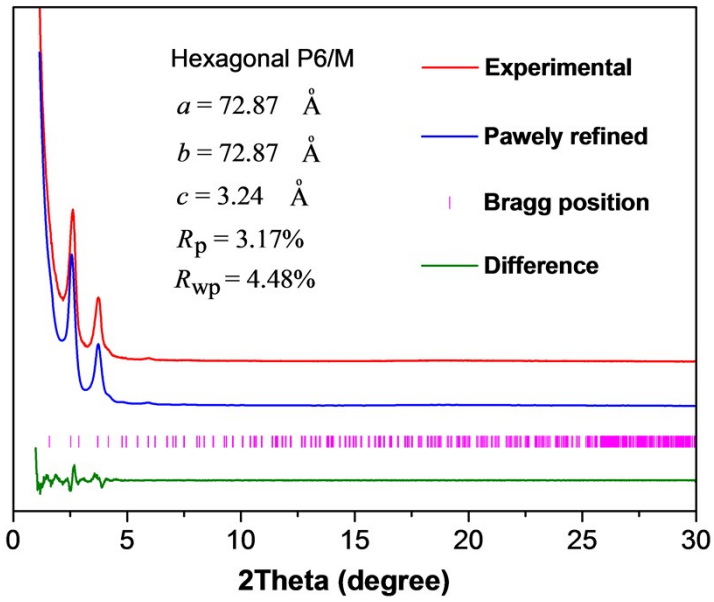


Figure S3. PXRD patterns of **htb** type BITA-PDA COF: experimental (red curve), Pawley refined (blue curve) and their difference (green curve). Purple ticks indicate the positions of reflections.

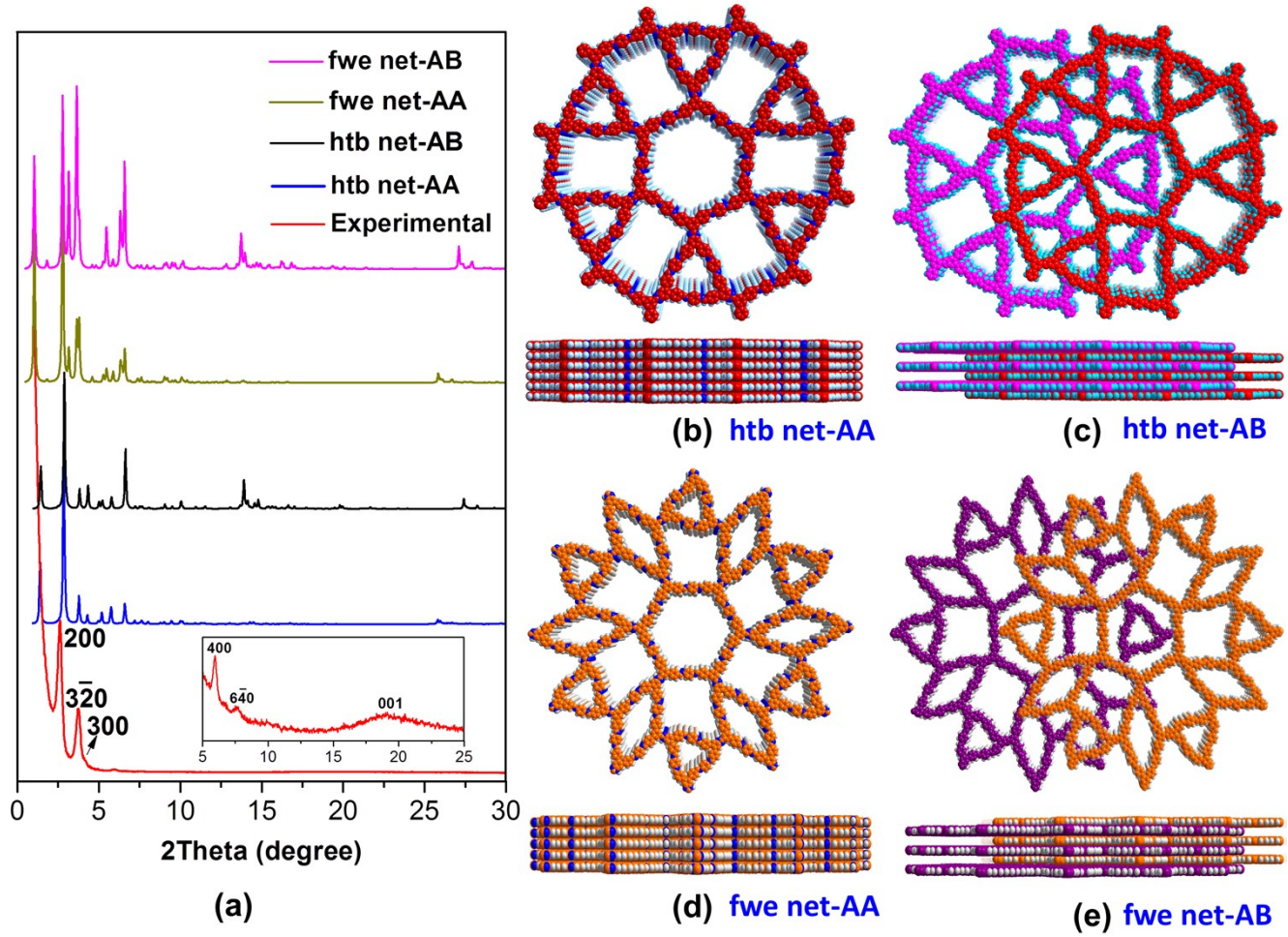


Figure S4. (**a**) Experimental PXRD pattern of BITA-PDA COF (red); Simulated PXRD patterns of BITA-PDA COF exhibiting an **htb** or **fwe** net topology**.** Space-filling models of BITA-PDA COF showing an **htb** or **fwe** net topology in (**b, d)** AA packing mode and **(c, e)** AB packing mode.

Section S4. Fourier-transform infrared (FT-IR) spectra.

The FT-IR spectra of starting materials including the building block BITA and 1,4-diaminobenzene (PDA), and the target product of the **htb** type BITA-PDA COF were determined on a Nicolet FT-IR-170SX spectrophotometer with KBr pellets in the range of 500−4000 cm^{-1}.

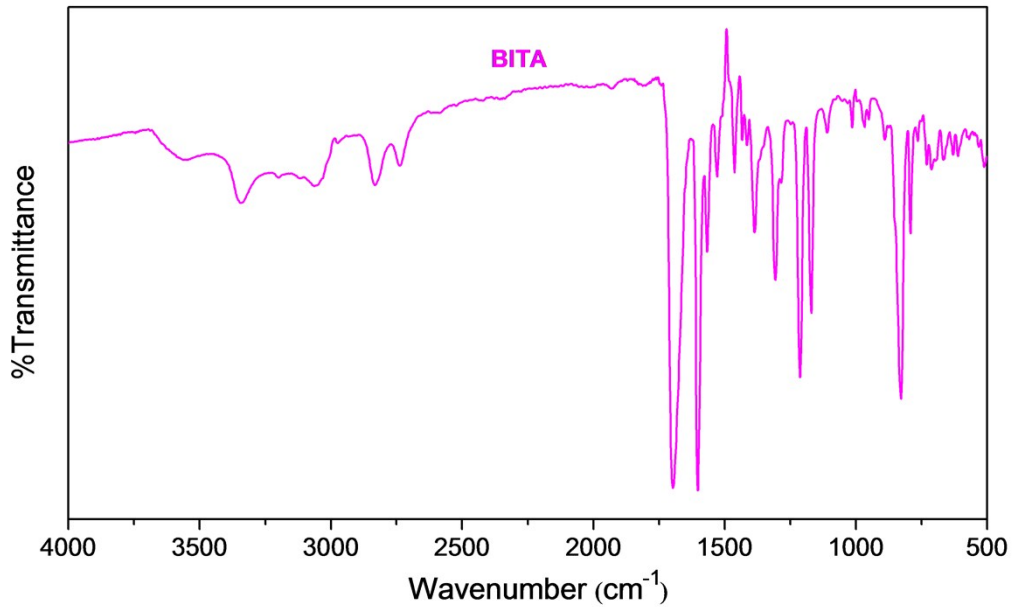


Figure S5. FT-IR spectrum of the building block BITA.

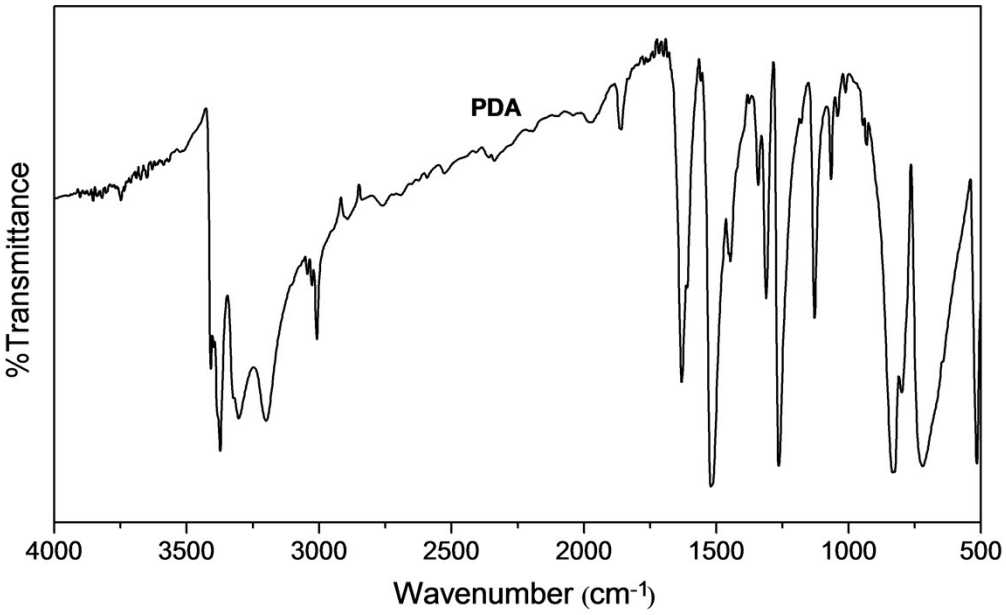


Figure S6. FT-IR spectrum of 1,4-diaminobenzene (PDA).

