Electronic Supplementary Information

Identification of two-dimensional covalent organic frameworks with mcm topology and their application in photocatalytic hydrogen evolution

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Instruments and Methods

Fourier-transform infrared spectroscopy (FT-IR)

Fourier-transform infrared spectroscopy (FT-IR) was carried out a Nicolet iS10 spectrometer. The samples were prepared as KBr pellets.

Solid-state nuclear magnetic resonance (NMR) spectroscopy

The ^{13}C CP/MAS NMR spectra of the COFs were recorded on an Agilent DD2 600 Solid NMR System with 3.2 mm zirconia rotors. The spinning rate is 8 kHz and the contact tome is 3ms.

Thermal gravimetric analysis

Thermal gravimetric analysis was conducted on a NETZSCH STA 449F3 instrument by heating the samples from room temperature to 900 °C under nitrogen atmosphere with a heating rate of 10 °C/min.

Powder X-ray diffraction

Powder X-ray diffraction measurements were carried out with an PANalytical X'Pert Powder system using monochromated Cu/Kα (λ = 0.1542 nm). The samples were spread on the square recess of a XRD sample holder as thin layers.

Structural simulation and powder X-ray diffraction analyses

Structural simulations were carried out with Materials Studio. The predicted structures were firstly optimized in geometry optimizations by the Forcite molecular dynamics module method, after which the simulated PXRD patterns were determined by Reflex module. Pawley refinement of the experimental PXRD patterns was conducted by the Reflex module.

Nitrogen adsorption-desorption isotherm measurement

The measurements were performed on a Quantanchrome autosorb IQ system. The as-prepared samples were activated by degassed for 30 minutes at 100 °C and 300 minutes

at 150 °C, respectively. The isotherms were collected at 77 K under liquid nitrogen bath. The Brunauer-Emmett-Teller (BET) method was utilized to calculate their specific surface areas. By using the quenched solid density functional theory (QSDFT), the pore size distributions were derived from the sorption data.

Solid-state UV-Vis diffuse reflectance spectroscopy

Solid-state UV-Vis diffuse reflectance spectra (DRS) were collected on a Hitachi UH4150 spectrophotometer equipped with integrating sphere with $BaSO_4$ as a reflectance standard.

X-ray photoelectron spectroscopy

X-ray photoelectron spectroscopy (XPS) was recorded on an ESCALAB 250Xi spectrophommeter with $Al\ K_\alpha$ radiation. The binding energy scale was calibrated using C 1*s* peak at 284.60 eV.

Transmission electron microscopy

Transmission electron microscopy (TEM) was performed on a JEOL JEM-2100 instrument.

Photoelectrochemical experiment

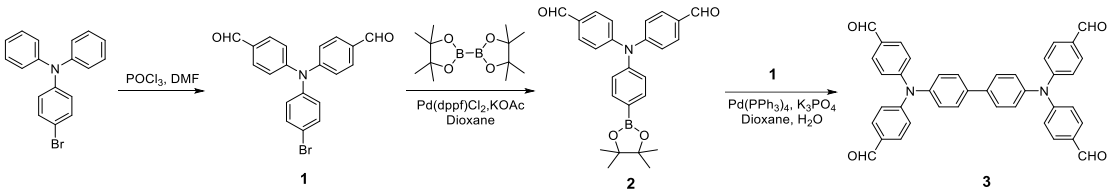
The photoelectrochemical measurement experiments were conducted with a CHI 660E electrochemical workstation (Shanghai Chenhua Instrument, China) in a conventional three electrode cell, using a Pt plate as the counter electrode and an Ag/AgCl electrode as the reference electrode. The working electrode was prepared on fluorine doped tin oxide (FTO) glass which was cleaned by sonication in ethanol for 30 min and dried at 353 K. The sample (1 mg) was dispersed in ethanol (1 mL) with a few droplets of 5 wt% Nafion by sonication to get a slurry. The slurry was spread onto pretreated FTO glass then dried in air as the working electrode. The electrolyte was 0.1 M Na_2SO_4 aqueous solution and the light source was provided by a 300 W Xe-lamp with an ultraviolet cut-

off filter (λ > 400 nm).

Photocatalytic H_2 evolution

A flask was charged with 5 mg COFs powder and 16 mL 0.1M ascorbate acid solution in PBS buffer (0.1 M, PH = 6.0). Then the suspensions were sonicated with a sonic tip (ultrasonic frequency:19-25 kHz) in ice bath for 20 min (period of 2 s with the interval for 2 s) using a power of 150 W. The mixture was transferred into a quartz top-irradiation reactor and 1 μL 8 wt% H_2PtCl_6 was added before the reactor was sealed. The reaction mixture was evacuated several times to ensure complete removal of air and filled with nitrogen, Then the reactor was illuminated with a 300 W Xe light source (λ > 400 nm). The temperature of the reaction solution was maintained at room temperature by the flow of cooling water. The evolved gases were analyzed by gas chromatography (Shimadzu GC2014) with helium as the carrier gas. Hydrogen was detected with a thermal conductivity detector (TCD) referencing standard gas with a known concentration of hydrogen.

Synthetic Procedures



4,4'-((4-bromophenyl)azanediyl)dibenzaldehyde (1)

4-Bromo-*N*,*N*-diphenylaniline (3.5 g, 10.8 mmol) was dissolved in DMF (25 mL) in a 250 mL flask. Under cooling with ice phosphorus oxychloride (20 mL) was added dropwise with stirring. During this process, precipitate was observed. After the addition was completed, the mixture was heated to 80 ^oC and stirred at this temperature for 36 h. The mixture was cooled to room temperature, poured into ice (100 g), and extracted with CH_2Cl_2 (100 mL × 3). The organic extracts were washed with brine (100 mL×2) and water (100 mL), dried with anhydrous Na_2SO_4, and concentrated. The residue was

purified by flash column chromatography (petroleum ether/dichloromethane (1/1), silica gel, 300-400 mesh) to give **1** as a light yellow solid (3.6 g, 88 %). ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C): δ 9.90 (s, 2H), 7.78 (d, J = 8.5 Hz, 4H), 7.50 (d, J = 8.6 Hz, 2H), 7.18 (d, J = 8.4 Hz, 4H), 7.05 (d, J = 8.6 Hz, 2H).

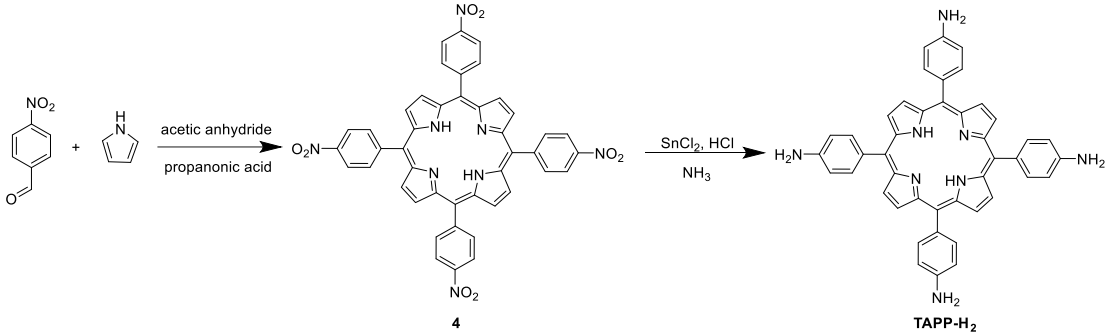
4,4'-((4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)azanediyl) dibenzaldehyde (2).

Compound **1** (13.50 g, 35.5 mmol), bis(pinacolato)diborane (11.00 g, 39.7 mmol), potassium acetate (10.45 g, 106.5 mmol), $Pd(dppf)_2Cl_2$ (1.28 g, 1.75 mmol), and dried 1,4-dioxane (200 mL) were added in a 500 mL flask. The mixture was degassed through three freeze-pump-thaw cycles under an argon atmosphere and then stirred at 100 °C for 24 h. After the reaction was completed, the reaction solution was filtered and the solvent was removed under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/ethyl acetate (10/1; 5/1); silica gel, 300-400 mesh) to give **2** as a light yellow solid (14.2 g, 94%). ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C): δ 9.90 (s, 2H), 7.81 (d, J = 8.2 Hz, 2H), 7.77 (d, J = 8.5 Hz, 4H), 7.19 (d, J = 8.5 Hz, 4H), 7.15 (d, J = 8.2 Hz, 2H), 1.35 (s, 12H).

4,4',4'',4'''-([1,1'-biphenyl]-4,4'-diylbis(azanetriyl))tetrabenzaldehyde (BATA, 3).

To a mixture of 4,4'-((4-bromophenyl)azanediyl)dibenzaldehyde (1.41 g, 3.3 mmol, 1.1eq), 4,4'-((4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)azanediyl) dibenzaldehyde (1.14 g, 3 mmol, 1 eq), K_3PO_4 (1.91 g, 9 mmol, 3 eq) and $Pd(PPh_3)_4$ (173 mg, 0.15 mmol, 0.05 eq), a degassed mixture of 1,4-dioxane (100 mL) and H_2O (5 mL) was added. The mixture was heated at 100 ^{o}C for 24 h under the protection of nitrogen. After cooling to room temperature, the solvent was removed under vacuum and the residue was purified by flash column chromatography (petroleum ether/dichloromethane/ethyl acetate (5/1/1), silica gel, 300-400 mesh) to give compound **3** a yellow solid (1.73 g, 96%).^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) : δ 9.86

(s, 4H), 7.83 (d, *J* = 8.6 Hz, 8H), 7.74 (d, *J* = 8.6 Hz, 4H), 7.24 (d, *J* = 8.6 Hz, 4H), 7.19 (d, *J* = 8.6 Hz, 8H).

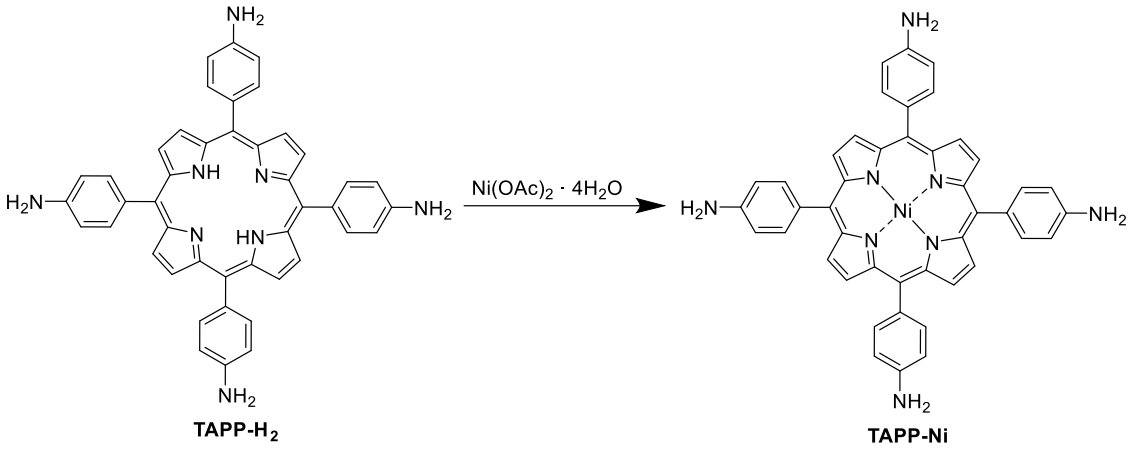


Tetrakis(4-nitrophenyl)porphyrin (4)

4-nitrobenzaldehyde (22.0 g, 0.145 mol) and acetic anhydride (24 mL, 0.24 mol) were dissolved in 600 mL propanoic acid. The solution was refluxed, to which pyrrole (10.0 mL, 0.144 mol) was added slowly. After refluxing for 30 min, the resulting mixture was cooled to room temperature to give a precipitate which was collected by filtration. The precipitate was washed with water and methanol, respectively, and dried under vacuum. The resulting power was mixed with pyridine (160 mL) and was refluxed for 1 h. After cooled to room temperature, the precipitate was collected by filtration and washed with acetone, and dried under vacuum to give **4** as a purple solid (5.6 g, 20.8%). MS (MALDI) m/z: 794.2. Its solubility is extremely poor so ^{1}H NMR was not conducted.