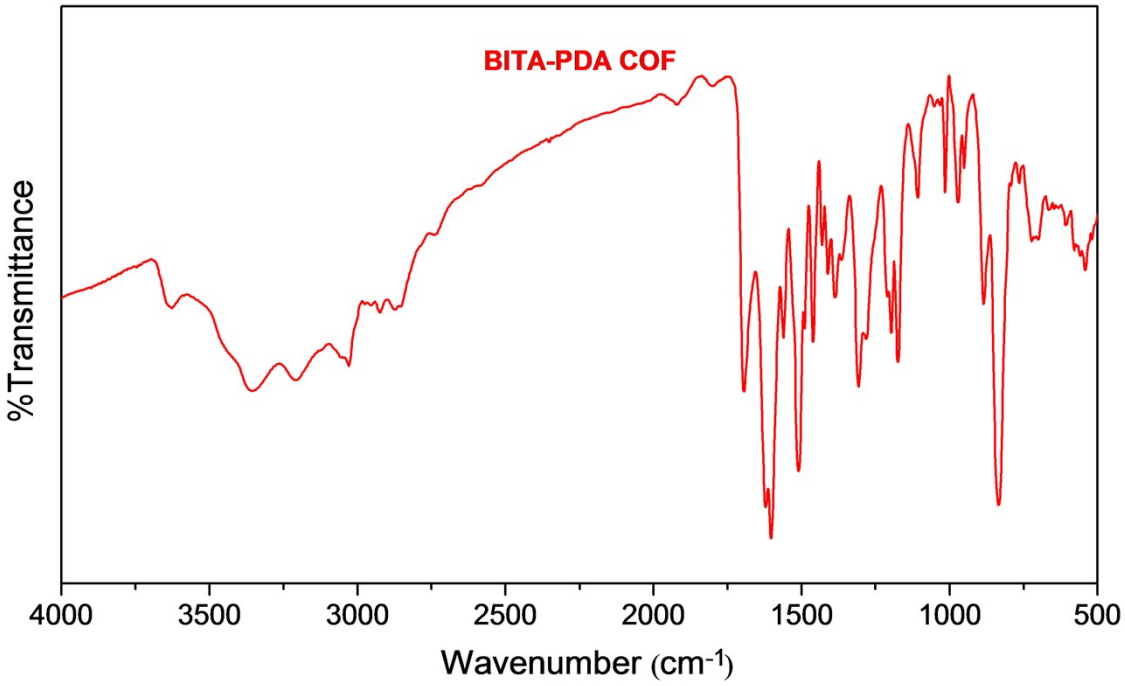


Figure S7. FT-IR spectrum of the **htb** type BITA-PDA COF.

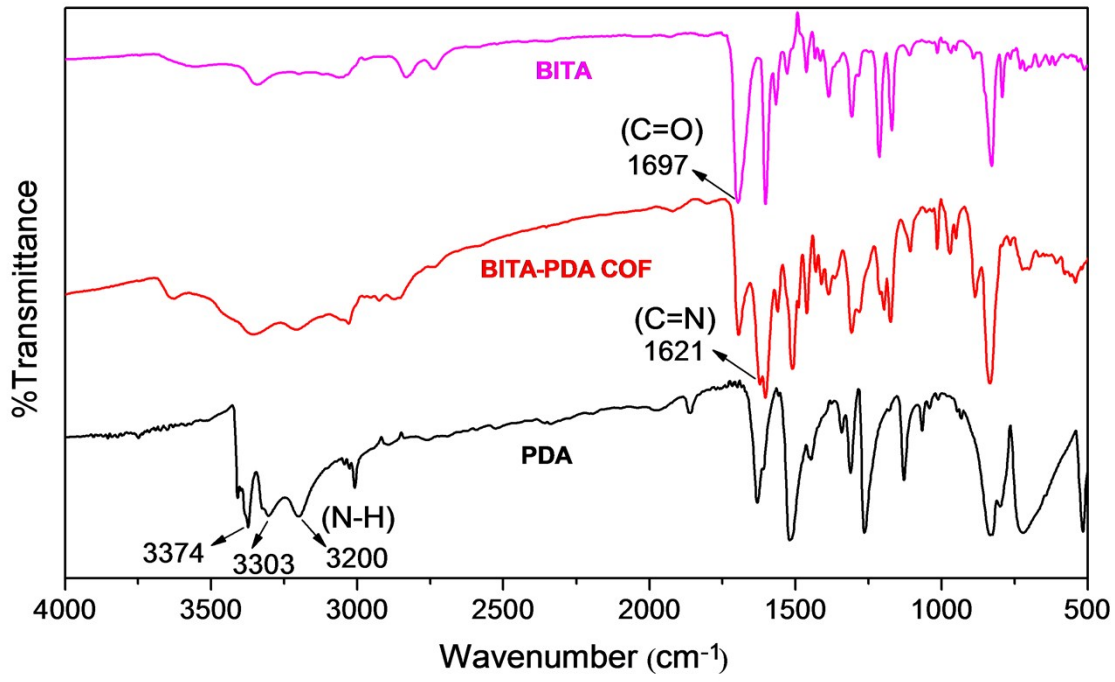


Figure S8. Stack plot of the FT-IR spectra for the comparison between starting materials of BITA and PDA, and the resulting **htb** type BITA-PDA COF.

Section S5. Solid-state nuclear magnetic resonance (SSNMR) spectroscopy.

The solid-state nuclear magnetic resonance (SSNMR) spectrum was acquired at ambient pressure on an Agilent-NMR-vnmrs 600 spectrometer (Agilent Technologies, Santa Clara, CA, USA). The spectrum was recorded at a resonance frequency of 150.15 MHz using a 4-mm magic angle-spinning (MAS) NMR probe with a spinning rate of 15 kHz at room temperature. The recycle delay was 5 s, and the accumulation number was set to be 2048.

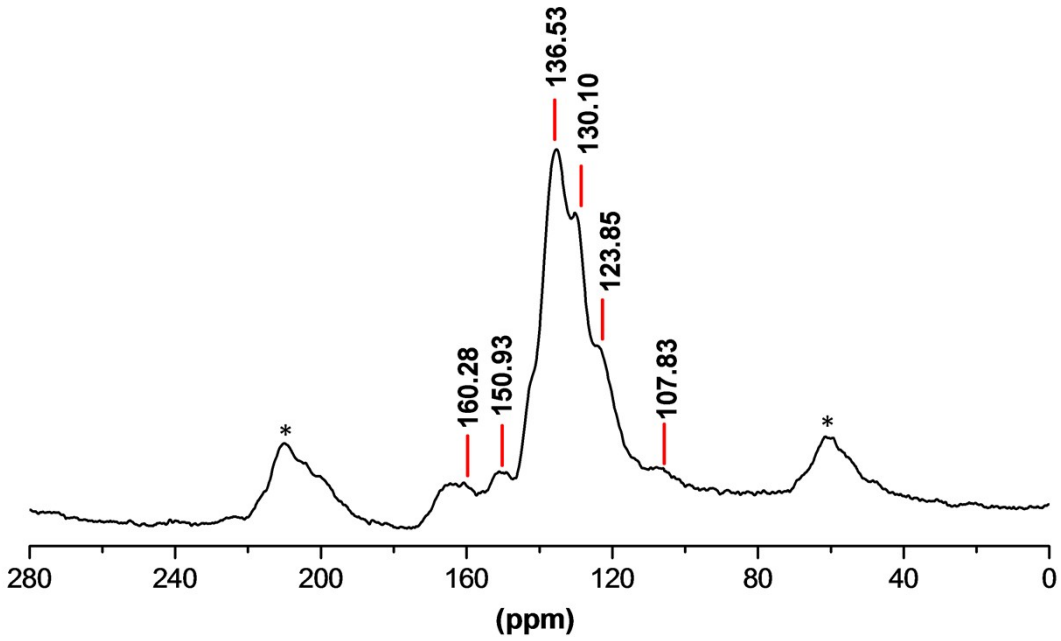


Figure S9. Solid state ^{13}C NMR spectrum of BITA-DPA COF.

Section S6. Scanning electron microscopy (SEM).

Scanning electron microscopy (SEM) images were recorded on a MAIA3 TESCAN Analytical Scanning Electron Microscope (USA) using an accelerating voltage of 4.0 kV.