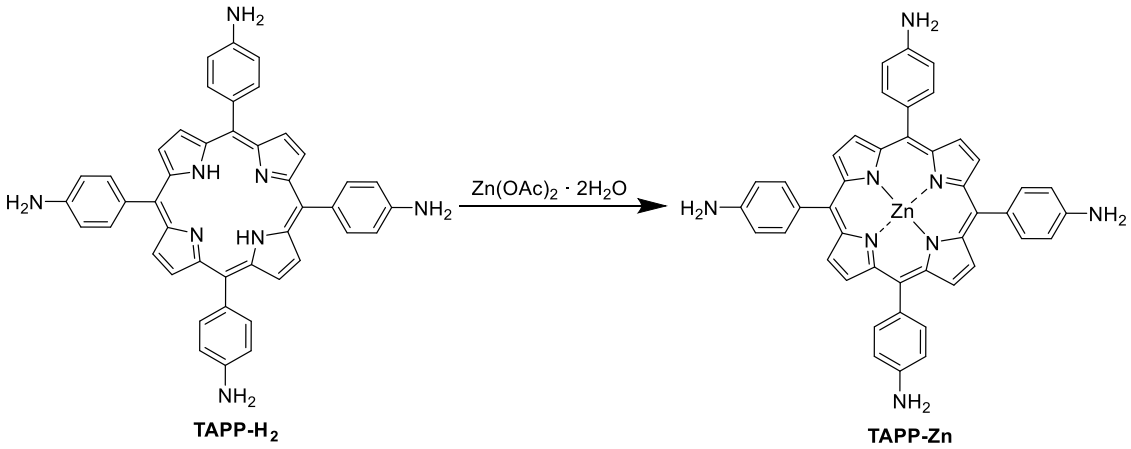
tetrakis(4-aminophenyl)porphyrin (TAPP-H_2)

A mixture of tetrakis(4-nitrophenyl)porphyrin (5.6 g, 7.5 mmol) and $SnCl_2 \cdot 2H_2O$ (28.9 g, 113 mmol) in concentrated HCl (460 mL) was stirred for 30 min at 60 °C. After cooled to room temperature, aqueous ammonia was added to the mixture slowly to de-acidification and a dark violet precipitate was obtained. After filtration and dried under vacuum, the raw product was purified by soxhlet extraction with chloroform to give **TAPP-H_2** as a violet powder (2.8 g, 55.3%). ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ 8.84 (s, 8H), 7.81 (d, *J* = 8.2 Hz, 8H), 6.96 (d, *J* = 8.3 Hz, 8H), 5.55 (s, 8H), -2.79 (s, 2H).



TAPP-Ni

TAPP-H_2 (674.8 mg, 1 mmol) and $Ni(OAc)_2 \cdot 4H_2O$ (500.0 mg, 2mmol) were added into a mixture of MeOH (40 mL), DMF (60 mL), and chloroform (180 mL). The reaction was stirred for 24 h at 80 ºC under N_2. The reaction was cooled to room temperature and the solvent was removed under reduced pressure. The crude product was washed with water and dried under vacuum to give **TAPP-Ni** as a purple solid (648 mg, 88.6%). ^{1}H NMR (400 MHz, DMSO-d_6, 25 ºC): δ 8.73 (s, 8H), 7.59 (d, J = 8.3 Hz, 8H), 6.88 (d, J = 8.3 Hz, 8H), 5.48 (s, 8H).



TAPP-Zn

TAPP-H_2 (337 mg, 0.5 mmol) and $Zn(OAc)_2 \cdot 2H_2O$ (2.2 g, 10mmol) was dissolved in MeOH (40 mL). The reaction was stirred for 12 h at room temperature and the solvent was removed under reduced pressure. The crude product was washed with water and dried under vacuum to give **TAPP-Zn** as a purple solid (360 mg, 97.6%). ^{1}H NMR (400 MHz, DMSO-d_6, 25 ºC): δ 8.79 (s, 8H), 7.77 (d, J = 8.3 Hz, 8H), 6.93 (d, J = 8.3 Hz, 8H), 5.43 (s, 8H).

Synthesis of COF-BATA-TAPP-H_2

A glass ampoule was charged with BATA (54 mg, 0.09 mmol), TAPP-H_2 (60.7 mg, 0.09 mmol), a mixture of mesitylene (1.4 mL), *n*-butanol (0.6 mL), and acetic acid (6 M (aq.), 0.2 mL). After being degassed through three freeze-pump-thaw cycles, the ampoule was flame-sealed and then heated at 120 °C for three days to afford a purple solid at the bottom of the tube. The solid was collected through filtration and washed three times with tetrahydrofuran, and then followed by Soxhlet extraction with anhydrous THF for 24 h. The resulting powder was dried under dynamic vacuum at 120 °C for 4 h to afford a purple powder (89.4 mg, 83.0%)

Synthesis of COF-BATA-TAPP-Ni

A glass ampoule was charged with BATA ((24.0 mg, 0.04 mmol), TAPP-Ni (29.3 mg, 0.04 mmol), a mixture of mesitylene (0.5 mL), DMAc (0.5 mL) and acetic acid (6 M (aq.), 0.1 mL). After being was degassed through three freeze-pump-thaw cycles, the ampoule was flame-sealed and heated at 120 °C for three days to give a purple solid at the bottom of the tube. The solid was collected through filtration and washed three times with tetrahydrofuran, and then followed by Soxhlet extraction with anhydrous THF for 24 h. The resulting powder was dried under dynamic vacuum at 120 °C for 4 h to afford a purple powder (37.6 mg, 74.7%)

Synthesis of COF-BATA-TAPP-Zn

A glass ampoule was charged with BATA ((24.0 mg, 0.04 mmol), TAPP-Zn (29.5 mg, 0.04 mmol), and a mixture of *o*-xylene (0.67 mL), DMAc (1.33 mL) and acetic acid (9 M (aq.), 0.2 mL). After being degassed through three freeze-pump-thaw cycles, the ampoule was flame-sealed and then heated at 120 °C for three days to yield a purple solid at the bottom of the tube. The solid was collected through filtration and washed three times with tetrahydrofuran, and then followed by Soxhlet extraction with anhydrous THF for 24 h. The resulting powder was dried under dynamic vacuum at 120 °C for 4 h to afford a purple powder (25.2 mg, 49.8%).

Supplementary Figures

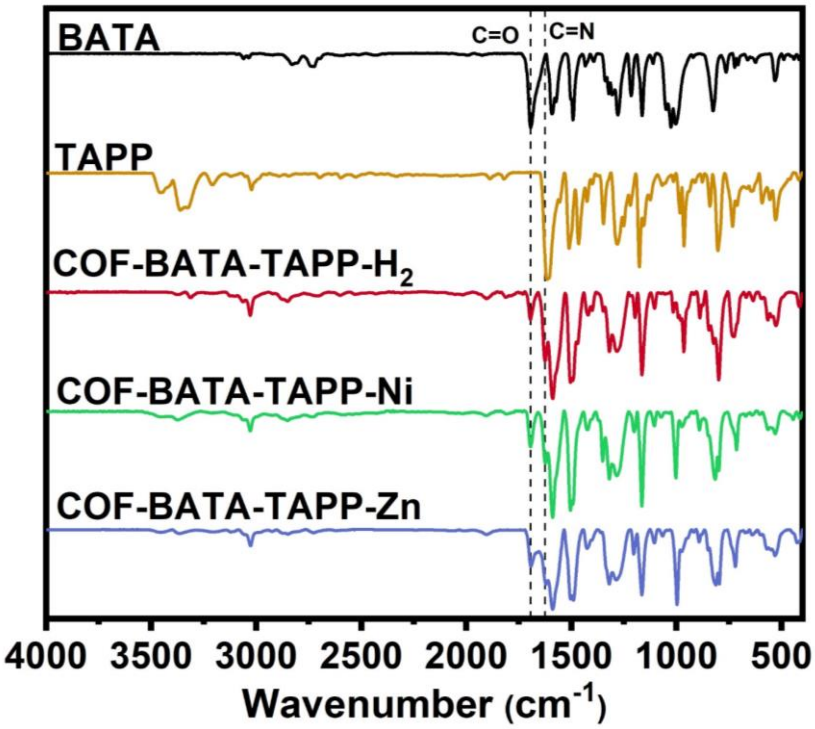


Figure S1. FT-IR spectra of the monomers and the COFs.

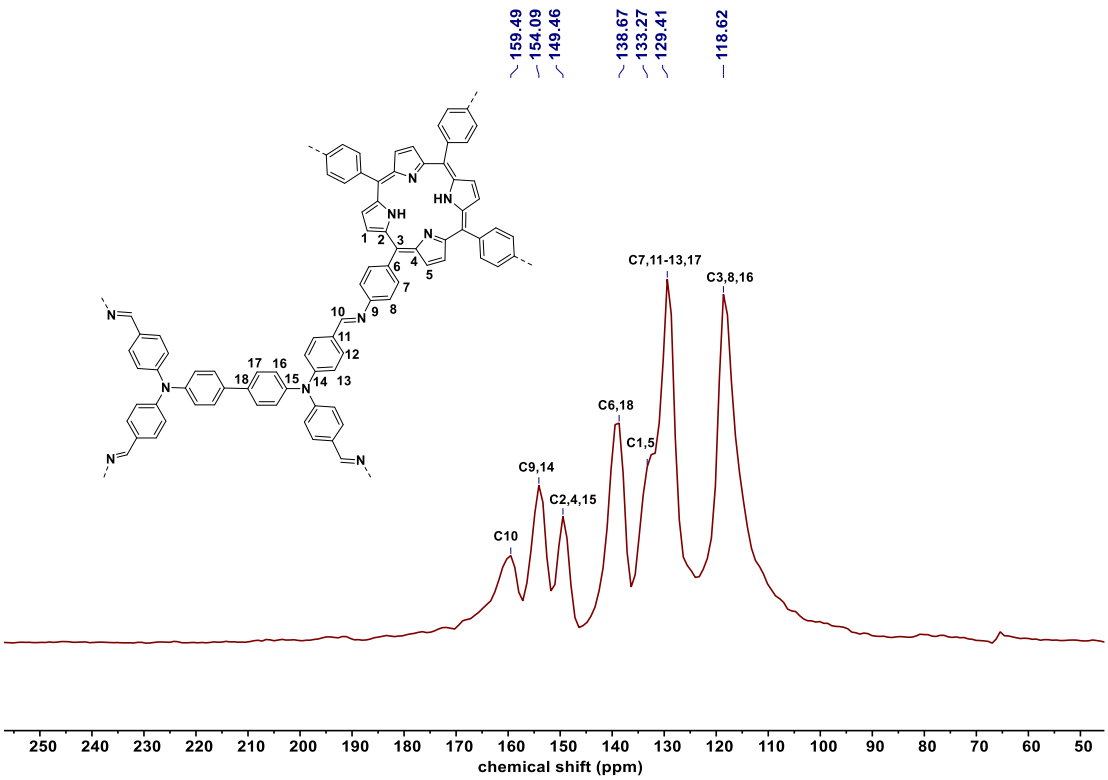


Figure S2. Solid-state ^{13}C CP/MAS NMR spectrum of COF-BATA-TAPP-H_2.