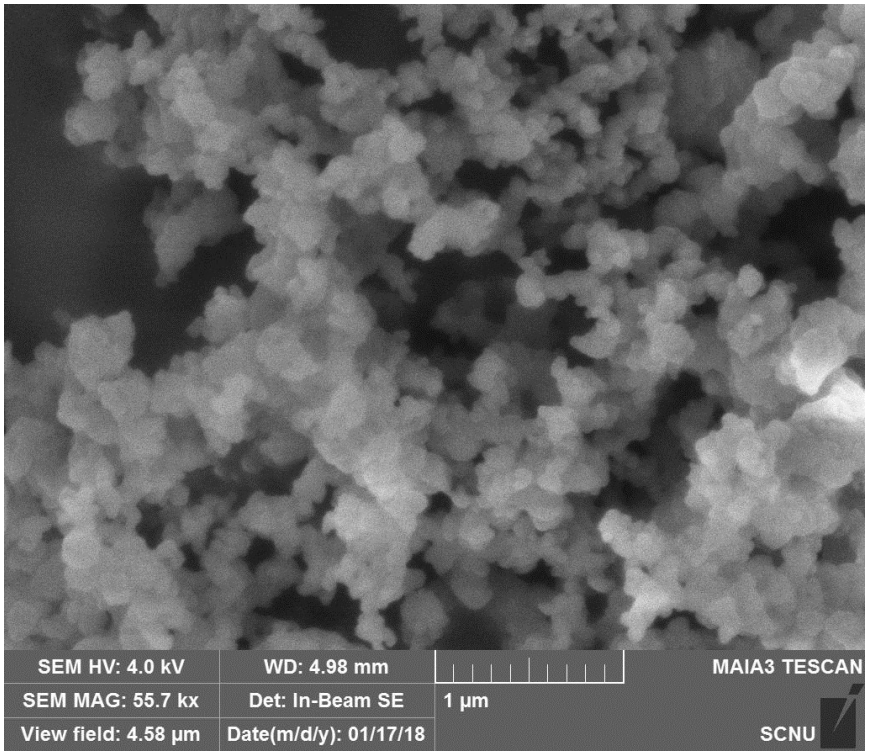


Figure S10. SEM image of BITA-PDA COF.

Section S6. *Thermogravimetric analysis (TGA).*

Thermogravimetric analysis (TGA) was measured by employing on a Perkin-Elmer TGA7 analyzer from room temperature to 800 °C at a heating rate of 10 °C/min under an air atmosphere.

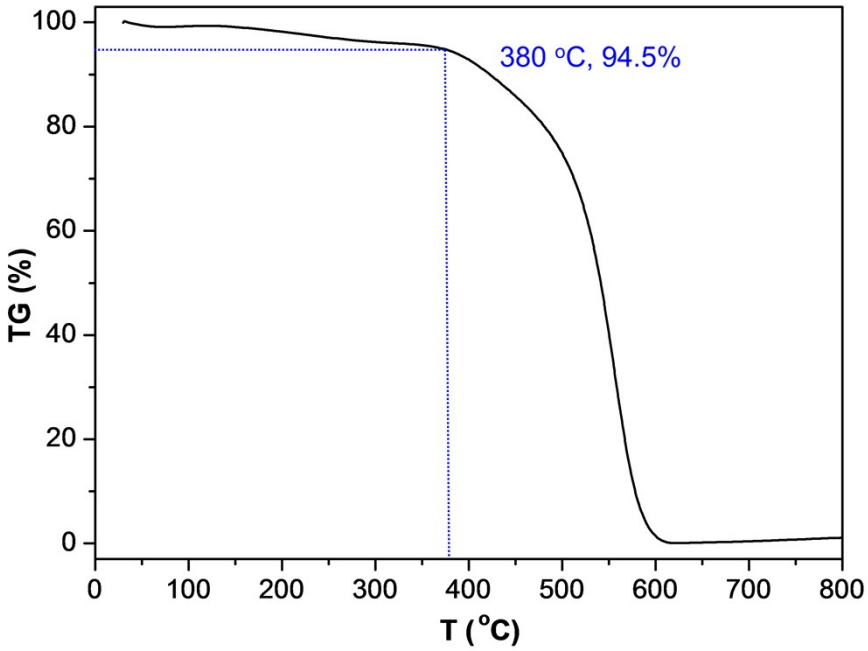


Figure S11. TGA curve of BITA-DPA COF.

Section 8. *Nitrogen adsorption−desorption measurement.*

Nitrogen adsorption-desorption measurement was conducted by using an ASAP 2020 Plus gas adsorption instrument (Micromeritics, USA). The cryogenic temperature of 77 K required for nitrogen sorption test was controlled using liquid nitrogen bath. The initial outgassing process for the sample was carried out under a dynamic vacuum (about 10^{-5} torr) at 120 °C for 12 h. The desolvated sample and sample tube were precisely weighed and transferred to the analyzer. Both the Brunauer-Emmett-Teller (BET) model and Langmuir model were utilized to evaluate the specific surface areas.

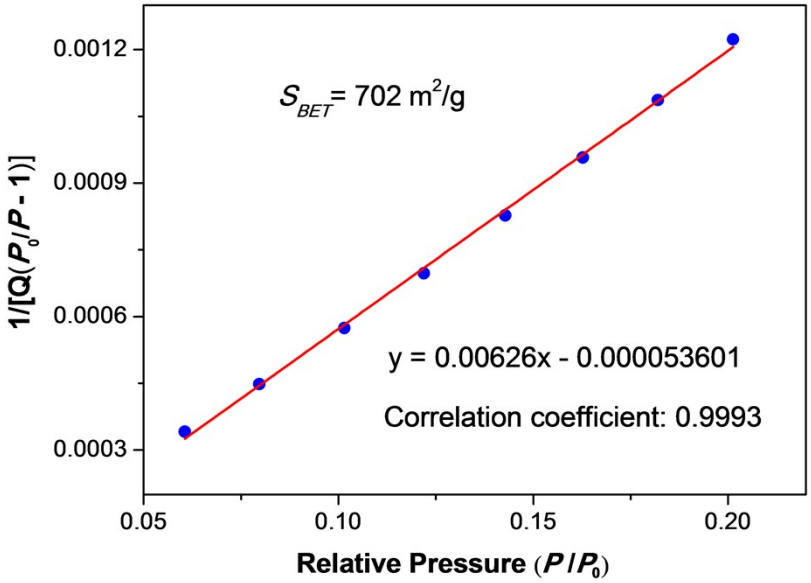


Figure S12. BET surface area plot for the **htb** type BITA-PDA COF calculated from the isotherm.

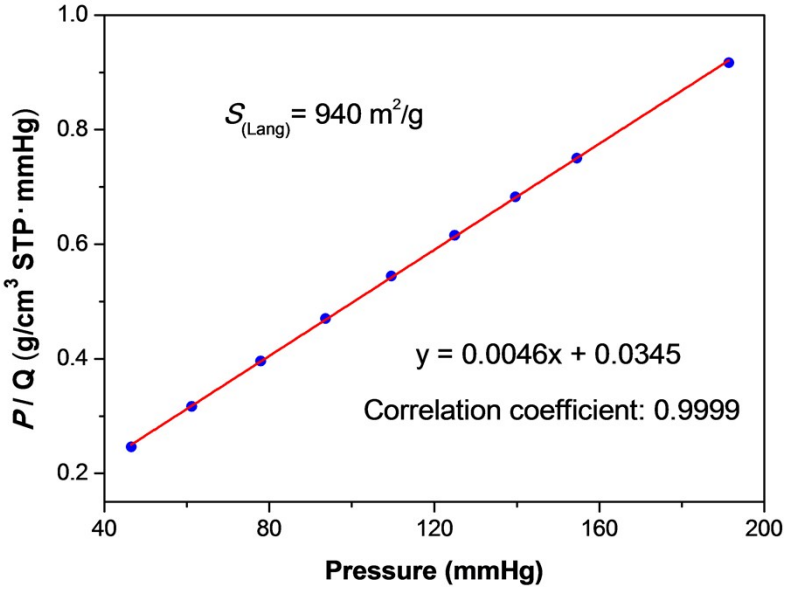


Figure S13. Langmuir surface area plot for the **htb** type BITA-PDA COF calculated from the isotherm.

Section S9. *Fluorescence spectroscopy*

Fluorescence spectra were measured at ambient temperature employing a Hitachi F-4600 fluorescence spectrophotometer (Hitachi, Japan) with a PMT voltage being 700 V and a scan speed being 1200 nm/min, and the slit width for both excitation and emission was set to 5 nm. For the fluorescence measurements, the fine powder of BITA-PDA COF was immersed in dimethylformamide (DMF) and then ultrasonicated for a couple of hours to obtain almost transparent suspensions. All the emission spectra of BITA-PDA COF suspensions before and after the addition of metal ions were recorded from 390 to 600 nm upon excitation at 322 nm. The fluorescence quenching efficiency was estimated employing Stern–Volmer equation, $I_o/I = K_{SV}[M] + 1$, in which I and I_o are the luminescence intensity with and without addition of Fe^{3+} cations, respectively, K_{SV} represents the quenching constant and [M] is the concentration of Fe^{3+} cations.

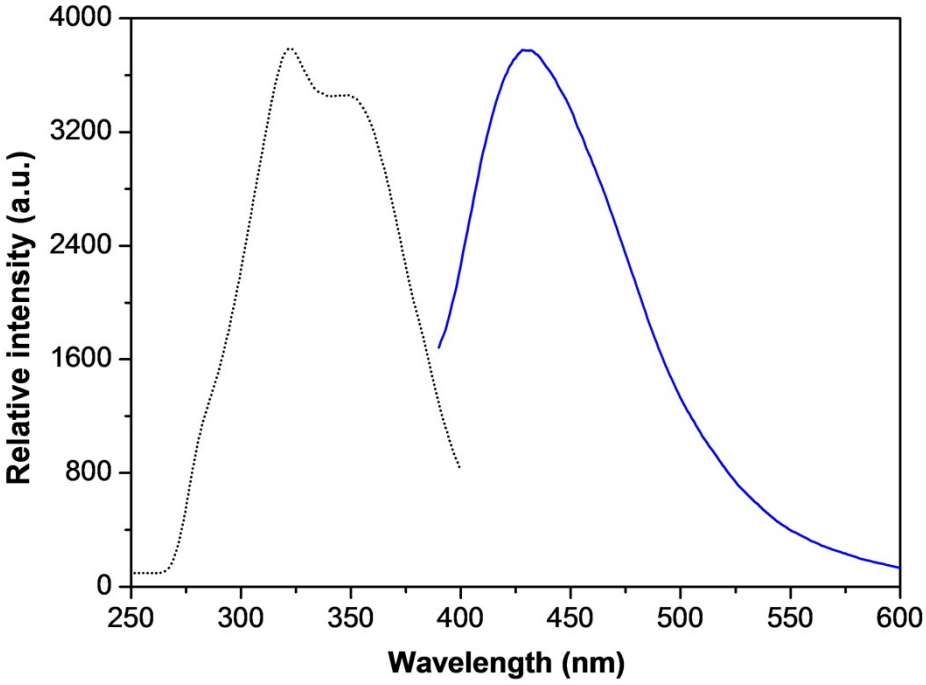


Figure S14. Excitation (λ_{em} = 432 nm) and emission (λ_{ex} = 322 nm) spectra of BITA-PDA COF (10 mg / L) in DMF suspension.

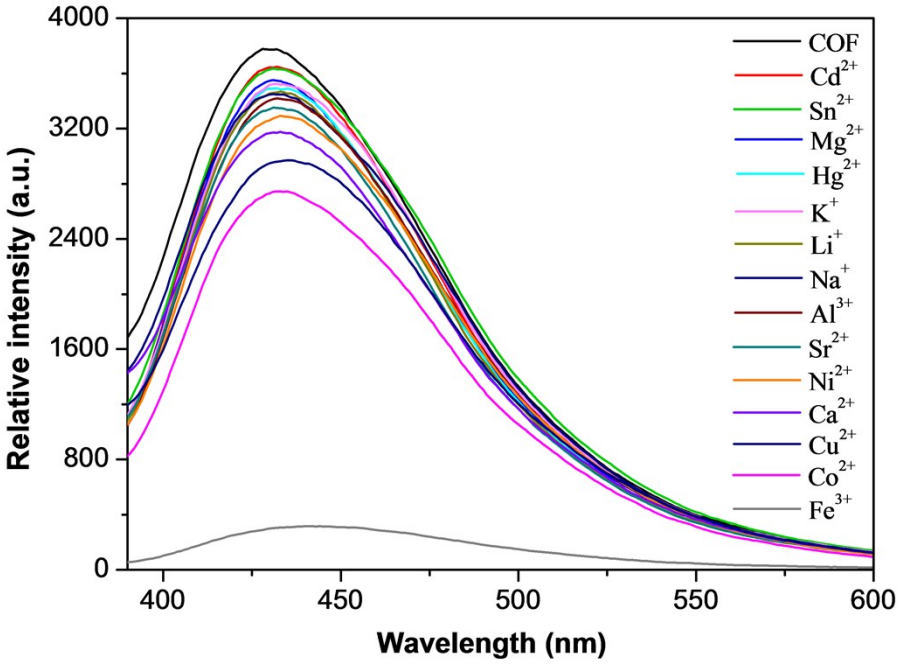


Figure S15. Emission spectra (λ_{ex} = 322 nm) of BITA-PDA COF in DMF suspensions containing 1×10^{-4} mol/L of Cd^{2+}, Sn^{2+}, Mg^{2+}, Hg^{2+}, K^{+}, Li^{+}, Na^{+}, Al^{3+}, Sr^{2+}, Ni^{2+}, Ca^{2+}, Cu^{2+}, Co^{2+} and Fe^{3+}, respectively.

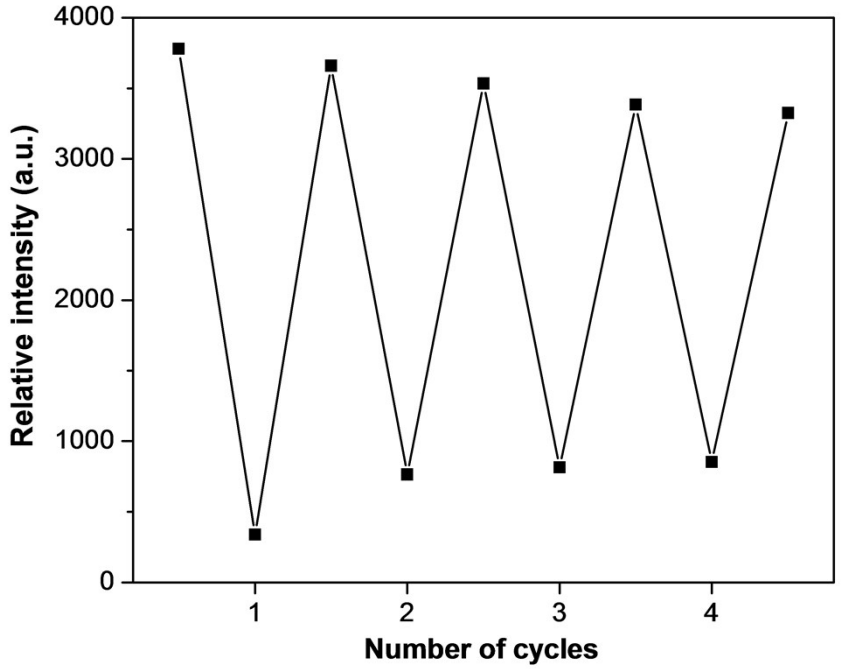


Figure S16. Recycled use of the BITA-PDA COF for the detection of Fe^{3+} ions.

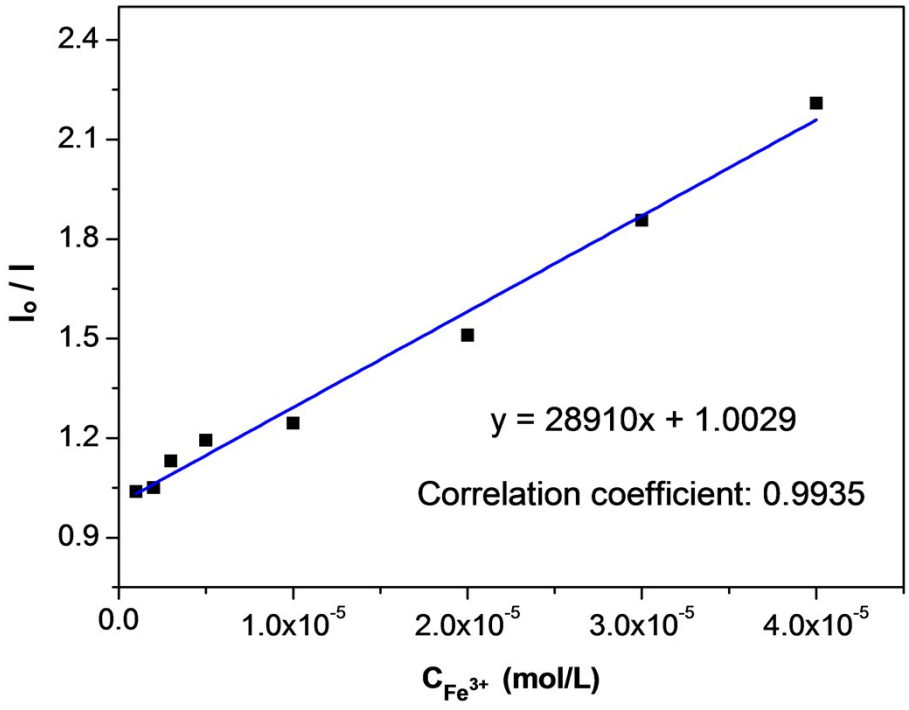


Figure S17. Stern–Volmer plot of photoluminescent quenching efficiency (I_0/I) versus Fe^{3+} concentration in the BITA-PDA COF suspension.

Section S10. X-ray photoelectron spectroscopy (XPS)

The Fe 2p X-ray photoelectron spectroscopy (XPS) experiment of the Fe^{3+}-incorporated BITA-PDA COF was carried out on an ESCALAB 250 instrument (XPS, ESCALAB 250, Thermo Scientific, America) by employing aluminum Kα X-ray radiation under ultra-high vacuum. The BITA-PDA COF powder was firstly immersed in a DMF solution containing 10^{-2} mol/L Fe^{3+} ion for overnight, then collected by filtration, washed with DMF several times and dried under vacuum, and the resulting Fe^{3+}-incorporated BITA-PDA COF sample was finally subjected to XPS study.