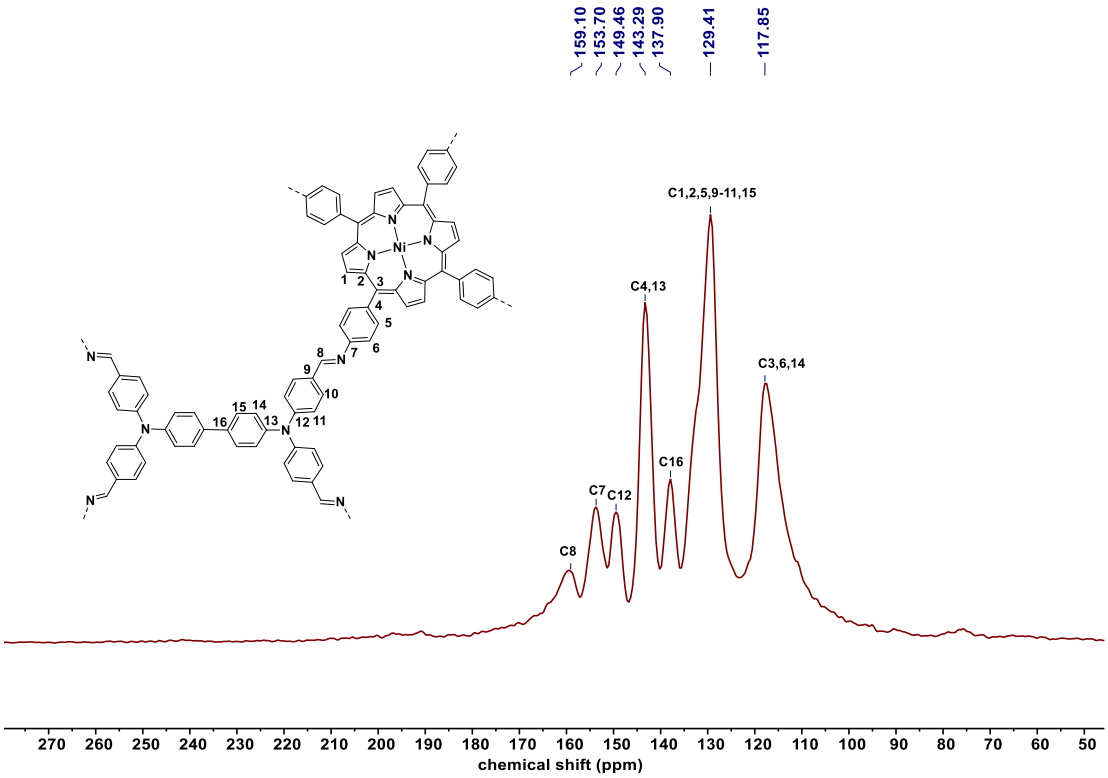


Figure S3. Solid-state ^{13}C CP/MAS NMR spectrum of COF-BATA-TAPP-Ni.

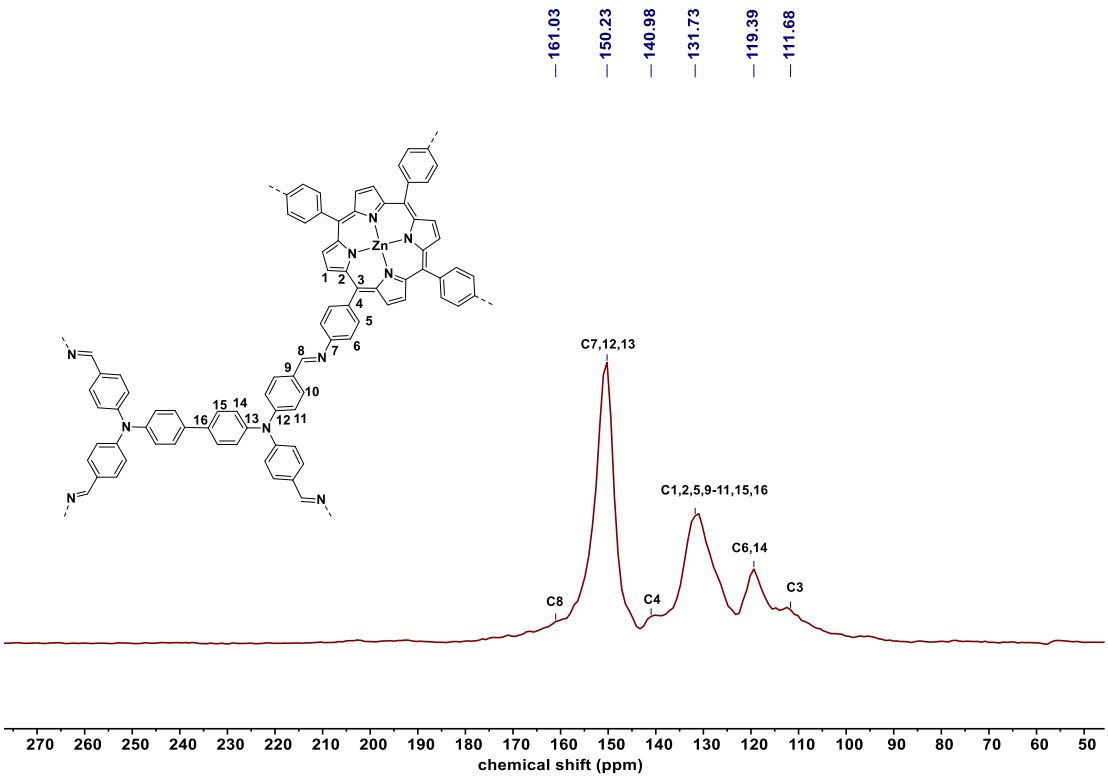


Figure S4. Solid-state ^{13}C CP/MAS NMR spectrum of COF-BATA-TAPP-Zn.

Table S1. The metal content of COF-BATA-TAPP-M from XPS measurement

	C (At. %)	N (At. %)	M (At. %)
COF-BATA-TAPP-Ni (calcd.)	88.4	10.5	1.1
COF-BATATAPP-Ni (found)	88.7	10.1	1.2
COF-BATATAPP-Zn (calcd.)	88.4	10.5	1.1
COF-BATATAPP-Zn (found)	88.0	10.8	1.2

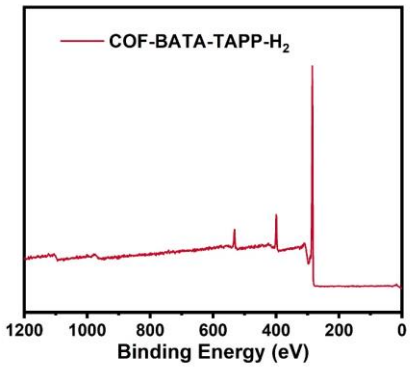


Figure S5. XPS survey of COF-BATA-TAPP-H_2.

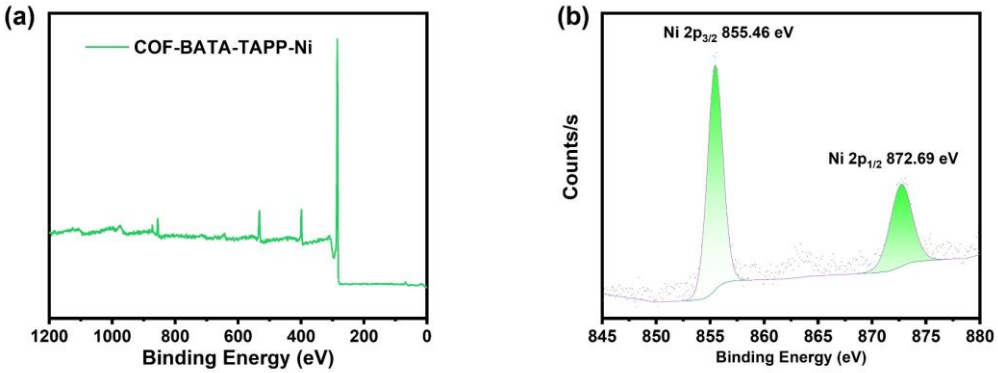


Figure S6. (a) XPS survey and (b) high-resolution XPS spectrum of COF-BATA-TAPP-Ni.

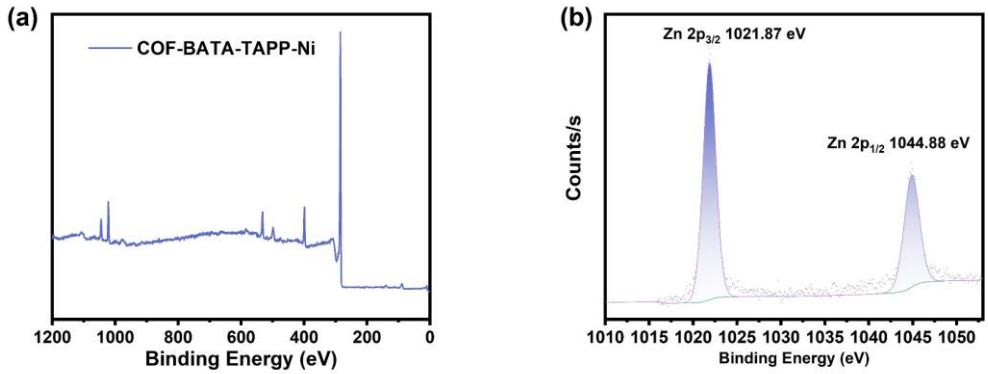


Figure S7. (a) XPS survey and (b) high-resolution XPS spectrum of COF-BATA-TAPP-Zn.