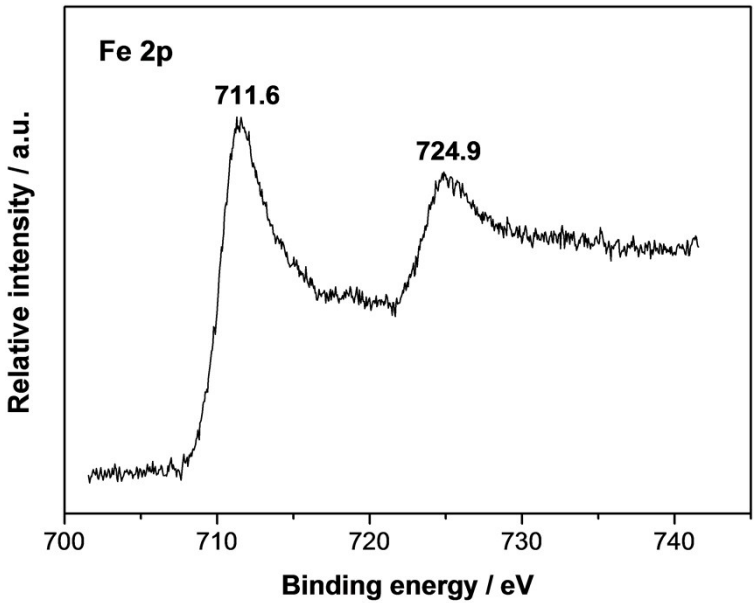


Figure S18. The Fe 2p XPS spectrum of the Fe^{3+}-incorporated BITA-PDA COF sample.

Section S11. *Proton and carbon nuclear magnetic resonance (^{1}H-NMR and ^{13}C-NMR) spectra.*

Liquid proton and carbon nuclear magnetic resonance (^{1}H-NMR and ^{13}C-NMR) spectra were recorded on a Varian 400 (400 MHz) NMR spectrometer at 298 K, utilizing the deuterated solvent as lock and tetramethylsilane as an internal standard. All chemical shifts are quoted using the δ scale, and all coupling constants (J) are expressed in Hertz (Hz).

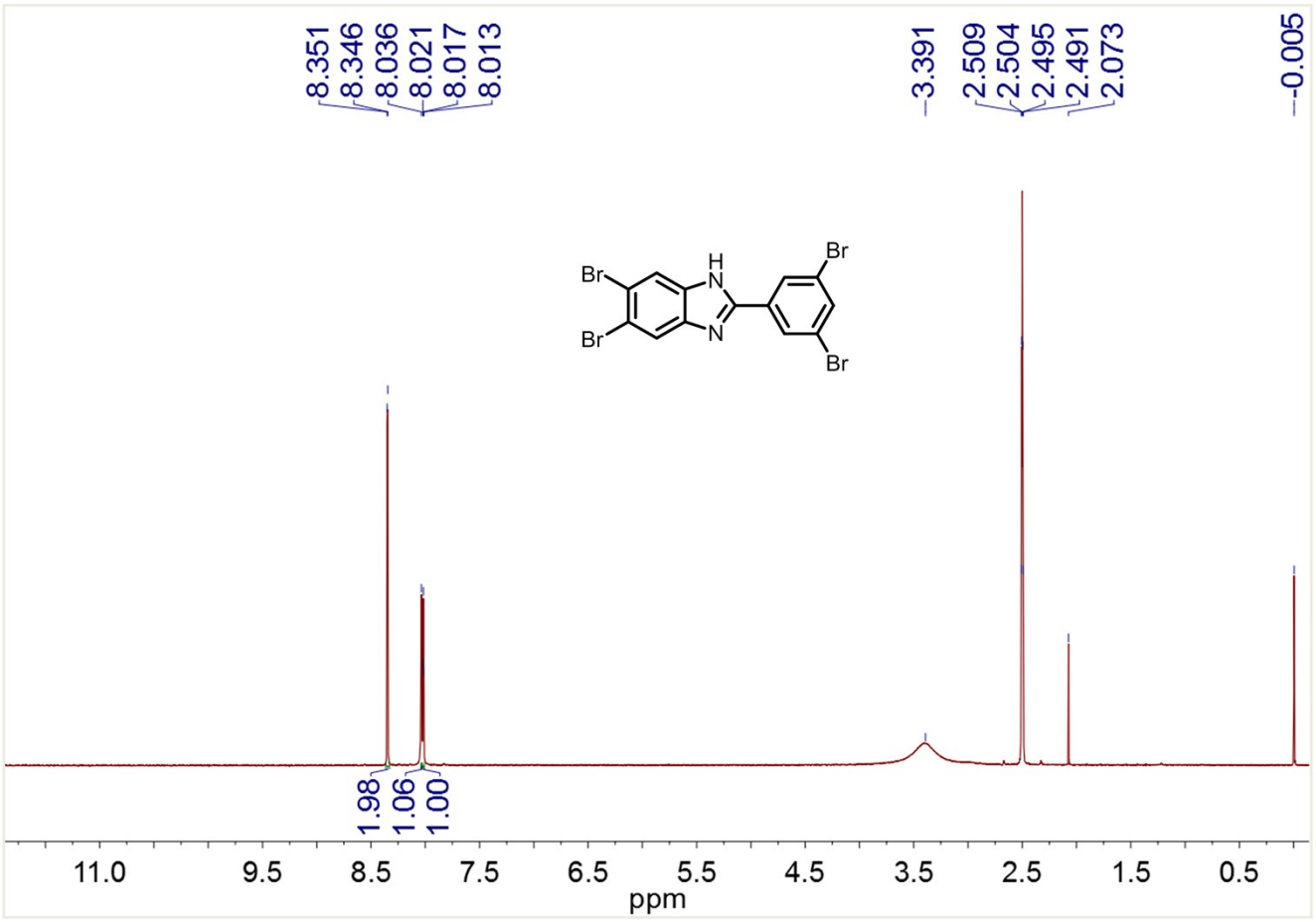


Figure S19. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 400 MHz) of compound **1**.

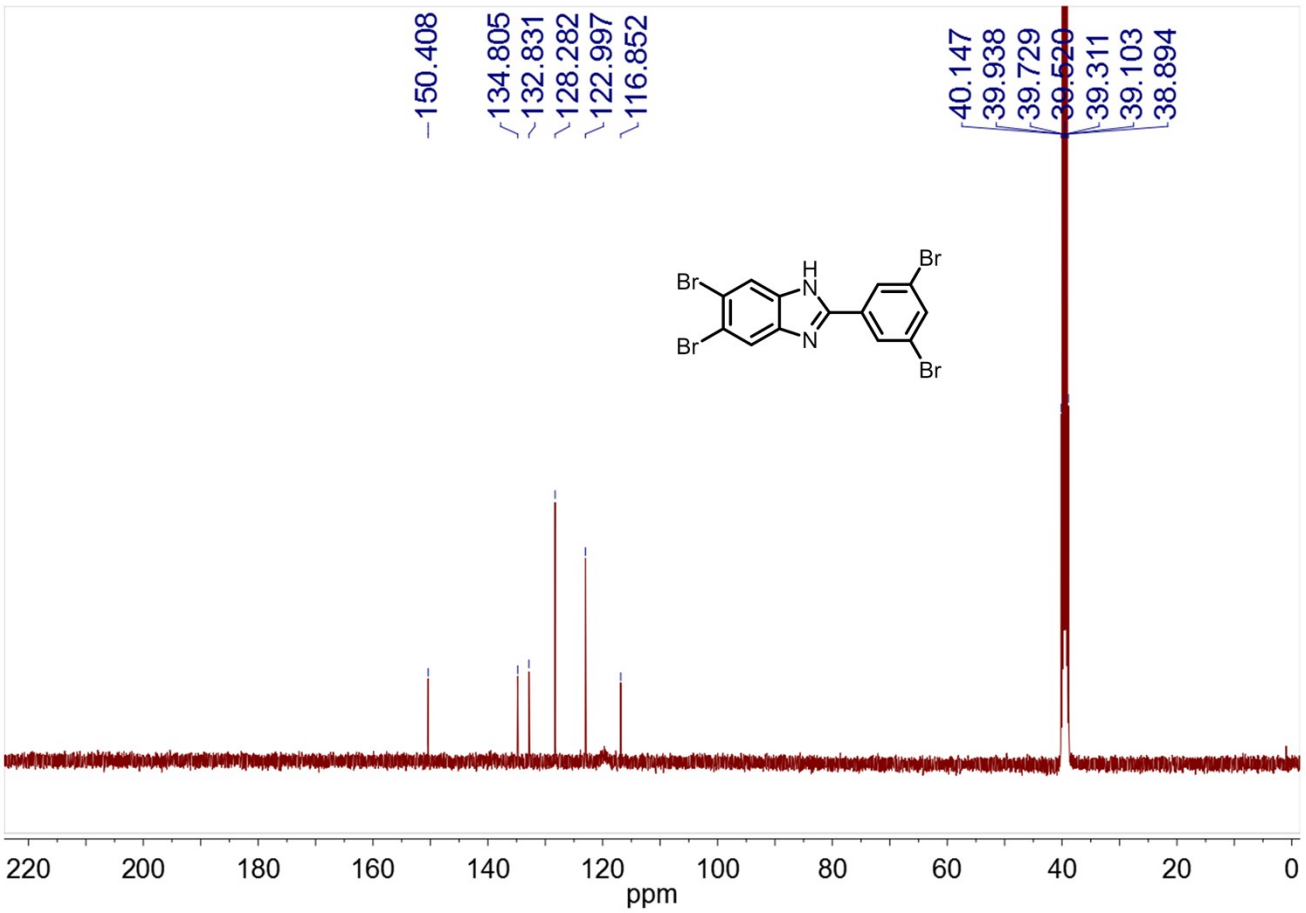


Figure S20. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 100 MHz) of compound **1**.