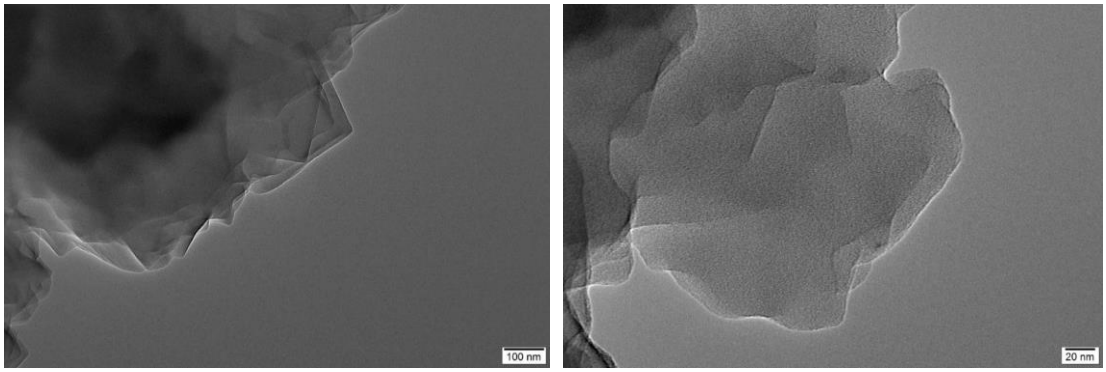


Figure S8. TEM images of COF-BATA-TAPP-H_2.

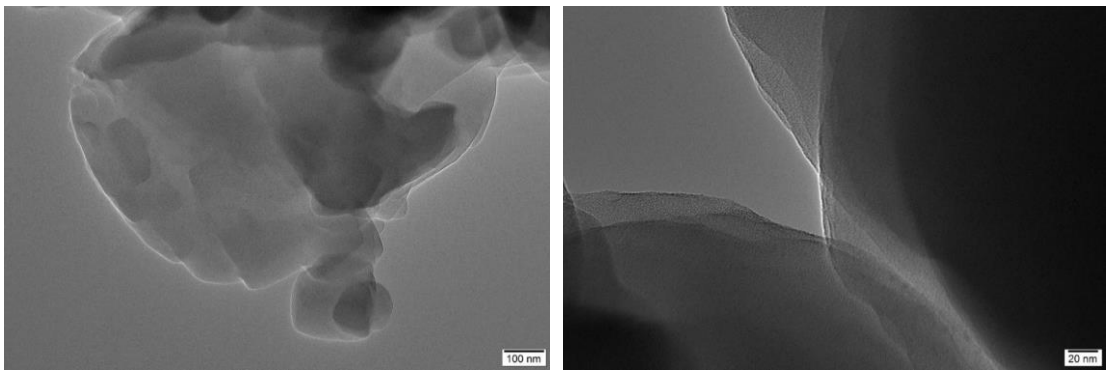


Figure S9. TEM images of COF-BATA-TAPP-Ni.

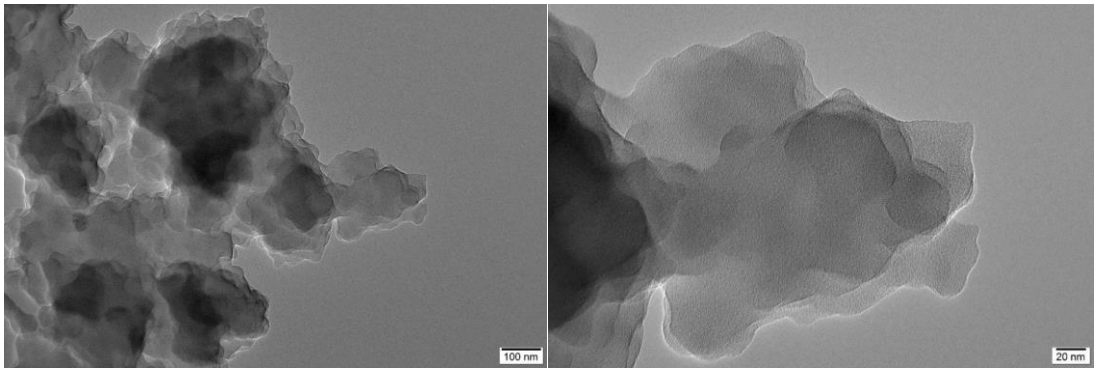


Figure S10. TEM images of COF-BATA-TAPP-Zn.

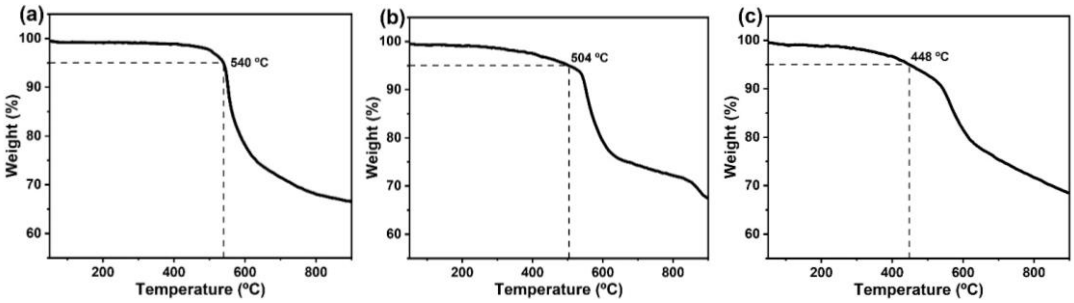


Figure S11. TGA profiles of (a) COF-BATA-TAPP-H_2, (b) COF-BATA-TAPP-Ni, and (c) COF-BATA-TAPP-Zn.

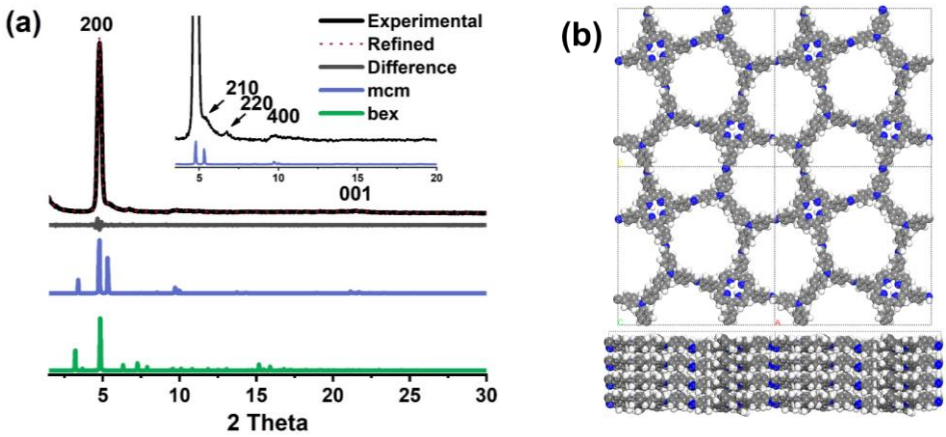


Figure S12. (a) Experimental (black) and Pawley refined (red) PXRD patterns, and their difference (gray), and simulated PXRD patterns for COF-BATA-TAPP-H_2 with **mcm** net (blue) and **bex** net (green). (b) Lattice structure of COF-BATA-TAPP-H_2 from top and side view (gray, carbon; white, hydrogen; blue, nitrogen).

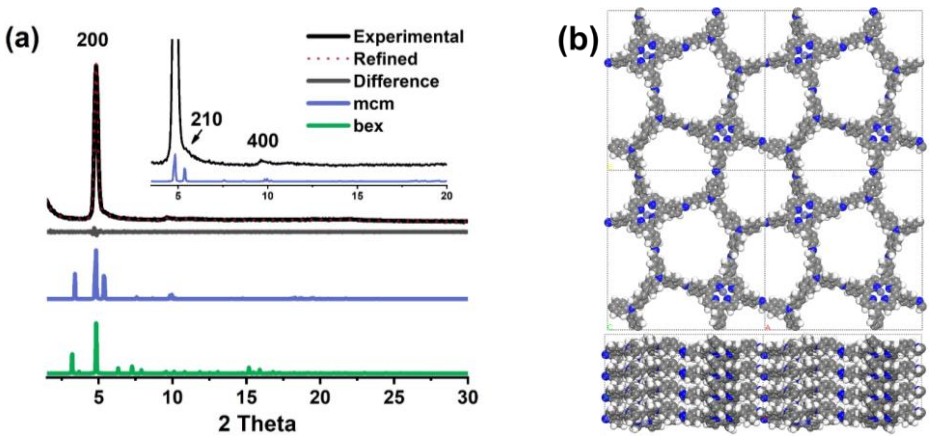


Figure S13. (a) Experimental (black) and Pawley refined (red) PXRD patterns, and their difference (gray), and simulated PXRD patterns for COF-BATA-TAPP-Ni with **mcm** net (blue) and **bex** net (green). (b) Lattice structure of COF-BATA-TAPP-Ni from top and side view (gray, carbon and nickel; white, hydrogen; blue, nitrogen).

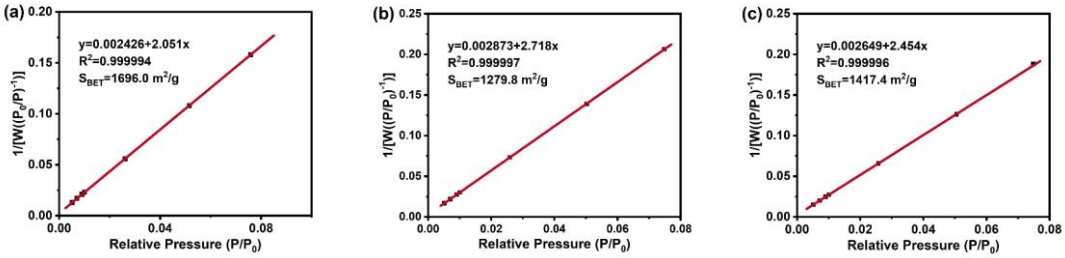


Figure S14. BET surface area plots of (a) COF-BATA-TAPP-H_2, (b) COF-BATA-TAPP-Ni, and (c) COF-BATA-TAPP-Zn.

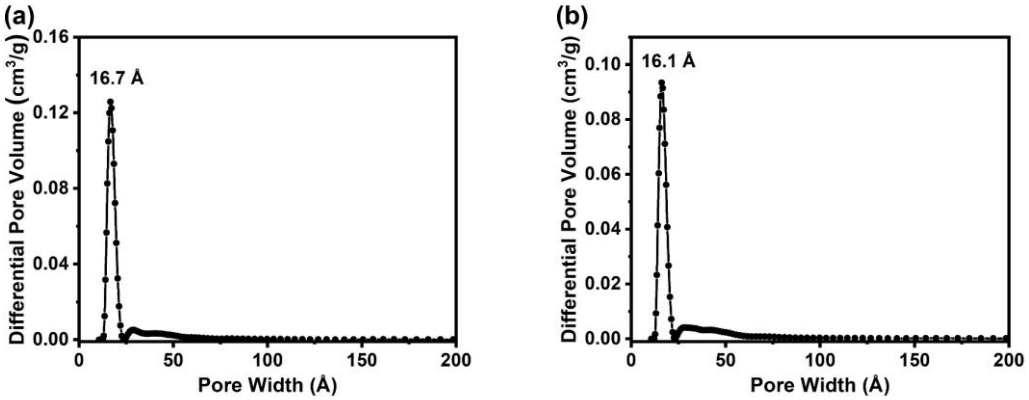


Figure S15. Pore size distribution profiles of (a) COF-BATA-TAPP-H_2 and (b) COF-BATA-TAPP-Ni.