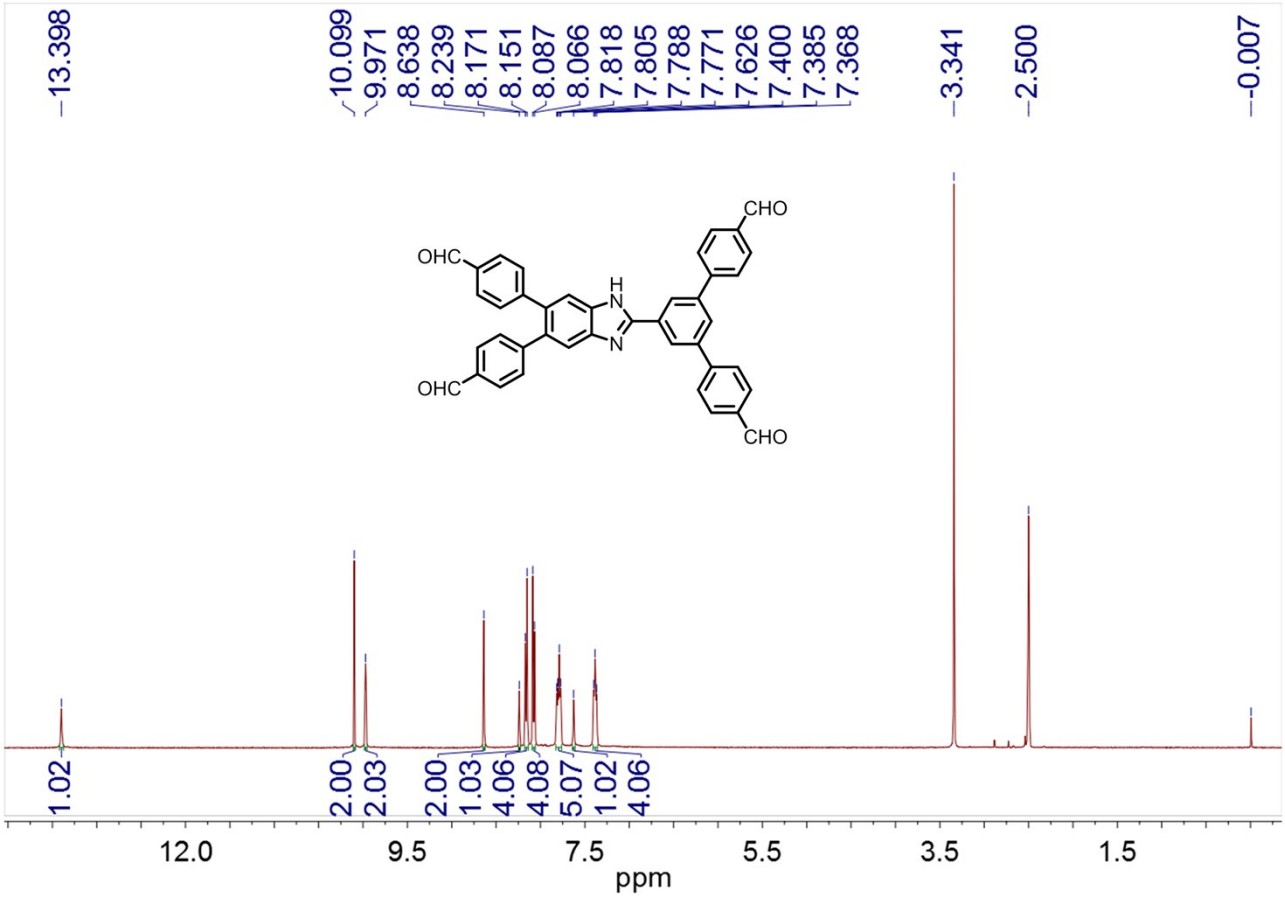


Figure S21. ^{1}H NMR spectrum (DMSO-d_6, 298 K, 400 MHz) of the building block BITA.

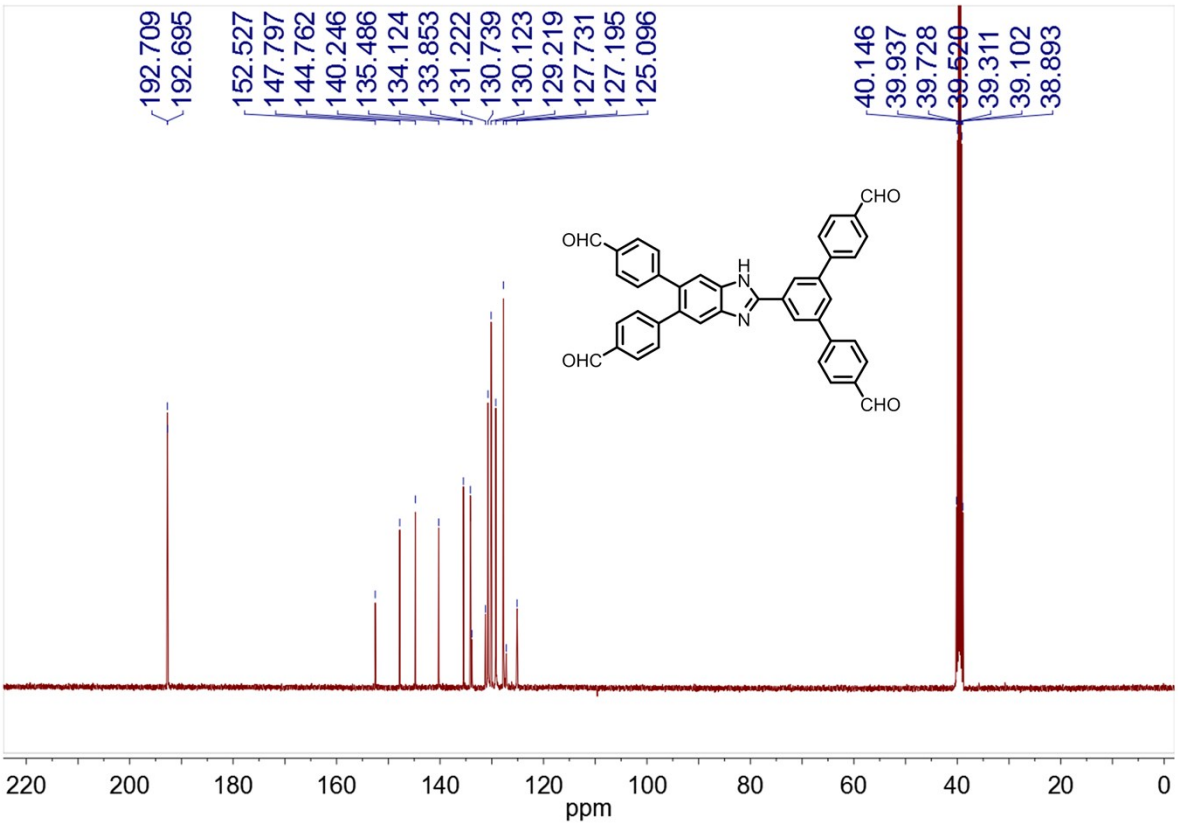


Figure S22. ^{13}C NMR spectrum (DMSO-d_6, 298 K, 100 MHz) of the building block BITA.

Section S12. *Mass spectra (MS)*

Mass detections were recorded by employing an LC-MS instrument equipped with a Waters SQ detector through an electrospray ionization (ESI) interface. Measurements were carried out in positive ion mode for compound **1** and negative ion mode for the building block BITA. To better obtain the fragment ions, cone voltage was set at 42 V. Other MS detection conditions were as follows: capillary voltage, 3.0 kV; source temperature, 120 °C; desolvation temperature, 350 °C; and desolvation gas flow was 500 L/h.

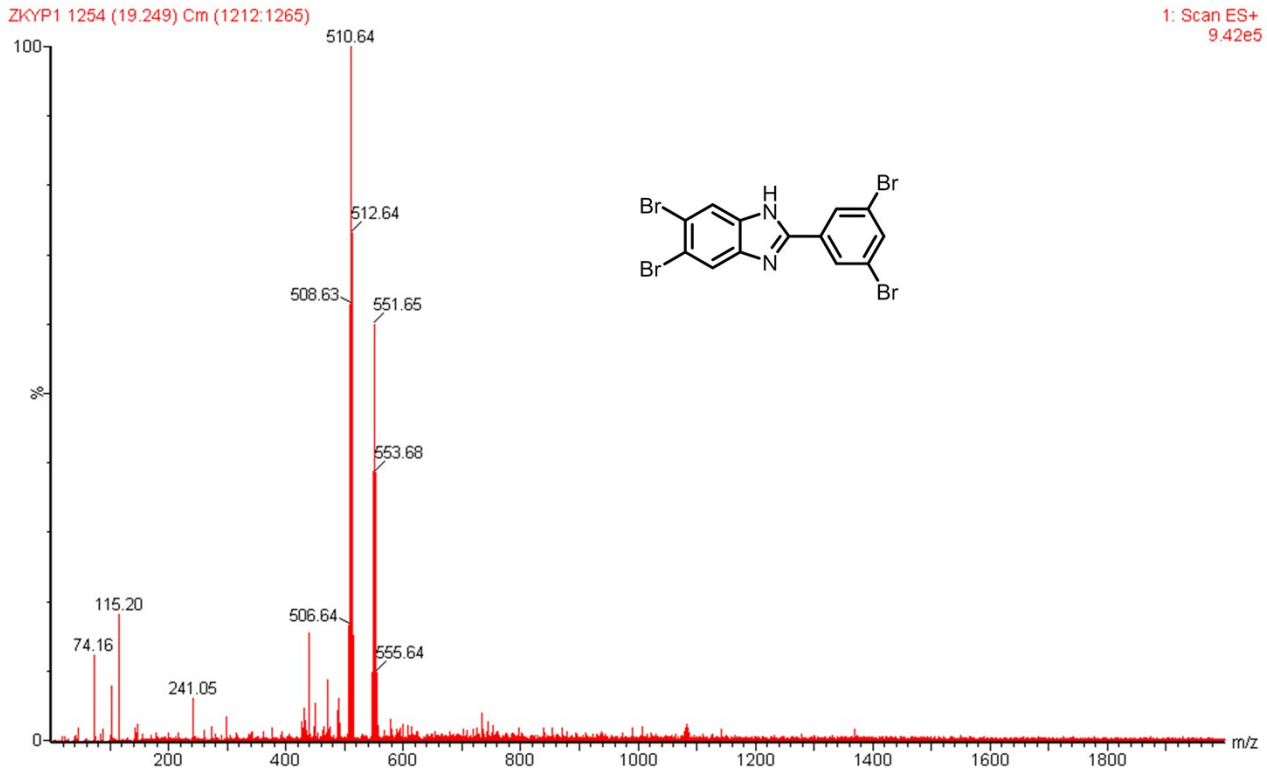


Figure S23. MS of compound **1**.

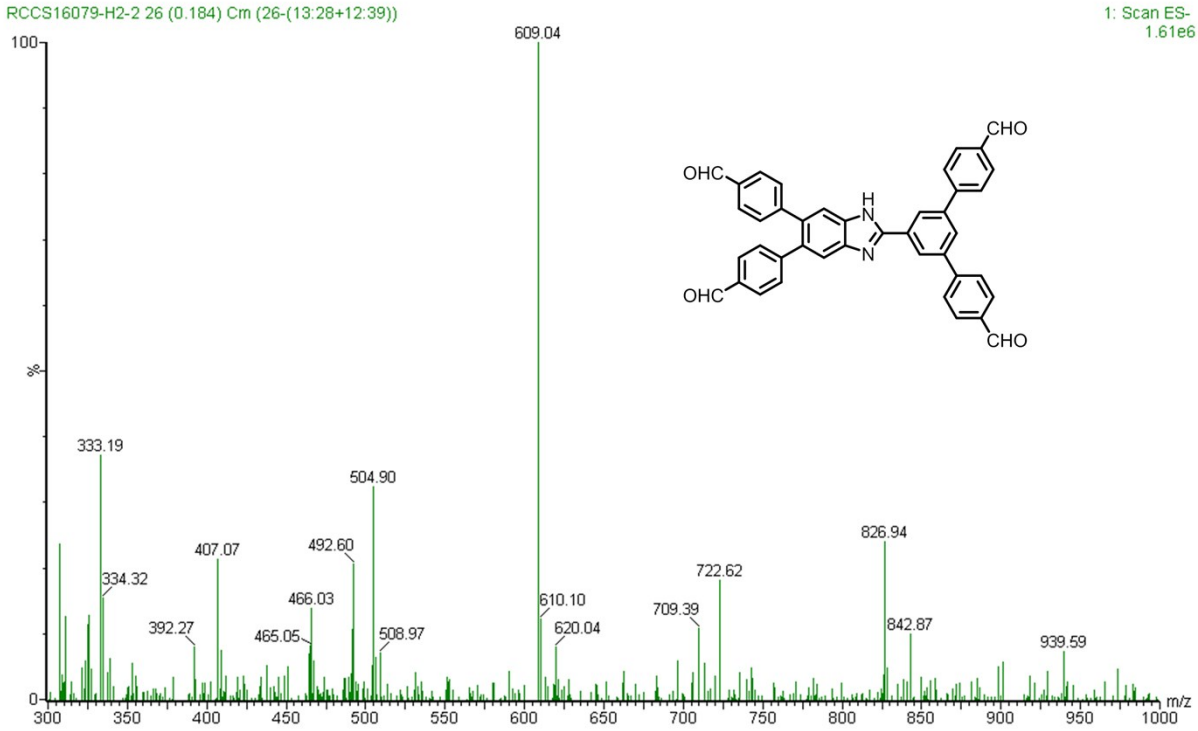


Figure S24. MS of the building block BITA.

Table S1. *Fractional atomic coordinates for the unit cell of the* ***htb*** *type BITA-PDA COF with AA packing.*

htb type BITA-PDA COF with AA packing			
Space group: *P6/M* (No. 175) $a = b = 70.26$ Å, $c = 3.44$ Å $\alpha = \beta = 90°$, $\gamma = 120°$ $V = 14712$ Å^3			
Atom	x/a	y/b	z/c
C1	0.20849	0.45737	0.00000
C2	0.21046	0.43894	0.00000
C3	0.24932	0.48018	0.00000
N4	0.22697	0.41844	0.00000
C5	0.20909	0.37144	0.00000
C6	0.20026	0.34847	0.00000
C7	0.21843	0.49740	0.00000
C8	0.13796	0.32942	0.00000
C9	0.23051	0.52120	0.00000
C10	0.22111	0.53459	0.00000
C11	0.19861	0.52607	0.00000
C12	0.18553	0.50347	0.00000
C13	0.19492	0.48982	0.00000
C14	0.23833	0.35167	0.00000
C15	0.25191	0.34242	0.00000
C16	0.24295	0.31966	0.00000
C17	0.22008	0.30619	0.00000
C18	0.20641	0.31532	0.00000
C19	0.37826	0.58024	0.00000
C20	0.37896	0.60069	0.00000
C21	0.41858	0.60032	0.00000
C22	0.26169	0.27757	0.00000
C23	0.24967	0.25459	0.00000
C24	0.29547	0.27591	0.00000
C25	0.20576	0.40525	0.00000
C26	0.19565	0.38091	0.00000
C27	0.17707	0.33524	0.00000
C28	0.22970	0.43991	0.00000
C29	0.24884	0.45949	0.00000
C30	0.22700	0.47962	0.00000
N31	0.19355	0.41665	0.00000
C32	0.16287	0.34412	0.00000
C33	0.17280	0.36724	0.00000
C34	0.27371	0.49927	0.00000
C35	0.21508	0.33841	0.00000
C36	0.29331	0.49742	0.00000
C37	0.31466	0.51613	0.00000

C38	0.31723	0.53721	0.00000
C39	0.29841	0.53895	0.00000
C40	0.27793	0.52026	0.00000
C41	0.12777	0.30615	0.00000
C42	0.10493	0.29276	0.00000
C43	0.09129	0.30192	0.00000
C44	0.10089	0.32481	0.00000
C45	0.12373	0.33831	0.00000
C46	0.39880	0.62022	0.00000
C47	0.41864	0.62035	0.00000
C48	0.39838	0.58035	0.00000
C49	0.26031	0.24228	0.00000
C50	0.28344	0.25292	0.00000
C51	0.28482	0.28822	0.00000
C52	0.78044	0.33843	0.00000
N53	0.79821	0.35769	0.00000
N54	0.79627	0.43788	0.00000
C55	0.81040	0.45876	0.00000
N56	0.29545	0.24129	0.00000
C57	0.28733	0.22012	0.00000
C58	0.25768	0.31032	0.00000
N59	0.24966	0.28917	0.00000
H60	0.19157	0.45228	0.00000
H61	0.22651	0.38253	0.00000
H62	0.24713	0.53332	0.00000
H63	0.23196	0.55233	0.00000
H64	0.16780	0.49616	0.00000
H65	0.18184	0.47326	0.00000
H66	0.24674	0.36932	0.00000
H67	0.26957	0.35320	0.00000
H68	0.21263	0.28846	0.00000
H69	0.18910	0.30363	0.00000
H70	0.36460	0.60243	0.00000
H71	0.43384	0.60006	0.00000
H72	0.23188	0.24615	0.00000
H73	0.31326	0.28435	0.00000
H74	0.17001	0.31792	0.00000
H75	0.26282	0.45734	0.00000
H76	0.17664	0.41060	0.00000
H77	0.16306	0.37502	0.00000
H78	0.29345	0.48223	0.00000
H79	0.32894	0.51408	0.00000
H80	0.29936	0.55483	0.00000
H81	0.26475	0.52132	0.00000
H82	0.13681	0.29753	0.00000
H83	0.09788	0.27508	0.00000