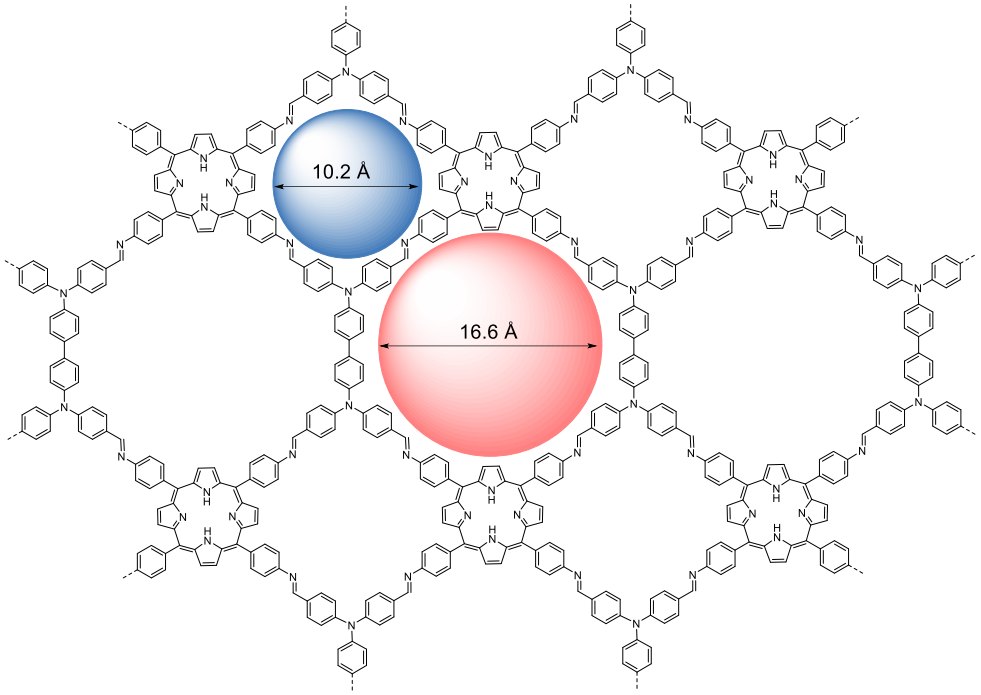


Figure S16. Illustration for the structure of the proposed COF with **bex** topology.

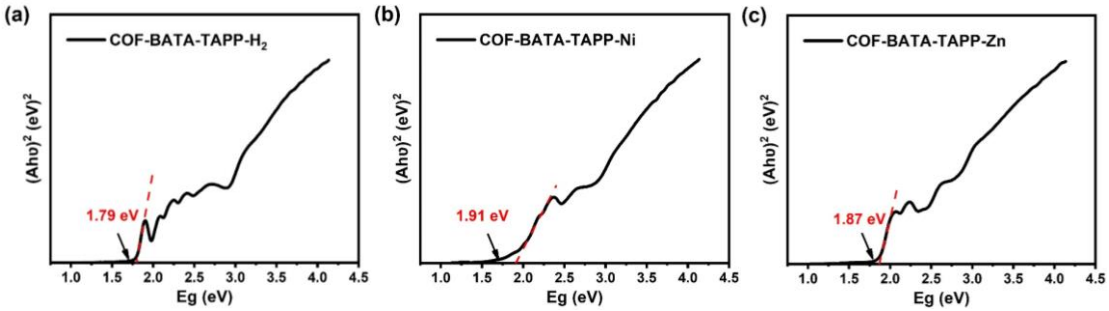


Figure S17. Tauc plots of (a) COF-BATA-TAPP-H_2, (b) COF-BATA-TAPP-Ni, and (c) COF-BATA-TAPP-Zn.

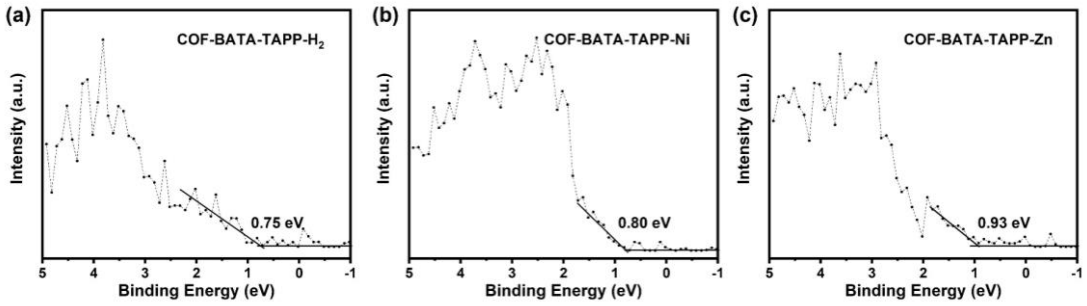


Figure S18. Valence band XPS spectra of (a) COF-BATA-TAPP-H_2, (b) COF-BATA-TAPP-Ni, and (c) COF-BATA-TAPP-Zn. The binding energy scale was calibrated using *C 1s* peak at 284.60 eV.

Table S2. Comparison of the results of the HOMO from valence band XPS spectroscopy and the HOMO from Mott-Schottky plots and Tauc plots.

Samples	HOMO *vs* vacuum (M-S and Tauc)	HOMO *vs* NHE (M-S and Tauc)	XPS (valence band) *vs* NHE
COF-BATA-TAPP-H_2	5.07	0.63	0.75
COF-BATATAPP-Ni	5.17	0.73	0.80
COF-BATATAPP-Zn	5.36	0.92	0.93

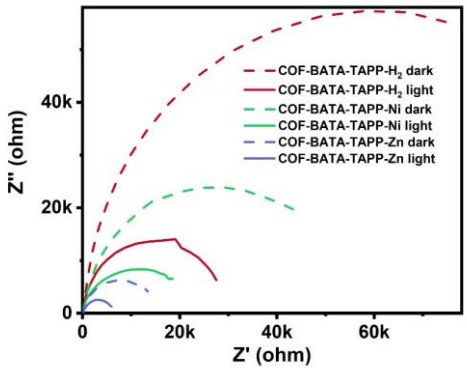


Figure S19. Impedance analysis with and without light.

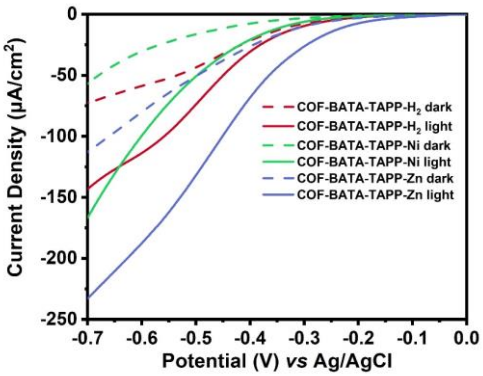


Figure S20. LSV curves measured with and without light.

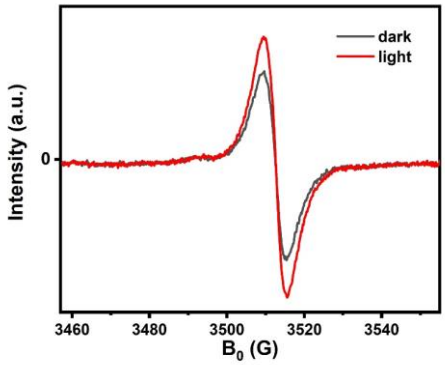


Figure S21. EPR spectra of COF-BATA-TAPP-H_2 with and without light.

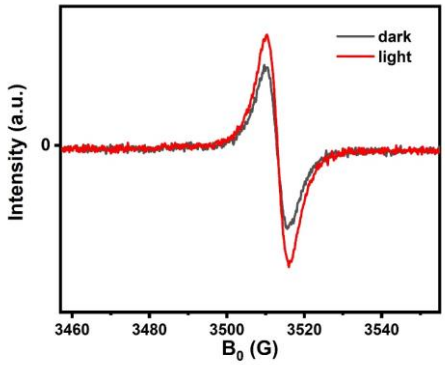


Figure S22. EPR spectra of COF-BATA-TAPP-Zn with and without light.

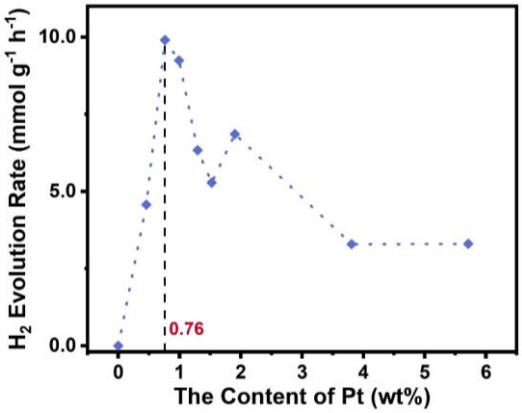


Figure S23. H_2 evolution rate of COF-BATA-TAPP-Zn with different amount of Pt.

Table S3. Summary of H_2 evolution activity of some COF and POP-based photocatalyts.

Photocatalysts	**Co-catalyst**	**Sacrificial reagent**	**HER (mmol g^{-1} h^{-1})**	**Ref.**
COF-BATA-TAPP-Zn	0.76 wt% Pt	ascorbic acid	10.0	This work
PCZN-4	15 wt% Pt	TEOA	7.16	*Chin. J. Chem.*, 2023, **41**, 2518-.
TzSPy	3 wt% Pt	TEOA	10.3	*Polym. Chem.*, 2022, **13**, 5769.
TzDTDO	3 wt% Pt	ascorbic acid	45.1	*Polym. Chem.*, 2023, **14**, 1507.
PyT-BTDO-2	3 wt% Pt	ascorbic acid	302.29	*ACS Appl. Mater. Interfaces*, 2023, **15**, 36404.
CMP-1	3 wt% Pt	TEOA	9.7	*Front. Chem.*, 2022, **10**, 854018.
COF-954	5 wt% Pt	ascorbic acid	137.226	*Adv. Mater.*, 2024, **36**, 2308251.
COF-JLU100	12 wt% Pt	TEOA	107.308	*Angew. Chem., Int. Ed.*, 2022, **61**, e202208919.
2.5% g_2T-T@COF	3 wt% Pt	ascorbic acid	1.56	*J. Mater. Chem. A*, 2023, **11**, 25899-25909.
COF-923	3 wt% Pt	ascorbic acid	7.82	*Angew. Chem., Int. Ed.*, 2023, **62**, e202216073.
COF-935	3 wt% Pt	ascorbic acid	67.55	*Angew. Chem., Int. Ed.*, 2023, **62**, e202304611.
N_3-COF	0.68 wt% Pt	TEOA	1.7	*Nat. Commun.*, 2015, **6**, 8508.
Tta-Tb	2.2 wt% Pt	ascorbic acid	6.286	*ChemSusChem*, 2022, **15**, e202101510.
ZnPor-DETH-COF	8 wt% Pt	TEOA	0.413	*Nat. Commun.*, 2021, **12**, 1354.
v-2D-COF-NO1	8 wt% Pt	TEA	1.97	*J. Am. Chem. Soc.*, 2022, **144**,13953.

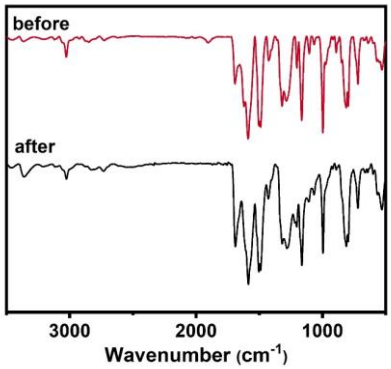


Figure S24. FT-IR spectra of COF-BATA-TAPP-Zn before and after 4 h photocatalysis experiment.

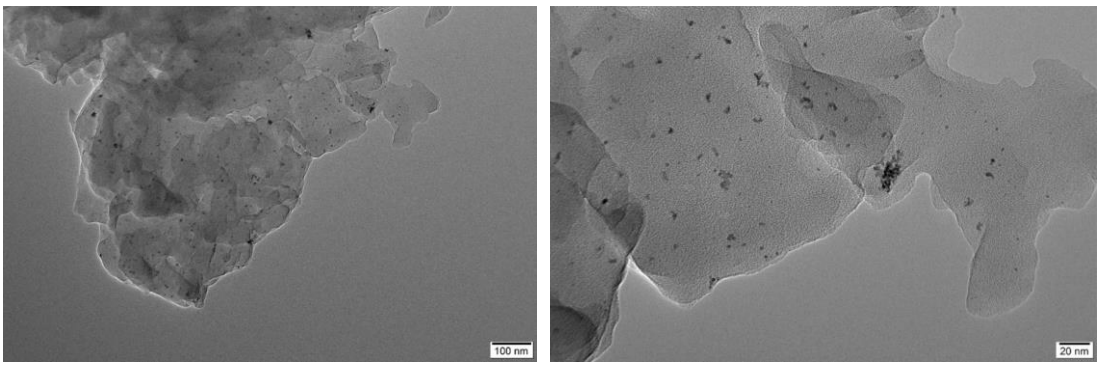


Figure S25. TEM images of COF-BATA-TAPP-H_2 after 4 h photocatalysis experiment.

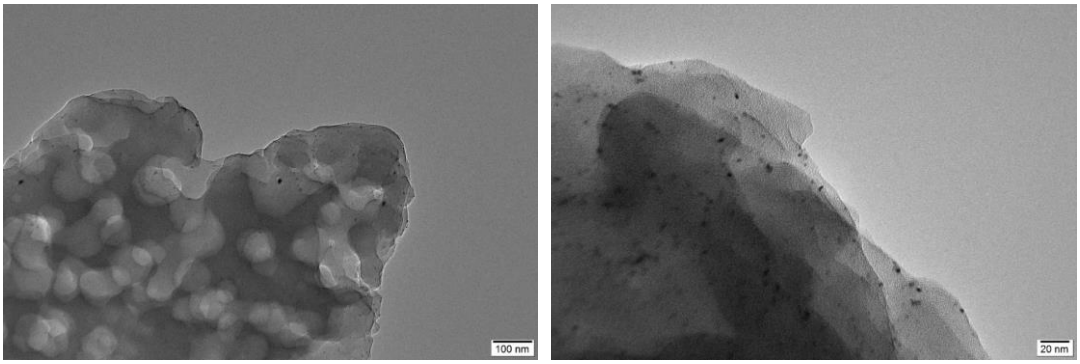


Figure S26. TEM images of COF-BATA-TAPP-Ni after 4 h photocatalysis experiment.

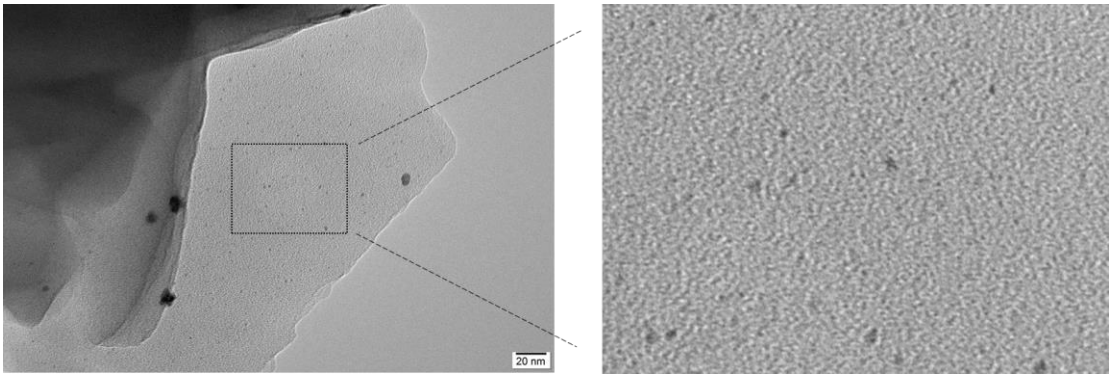


Figure S27. TEM images of COF-BATA-TAPP-Zn after 4 h photocatalysis experiment.

Fractional Atomic Coordinates of COFs

Table S4. Fractional atomic coordinates for the unit cell of COF-BATA-TAPP-H_2 with AA stacking.

P1							
a = 37.69508 Å, b = 37.96376 Å, c = 4.22048 Å, $\alpha = \beta = \gamma = 90^o$							
C1	0.72814	-0.23313	-1.00755	C149	0.93222	-0.7905	-0.53778
C2	0.70274	-0.20699	-0.97426	C150	0.89637	-0.78456	-0.49901
C3	0.67619	-0.20859	-0.73956	C151	0.59161	-0.76295	-1.12587
C4	0.67483	-0.24006	-0.56274	C152	0.55587	-0.75549	-1.10938
C5	0.69883	-0.26718	-0.60711	C153	0.54211	-0.7291	-0.91131
C6	0.72782	-0.26441	-0.82098	C154	0.56678	-0.70992	-0.72964
N7	0.65181	-0.17972	-0.67895	C155	0.60241	-0.71797	-0.72844
C8	0.75487	-0.29132	-0.84283	C156	0.68952	-0.91287	-0.42161
C9	0.79057	-0.28347	-0.9273	C157	0.68107	-0.94817	-0.41935
C10	0.81663	-0.30909	-0.93822	C158	0.69881	-0.97295	-0.60841
C11	0.80989	-0.34448	-0.85523	C159	0.72584	-0.96001	-0.80725
C12	0.77466	-0.35259	-0.77015	C160	0.73359	-0.9246	-0.82798
C13	0.74804	-0.32745	-0.77491	N161	0.79423	-0.53824	-1.07259
N14	0.83785	-0.37079	-0.85933	N162	0.50498	-0.72249	-0.91151
C15	0.61505	-0.18728	-0.75781	C163	0.80813	-0.52083	-0.83616
C16	0.66363	-0.14316	-0.69823	C164	0.4884	-0.70635	-0.68083
C17	0.83013	-0.40816	-0.8595	C165	0.14167	1.77195	0.14808
C18	0.87427	-0.36028	-0.80486	C166	0.16071	1.80209	0.14286
C19	0.85039	-0.43217	-0.68123	C167	0.19691	1.79354	0.12213
C20	0.84218	-0.46791	-0.67141	N168	0.19805	1.75774	0.13816
C21	0.81477	-0.48287	-0.85284	C169	0.16516	1.74316	0.15928
C22	0.79554	-0.4589	-1.04066	C170	0.22464	1.81832	0.07809
C23	0.80248	-0.42278	-1.04126	C171	0.26049	1.80974	0.03291
C24	0.90281	-0.37798	-0.94942	C172	0.29036	1.83416	-0.03173

C25	0.93772	-0.36663	-0.91161	C173	0.32034	1.81626	-0.00402
C26	0.94698	-0.33824	-0.71383	C174	0.31127	1.77931	0.07562
C27	0.91843	-0.3221	-0.5555	N175	0.27511	1.778	0.1197
C28	0.88329	-0.33217	-0.60351	C176	0.33429	1.75203	0.16387
C29	0.59634	-0.1678	-0.9874	C177	0.32371	1.71695	0.2279
C30	0.56039	-0.17341	-1.04773	C178	0.34592	1.69097	0.35862
C31	0.54038	-0.19912	-0.88729	C179	0.32681	1.66123	0.40187
C32	0.55974	-0.21982	-0.67257	C180	0.2921	1.66697	0.2892
C33	0.59563	-0.21441	-0.61076	N181	0.29168	1.70101	0.18934
C34	0.64002	-0.11478	-0.64841	C182	0.26489	1.64146	0.29353
C35	0.65102	-0.07974	-0.66567	C183	0.22871	1.64826	0.25105
C36	0.68596	-0.07014	-0.74288	C184	0.19901	1.62266	0.24026
C37	0.70973	-0.09848	-0.77379	C185	0.16896	1.64064	0.22978
C38	0.69963	-0.13336	-0.72143	C186	0.17785	1.67869	0.21411
N39	0.68907	-0.00903	-0.58431	N187	0.2143	1.68167	0.23593
C40	0.69776	-0.03374	-0.78544	C188	0.15475	1.70736	0.18618
N41	1.00781	-0.33163	-0.8818	H189	0.74881	-0.2297	-1.18913
C42	0.98343	-0.32603	-0.66751	H190	0.70376	-0.18409	-1.13494
C43	0.19762	-0.78089	-0.50636	H191	0.65589	-0.24302	-0.36642
C44	0.17172	-0.80669	-0.52378	H192	0.69679	-0.29037	-0.45149
C45	0.17751	-0.83883	-0.68275	H193	0.79789	-0.25618	-0.98517
C46	0.21048	-0.84289	-0.83603	H194	0.84351	-0.30111	-1.01099
C47	0.23583	-0.81656	-0.83792	H195	0.76763	-0.37961	-0.69799
C48	0.23097	-0.78408	-0.6691	H196	0.72103	-0.33565	-0.70919
N49	0.151	-0.8665	-0.69181	H197	0.87214	-0.42242	-0.53074
C50	0.25722	-0.75707	-0.66673	H198	0.85863	-0.48456	-0.5163
C51	0.25071	-0.72263	-0.79476	H199	0.7737	-0.46852	-1.19102
C52	0.27622	-0.69645	-0.78965	H200	0.78649	-0.40548	-1.19517
C53	0.31091	-0.70248	-0.6766	H201	0.89747	-0.40029	-1.10938