H84	0.09075	0.33241	0.00000
H85	0.12955	0.35566	0.00000
H86	0.39876	0.63562	0.00000
H87	0.39839	0.56495	0.00000
H88	0.25022	0.22461	0.00000
H89	0.29489	0.30589	0.00000
H90	0.76446	0.33693	0.00000
H91	0.82791	0.46482	0.00000
H92	0.26980	0.20897	0.00000
H93	0.27520	0.32154	0.00000

Table S2. *Fractional atomic coordinates for the unit cell of the* ***htb*** *type BITA-PDA COF with AB packing.*

htb type BITA-PDA COF with AB packing			
Space group: *P63/M* (No. 176) $a = b = 70.21$ Å, $c = 6.49$ Å $\alpha = \beta = 90°$, $\gamma = 120°$ $V = 27729$ Å^3			
Atom	*x/a*	*y/b*	*z/c*
C1	1.54537	0.12346	0.25000
C2	1.54774	0.10525	0.25000
C3	1.58616	0.14685	0.25000
N4	1.56471	0.08515	0.25000
C5	1.54699	0.03796	0.25000
C6	1.53810	0.01495	0.25000
C7	1.55450	0.16324	0.25000
C8	1.47577	0.99607	0.25000
C9	1.56616	0.18706	0.25000
C10	1.55631	0.20007	0.25000
C11	1.53373	0.19111	0.25000
C12	1.52103	0.16845	0.25000
C13	1.53087	0.15519	0.25000
C14	1.57617	0.01805	0.25000
C15	1.58968	0.00870	0.25000
C16	1.58059	0.98589	0.25000
C17	1.55768	0.97252	0.25000
C18	1.54410	0.98173	0.25000
C19	1.71436	0.24890	0.25000
C20	1.71452	0.26911	0.25000
C21	1.75471	0.26983	0.25000
C22	1.59829	0.94298	0.25000

C23	1.58576	0.92000	0.25000
C24	1.63153	0.94033	0.25000
C25	1.54352	0.07175	0.25000
C26	1.53355	0.04742	0.25000
C27	1.51486	0.00172	0.25000
C28	1.56713	0.10653	0.25000
C29	1.58610	0.12634	0.25000
C30	1.56360	0.14585	0.25000
N31	1.53105	0.08290	0.25000
C32	1.50071	0.01065	0.25000
C33	1.51070	0.03375	0.25000
C34	1.61042	0.16629	0.25000
C35	1.55289	0.00484	0.25000
C36	1.63029	0.16490	0.25000
C37	1.65147	0.18390	0.25000
C38	1.65360	0.20481	0.25000
C39	1.63452	0.20611	0.25000
C40	1.61421	0.18716	0.25000
C41	1.46540	0.97277	0.25000
C42	1.44250	0.95954	0.25000
C43	1.42905	0.96894	0.25000
C44	1.43886	0.99186	0.25000
C45	1.46170	0.00516	0.25000
C46	1.73411	0.28892	0.25000
C47	1.75422	0.28960	0.25000
C48	1.73477	0.24956	0.25000
C49	1.59589	0.90720	0.25000
C50	1.61900	0.91732	0.25000
C51	1.62140	0.95313	0.25000
C52	1.11556	0.00819	0.25000
N53	1.13312	0.02762	0.25000
N54	1.12899	0.10665	0.25000
C55	1.14265	0.12763	0.25000
N56	1.63048	0.90515	0.25000
C57	1.62192	0.88390	0.25000
C58	1.59511	0.97630	0.25000
N59	1.58674	0.95508	0.25000
C60	1.12104	0.20964	0.25000
C61	1.11867	0.22784	0.25000
C62	1.08027	0.18621	0.25000
N63	1.10172	0.24798	0.25000

C64	1.11966	0.29540	0.25000
C65	1.12872	0.31847	0.25000
C66	1.11201	0.16991	0.25000
C67	1.19101	0.33693	0.25000
C68	1.10042	0.14610	0.25000
C69	1.11036	0.13317	0.25000
C70	1.13297	0.14223	0.25000
C71	1.14558	0.16486	0.25000
C72	1.13565	0.17803	0.25000
C73	1.09081	0.31580	0.25000
C74	1.07745	0.32534	0.25000
C75	1.08669	0.34817	0.25000
C76	1.10961	0.36139	0.25000
C77	1.12305	0.35197	0.25000
C78	1.95205	0.08450	0.25000
C79	1.95187	0.06429	0.25000
C80	1.91171	0.06363	0.25000
C81	1.06905	0.39121	0.25000
C82	1.08155	0.41420	0.25000
C83	1.03577	0.39384	0.25000
C84	1.12293	0.26138	0.25000
C85	1.13299	0.28577	0.25000
C86	1.15199	0.33155	0.25000
C87	1.09928	0.22657	0.25000
C88	1.08032	0.20673	0.25000
C89	1.10283	0.18723	0.25000
N90	1.13536	0.25019	0.25000
C91	1.16602	0.32248	0.25000
C92	1.15587	0.29935	0.25000
C93	1.05602	0.16677	0.25000
C94	1.11410	0.32882	0.25000
C95	1.03618	0.16820	0.25000
C96	1.01499	0.14926	0.25000
C97	1.01281	0.12835	0.25000
C98	1.03185	0.12697	0.25000
C99	1.05218	0.14586	0.25000
C100	1.20153	0.36025	0.25000
C101	1.22444	0.37337	0.25000
C102	1.23781	0.36387	0.25000
C103	1.22786	0.34093	0.25000
C104	1.20499	0.32773	0.25000

C105	1.93229	0.04452	0.25000
C106	1.91222	0.04386	0.25000
C107	1.93166	0.08389	0.25000
C108	1.07140	0.42698	0.25000
C109	1.04829	0.41684	0.25000
C110	1.04593	0.38105	0.25000
C111	1.55129	0.32542	0.25000
N112	1.53380	0.30594	0.25000
N113	1.53796	0.22684	0.25000
C114	1.52420	0.20586	0.25000
N115	1.03679	0.42899	0.25000
C116	1.04533	0.45024	0.25000
C117	1.07225	0.35790	0.25000
N118	1.08063	0.37913	0.25000
H119	1.52838	0.11806	0.25000
H120	1.56444	0.04905	0.25000
H121	1.58271	0.19940	0.25000
H122	1.56687	0.21787	0.25000
H123	1.50325	0.16080	0.25000
H124	1.51799	0.13852	0.25000
H125	1.58464	0.03572	0.25000
H126	1.60738	0.01941	0.25000
H127	1.55011	0.95477	0.25000
H128	1.52677	0.97009	0.25000
H129	1.69991	0.27045	0.25000
H130	1.77020	0.26999	0.25000
H131	1.56798	0.91195	0.25000
H132	1.64932	0.94837	0.25000
H133	1.50770	-0.01563	0.25000
H134	1.60029	0.12451	0.25000
H135	1.51410	0.07672	0.25000
H136	1.50097	0.04153	0.25000
H137	1.63075	0.14986	0.25000
H138	1.66597	0.18218	0.25000
H139	1.63512	0.22184	0.25000
H140	1.60084	0.18795	0.25000
H141	1.47434	0.96405	0.25000
H142	1.43528	0.94183	0.25000
H143	1.42889	0.99965	0.25000
H144	1.46759	0.02252	0.25000
H145	1.73363	0.30412	0.25000

H146	1.73521	0.23437	0.25000
H147	1.58543	0.88955	0.25000
H148	1.63180	0.97079	0.25000
H149	1.09943	0.00634	0.25000
H150	1.16026	0.13416	0.25000
H151	1.60432	0.87304	0.25000
H152	1.61270	0.98730	0.25000
H153	1.13803	0.21508	0.25000
H154	1.10219	0.28440	0.25000
H155	1.08388	0.13377	0.25000
H156	1.09987	0.11537	0.25000
H157	1.16336	0.17257	0.25000
H158	1.14850	0.19471	0.25000
H159	1.08225	0.29812	0.25000
H160	1.05975	0.31474	0.25000
H161	1.11730	0.37915	0.25000
H162	1.14042	0.36351	0.25000
H163	1.96643	0.06290	0.25000
H164	1.89623	0.06347	0.25000
H165	1.09934	0.42227	0.25000
H166	1.01798	0.38579	0.25000
H167	1.15925	0.34892	0.25000
H168	1.06613	0.20856	0.25000
H169	1.15230	0.25634	0.25000
H170	1.16553	0.29148	0.25000
H171	1.03573	0.18324	0.25000
H172	1.00051	0.15101	0.25000
H173	1.03119	0.11121	0.25000
H174	1.06550	0.14496	0.25000
H175	1.19266	0.36906	0.25000
H176	1.23176	0.39110	0.25000
H177	1.23777	0.33306	0.25000
H178	1.19897	0.31034	0.25000
H179	1.93274	0.02931	0.25000
H180	1.93124	0.09910	0.25000
H181	1.08183	0.44463	0.25000
H182	1.03553	0.36339	0.25000
H183	1.56745	0.32732	0.25000
H184	1.50661	0.19941	0.25000
H185	1.06292	0.46113	0.25000
H186	1.05466	0.34693	0.25000

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