C54	0.31808	-0.73638	-0.55647	H202	0.95859	-0.38102	-1.0406
C55	0.29219	-0.76218	-0.53927	H203	0.92314	-0.30011	-0.39074
N56	0.33766	-0.675	-0.68651	H204	0.86212	-0.31835	-0.47368
C57	0.16212	-0.90304	-0.68448	H205	0.61037	-0.14726	-1.12273
C58	0.11359	-0.85841	-0.6628	H206	0.5478	-0.15645	-1.22703
C59	0.37513	-0.68341	-0.6864	H207	0.54626	-0.24092	-0.53962
C60	0.32763	-0.63846	-0.6449	H208	0.60732	-0.23055	-0.42192
C61	0.39992	-0.66318	-0.51607	H209	0.61181	-0.1198	-0.5966
C62	0.43582	-0.67176	-0.51062	H210	0.63092	-0.05908	-0.62844
C63	0.45019	-0.69954	-0.68997	H211	0.738	-0.09348	-0.82062
C64	0.42534	-0.71906	-0.86659	H212	0.72075	-0.15336	-0.72553
C65	0.38901	-0.712	-0.85872	H213	0.71553	-0.02793	-0.98558
C66	0.34666	-0.61089	-0.78965	H214	0.98966	-0.31091	-0.45236
C67	0.33638	-0.57582	-0.75705	H215	0.19226	-0.75675	-0.37027
C68	0.30787	-0.56538	-0.5635	H216	0.14665	-0.8026	-0.39462
C69	0.28978	-0.59305	-0.4114	H217	0.21585	-0.86725	-0.96914
C70	0.29843	-0.62835	-0.45877	H218	0.26067	-0.82064	-0.96987
C71	0.14199	-0.92985	-0.82868	H219	0.22446	-0.71689	-0.89643
C72	0.15363	-0.96467	-0.83752	H220	0.26937	-0.6705	-0.88866
C73	0.1843	-0.97601	-0.67764	H221	0.34454	-0.74224	-0.45872
C74	0.20318	-0.94936	-0.51845	H222	0.29893	-0.78792	-0.43546
C75	0.1935	-0.91396	-0.53322	H223	0.39071	-0.6409	-0.37059
C76	0.09021	-0.88041	-0.4947	H224	0.45313	-0.65514	-0.36285
C77	0.05455	-0.87194	-0.45507	H225	0.43444	-0.74131	-1.01309
C78	0.03864	-0.84299	-0.60653	H226	0.37098	-0.72837	-1.00194
C79	0.06189	-0.82191	-0.78631	H227	0.3695	-0.61708	-0.94252
C80	0.09829	-0.82842	-0.80366	H228	0.35206	-0.55572	-0.88313
N81	-0.0180	-0.8217	-0.79509	H229	0.26728	-0.58744	-0.25297
C82	0.00053	-0.83665	-0.57094	H230	0.283	-0.64874	-0.33469

C83	0.21595	-0.14498	-0.9194	H231	0.11707	-0.92311	-0.94975
C84	0.37126	-0.23975	-0.82041	H232	0.13716	-0.98397	-0.96547
C85	0.27544	-0.39491	-0.69938	H233	0.22737	-0.95577	-0.38425
C86	0.11774	-0.30093	-0.83539	H234	0.20998	-0.89441	-0.40895
C87	0.23386	-0.12048	-0.7127	H235	0.10058	-0.90415	-0.37768
C88	0.22619	-0.08502	-0.71339	H236	0.03855	-0.88994	-0.30863
C89	0.19876	-0.07083	-0.90017	H237	0.05152	-0.79867	-0.91213
C90	0.18106	-0.09417	-1.10417	H238	0.11507	-0.81057	-0.94498
C91	0.18993	-0.12929	-1.12681	H239	-0.01291	-0.84668	-0.35779
C92	0.39803	-0.25814	-1.00078	H240	0.25428	-0.13056	-0.55026
C93	0.43361	-0.2505	-0.96849	H241	0.24132	-0.06824	-0.55059
C94	0.44575	-0.2239	-0.76415	H242	0.16012	-0.08384	-1.25982
C95	0.4202	-0.20492	-0.59347	H243	0.17588	-0.14612	-1.29843
C96	0.38453	-0.21206	-0.61828	H244	0.38979	-0.27947	-1.16039
C97	0.10408	-0.32643	-1.05753	H245	0.45289	-0.26588	-1.1063
C98	0.06908	-0.33676	-1.05381	H246	0.42888	-0.1843	-0.42845
C99	0.04371	-0.32067	-0.85851	H247	0.36559	-0.19705	-0.47448
C100	0.05587	-0.29396	-0.65441	H248	0.12239	-0.3391	-1.22565
C101	0.09131	-0.28543	-0.63076	H249	0.06036	-0.35719	-1.22116
C102	0.25976	-0.42025	-0.48685	H250	0.03746	-0.28034	-0.49456
C103	0.26751	-0.45567	-0.50652	H251	0.09977	-0.26605	-0.45169
C104	0.29431	-0.46861	-0.70745	H252	0.23951	-0.41136	-0.3168
C105	0.31201	-0.44387	-0.89726	H253	0.25308	-0.47352	-0.34792
C106	0.30332	-0.40864	-0.89739	H254	0.33306	-0.45302	-1.05765
N107	0.48223	-0.2169	-0.71734	H255	0.31726	-0.39072	-1.05996
N108	0.30375	-0.50472	-0.73158	H256	0.49037	-0.19504	-1.16445
C109	0.50234	-0.20408	-0.94128	H257	0.28255	-0.52181	-0.30052
C110	0.29728	-0.52866	-0.51678	H258	0.2127	-1.021	-0.4672
N111	0.18897	-1.03471	-0.89813	H259	0.64584	-0.68677	-1.15431

C112	0.19622	-1.01267	-0.66863	H260	0.70499	-0.65021	-1.17787
C113	0.67171	-0.69554	-1.06887	H261	0.84219	-0.6706	-0.87785
C114	0.70208	-0.67671	-1.08003	H262	0.87982	-0.72903	-0.78854
C115	0.72962	-0.69706	-0.94839	H263	0.84174	-0.86117	-0.46699
N116	0.71427	-0.72819	-0.86691	H264	0.78243	-0.8975	-0.43543
C117	0.67901	-0.72876	-0.93554	H265	0.64481	-0.8767	-0.72599
C118	0.76529	-0.68574	-0.93089	H266	0.60729	-0.81832	-0.82139
C119	0.79451	-0.70725	-0.86488	H267	0.81185	-0.65393	-1.34527
C120	0.83255	-0.69731	-0.85038	H268	0.8254	-0.5913	-1.38236
C121	0.85125	-0.72635	-0.80347	H269	0.74561	-0.56781	-0.68094
C122	0.82607	-0.75614	-0.76868	H270	0.73338	-0.63054	-0.61416
N123	0.79225	-0.74307	-0.81254	H271	0.86576	-0.84381	-1.04924
C124	0.83363	-0.79154	-0.70494	H272	0.92922	-0.85565	-1.08914
C125	0.80819	-0.81868	-0.67241	H273	0.95106	-0.77544	-0.3924
C126	0.81568	-0.85216	-0.54544	H274	0.88759	-0.76442	-0.32872
C127	0.78524	-0.87086	-0.53003	H275	0.60082	-0.78361	-1.28906
C128	0.75749	-0.85027	-0.65494	H276	0.53755	-0.77013	-1.26336
N129	0.77278	-0.81906	-0.73528	H277	0.55807	-0.68835	-0.57507
C130	0.72178	-0.86157	-0.67098	H278	0.62038	-0.70316	-0.57273
C131	0.69252	-0.84002	-0.73519	H279	0.67516	-0.89489	-0.26261
C132	0.65451	-0.84999	-0.753	H280	0.66047	-0.95748	-0.25508
C133	0.63584	-0.82098	-0.80282	H281	0.74095	-0.9779	-0.9603
C134	0.66103	-0.79119	-0.83534	H282	0.75391	-0.91562	-0.99678
N135	0.69485	-0.80424	-0.79016	H283	0.81717	-0.53516	-0.62474
C136	0.65356	-0.75589	-0.90394	H284	0.50331	-0.69626	-0.47612
C137	0.7721	-0.6488	-0.9671	H285	0.11273	1.77071	0.15092
C138	0.87042	-0.80124	-0.70132	H286	0.14941	1.82859	0.14147
C139	0.715	-0.89861	-0.64208	H287	0.28668	1.86172	-0.08997
C140	0.61683	-0.74615	-0.91761	H288	0.34734	1.82555	-0.03167

C141	0.79754	-0.63531	-1.19199	H289	0.37385	1.69449	0.41968
C142	0.80525	-0.59993	-1.21138	H290	0.3366	1.6366	0.50365
C143	0.78684	-0.57459	-1.03374	H291	0.20244	1.59433	0.24395
C144	0.76066	-0.58684	-0.82401	H292	0.14212	1.6304	0.22974
C145	0.75357	-0.62222	-0.78685	H293	0.72749	-0.7486	-0.77598
C146	0.88425	-0.82904	-0.89849	H294	0.75939	-0.79848	-0.82113
C147	0.92012	-0.83538	-0.92246	H295	0.22048	1.74378	0.1415
C148	0.9452	-0.81594	-0.74988	H296	0.27008	1.71328	0.10925

Table S5. Fractional atomic coordinates for the unit cell of COF-BATA-TAPP-Ni with AA stacking.

P1							
a = 37.65926 Å, b = 37.42621 Å, c = 4.95061 Å, $\alpha = \beta = \gamma$ = 90º							
C1	0.72491	-0.23557	-1.03887	C148	0.94456	-0.81276	-0.64053
C2	0.69896	-0.20869	-1.00347	C149	0.92898	-0.78939	-0.45128
C3	0.67541	-0.20893	-0.78126	C150	0.8921	-0.78242	-0.45354
C4	0.67802	-0.23839	-0.6043	C151	0.58884	-0.76093	-1.0255
C5	0.70342	-0.2656	-0.64223	C152	0.55245	-0.75174	-1.01002
C6	0.72821	-0.26488	-0.85816	C153	0.53967	-0.72773	-0.81275
N7	0.65265	-0.18069	-0.73725	C154	0.56506	-0.71193	-0.63871
C8	0.75521	-0.2916	-0.88474	C155	0.60134	-0.72117	-0.65271
C9	0.78872	-0.28419	-1.00362	C156	0.69218	-0.91329	-0.36953
C10	0.81592	-0.31009	-1.01692	C157	0.68391	-0.95006	-0.35427
C11	0.81198	-0.34481	-0.90584	C158	0.69811	-0.97466	-0.54065
C12	0.77822	-0.35241	-0.79257	C159	0.7208	-0.96129	-0.74433
C13	0.75059	-0.32698	-0.78705	C160	0.72784	-0.92437	-0.76667
N14	0.83968	-0.36927	-0.89988	N161	0.79503	-0.53845	-1.05239
C15	0.61718	-0.1869	-0.7879	N162	0.5039	-0.72159	-0.80235
C16	0.66544	-0.14671	-0.67228	C163	0.80572	-0.51677	-0.84775
C17	0.83311	-0.40555	-0.90394	C164	0.48442	-0.70335	-0.61606

C18	0.87422	-0.35764	-0.86896	C165	0.15032	1.77099	0.14093
C19	0.84838	-0.42847	-0.70841	C166	0.17077	1.80096	0.13275
C20	0.8397	-0.46504	-0.69521	C167	0.20562	1.79118	0.07543
C21	0.81536	-0.4805	-0.8788	N168	0.20615	1.75389	0.06279
C22	0.80109	-0.45821	-1.08235	C169	0.17192	1.74096	0.11227
C23	0.80982	-0.42146	-1.09398	C170	0.23112	1.81926	0.03507
C24	0.90233	-0.36985	-1.03509	C171	0.26746	1.81216	0.00814
C25	0.93752	-0.35748	-1.00029	C172	0.29443	1.83195	-0.11433
C26	0.94609	-0.3324	-0.79622	C173	0.32534	1.81209	-0.0901
C27	0.91805	-0.32037	-0.62869	C174	0.31653	1.78098	0.05029
C28	0.88307	-0.33287	-0.6639	N175	0.2824	1.7834	0.11492
C29	0.60004	-0.16924	-1.00451	C176	0.33726	1.75159	0.12771
C30	0.56324	-0.17302	-1.05194	C177	0.32056	1.71894	0.21139
C31	0.54224	-0.19601	-0.89073	C178	0.34024	1.69506	0.36699
C32	0.5594	-0.21496	-0.68138	C179	0.32024	1.66521	0.41107
C33	0.59586	-0.20986	-0.62819	C180	0.28758	1.66961	0.28287
C34	0.64283	-0.11683	-0.62306	N181	0.28724	1.70364	0.16973
C35	0.6558	-0.08161	-0.58966	C182	0.26322	1.64023	0.28682
C36	0.69255	-0.07423	-0.60086	C183	0.22655	1.64509	0.24995
C37	0.71563	-0.10381	-0.62415	C184	0.19967	1.6201	0.2061
C38	0.70238	-0.13881	-0.65348	C185	0.1685	1.639	0.16906
N39	0.68841	-0.00962	-0.52054	C186	0.17692	1.67537	0.18021
C40	0.70664	-0.03918	-0.59876	N187	0.211	1.67699	0.24966
N41	1.00908	-0.32704	-0.91466	C188	0.15609	1.706	0.13294
C42	0.98092	-0.31939	-0.75282	H189	0.74141	-0.23335	-1.20184
C43	0.19759	-0.78325	-0.50217	H190	0.69755	-0.18815	-1.13941
C44	0.17128	-0.81019	-0.51743	H191	0.66205	-0.23992	-0.4391
C45	0.17342	-0.83837	-0.7081	H192	0.70408	-0.28559	-0.50165
C46	0.20298	-0.83774	-0.88569	H193	0.79424	-0.2594	-1.07906

C47	0.22955	-0.81127	-0.86981	H194	0.83934	-0.30304	-1.10591
C48	0.22739	-0.78369	-0.67619	H195	0.77346	-0.37689	-0.70888
N49	0.14903	-0.86602	-0.71484	H196	0.72681	-0.33493	-0.70788
C50	0.25436	-0.75743	-0.66134	H197	0.86564	-0.41831	-0.5691
C51	0.24929	-0.72343	-0.77789	H198	0.85123	-0.48031	-0.54736
C52	0.2763	-0.69736	-0.767	H199	0.7838	-0.46858	-1.22138
C53	0.30957	-0.70357	-0.63947	H200	0.79878	-0.40596	-1.24174
C54	0.31411	-0.73796	-0.52316	H201	0.8971	-0.38789	-1.1846
C55	0.28728	-0.76437	-0.53431	H202	0.95702	-0.36693	-1.12556
N56	0.33534	-0.67716	-0.62247	H203	0.92282	-0.30232	-0.47733
C57	0.16213	-0.90044	-0.73027	H204	0.86368	-0.32385	-0.53705
C58	0.11263	-0.8604	-0.69959	H205	0.61459	-0.15292	-1.12752
C59	0.37126	-0.68482	-0.62318	H206	0.55192	-0.15892	-1.20691
C60	0.32529	-0.64188	-0.59323	H207	0.54514	-0.232	-0.56094
C61	0.39434	-0.66872	-0.4328	H208	0.60638	-0.22268	-0.46594
C62	0.43119	-0.67503	-0.43338	H209	0.61598	-0.12023	-0.61404
C63	0.44713	-0.69816	-0.62446	H210	0.63814	-0.06113	-0.56234
C64	0.42428	-0.7149	-0.8133	H211	0.74258	-0.10012	-0.62223
C65	0.38719	-0.70834	-0.81224	H212	0.72081	-0.15869	-0.66478
C66	0.33929	-0.61428	-0.75744	H213	0.73233	-0.03591	-0.66186
C67	0.32912	-0.57824	-0.72207	H214	0.98499	-0.30333	-0.58862
C68	0.30445	-0.56829	-0.51982	H215	0.19507	-0.76345	-0.36071
C69	0.29039	-0.59583	-0.35547	H216	0.15053	-0.80953	-0.38449
C70	0.30069	-0.63171	-0.3918	H217	0.20546	-0.85713	-1.02896
C71	0.1497	-0.92543	-0.92329	H218	0.2505	-0.81223	-1.00152
C72	0.16254	-0.96093	-0.93098	H219	0.22585	-0.71743	-0.87239
C73	0.18861	-0.97279	-0.74568	H220	0.27123	-0.67314	-0.85281
C74	0.20152	-0.94768	-0.55561	H221	0.33726	-0.74394	-0.42557
C75	0.18851	-0.91244	-0.54842	H222	0.29188	-0.78878	-0.44776

C76	0.08961	-0.88589	-0.57827	H223	0.38418	-0.65196	-0.28968
C77	0.05243	-0.8817	-0.57316	H224	0.44636	-0.66237	-0.29057
C78	0.03613	-0.85098	-0.68283	H225	0.43467	-0.732	-0.95413
C79	0.05853	-0.82452	-0.7949	H226	0.3716	-0.7206	-0.95348
C80	0.09581	-0.82946	-0.80602	H227	0.35709	-0.62048	-0.90552
N81	-0.01966	-0.81806	-0.63116	H228	0.33986	-0.55917	-0.84592
C82	-0.00131	-0.84849	-0.68434	H229	0.27243	-0.59006	-0.2063
C83	0.22215	-0.14368	-0.96385	H230	0.29018	-0.6508	-0.26883
C84	0.3749	-0.24346	-0.87254	H231	0.13091	-0.91766	-1.05968
C85	0.27501	-0.39568	-0.6764	H232	0.15265	-0.97821	-1.07264
C86	0.11866	-0.30026	-0.8823	H233	0.22052	-0.95485	-0.4177
C87	0.23735	-0.1211	-0.76565	H234	0.19827	-0.89535	-0.40637
C88	0.22868	-0.0846	-0.75036	H235	0.09986	-0.90842	-0.49235
C89	0.20386	-0.06908	-0.92985	H236	0.03731	-0.9014	-0.48716
C90	0.18904	-0.09137	-1.13057	H237	0.04762	-0.80178	-0.87443
C91	0.19814	-0.12798	-1.1492	H238	0.11083	-0.81015	-0.89654
C92	0.39801	-0.26763	-1.0055	H239	-0.01534	-0.87147	-0.71973
C93	0.43518	-0.26251	-1.0044	H240	0.25492	-0.13123	-0.6276
C94	0.45049	-0.23267	-0.87549	H241	0.24066	-0.06972	-0.60399
C95	0.42778	-0.20844	-0.74206	H242	0.1713	-0.08081	-1.2651
C96	0.39075	-0.21401	-0.73782	H243	0.18693	-0.14323	-1.29825
C97	0.10382	-0.32162	-1.09003	H244	0.38788	-0.28936	-1.10404
C98	0.06733	-0.33037	-1.09375	H245	0.45126	-0.28052	-1.10015
C99	0.04381	-0.31701	-0.89684	H246	0.43829	-0.18689	-0.64352
C100	0.05816	-0.29457	-0.69468	H247	0.37529	-0.19618	-0.63431
C101	0.09487	-0.28713	-0.68428	H248	0.11979	-0.33156	-1.23978
C102	0.2611	-0.41764	-0.46874	H249	0.05778	-0.34671	-1.24265
C103	0.27045	-0.45404	-0.44914	H250	0.04216	-0.28379	-0.54982
C104	0.29464	-0.46967	-0.63306	H251	0.10422	-0.27201	-0.52722

C105	0.30995	-0.44738	-0.83091	H252	0.24352	-0.4073	-0.33142
C106	0.30033	-0.41104	-0.85309	H253	0.25921	-0.46899	-0.29962
N107	0.48634	-0.22866	-0.87465	H254	0.32798	-0.45786	-0.96371
N108	0.30382	-0.50486	-0.63762	H255	0.31155	-0.39597	-1.00321
C109	0.50522	-0.19868	-0.93165	H256	0.49211	-0.17699	-1.00913
C110	0.29345	-0.53255	-0.47865	H257	0.27646	-0.52754	-0.32199
N111	0.19316	-1.03426	-0.91972	H258	0.21898	-1.01435	-0.58706
C112	0.20184	-1.00816	-0.74005	H259	0.64753	-0.69445	-1.10155
C113	0.67147	-0.70229	-1.02497	H260	0.70374	-0.65937	-1.15418
C114	0.70207	-0.68309	-1.05237	H261	0.83917	-0.66741	-0.84161
C115	0.72941	-0.70128	-0.92142	H262	0.87672	-0.7225	-0.72987
N116	0.71483	-0.73251	-0.81563	H263	0.83796	-0.85882	-0.55356
C117	0.67886	-0.73343	-0.88128	H264	0.78298	-0.89449	-0.52177
C118	0.7639	-0.68501	-0.91901	H265	0.64143	-0.87578	-0.60833
C119	0.79496	-0.70458	-0.86456	H266	0.60516	-0.81937	-0.70087
C120	0.82988	-0.69299	-0.82871	H267	0.80079	-0.65292	-1.31959
C121	0.85005	-0.72273	-0.76632	H268	0.81436	-0.59031	-1.36577
C122	0.82701	-0.75198	-0.75423	H269	0.7508	-0.5673	-0.69111
N123	0.79552	-0.73984	-0.83335	H270	0.73733	-0.62981	-0.63956
C124	0.83302	-0.78762	-0.67547	H271	0.87025	-0.83235	-0.9913
C125	0.80447	-0.81262	-0.63194	H272	0.93253	-0.84601	-0.97376
C126	0.81325	-0.84808	-0.57811	H273	0.94465	-0.77747	-0.30853
C127	0.7829	-0.86773	-0.56139	H274	0.88172	-0.76576	-0.30954
C128	0.75364	-0.84564	-0.60592	H275	0.59695	-0.77863	-1.17072
N129	0.76739	-0.81097	-0.61965	H276	0.53496	-0.76299	-1.14327
C130	0.71888	-0.86186	-0.61743	H277	0.55747	-0.69363	-0.49751
C131	0.68785	-0.84228	-0.67688	H278	0.61862	-0.70948	-0.52039
C132	0.65193	-0.85155	-0.65801	H279	0.68193	-0.89642	-0.22636
C133	0.63218	-0.82117	-0.71039	H280	0.66747	-0.95905	-0.20452

C134	0.65611	-0.79401	-0.77399	H281	0.73161	-0.97832	-0.88306
N135	0.68822	-0.80878	-0.76554	H282	0.74348	-0.9157	-0.92281
C136	0.65013	-0.75779	-0.83365	H283	0.80789	-0.5276	-0.65805
C137	0.76886	-0.64776	-0.96816	H284	0.49762	-0.69246	-0.45542
C138	0.86966	-0.79729	-0.65415	H285	0.12355	1.77207	0.16701
C139	0.7134	-0.89941	-0.58158	H286	0.16087	1.82608	0.16136
C140	0.61387	-0.74659	-0.84113	H287	0.29192	1.85609	-0.20839
C141	0.79024	-0.63521	-1.18382	H288	0.34971	1.81893	-0.16411
C142	0.79815	-0.59852	-1.2121	H289	0.36544	1.69848	0.43852
C143	0.78481	-0.57318	-1.0277	H290	0.32861	1.64359	0.52035
C144	0.7617	-0.58529	-0.82243	H291	0.2022	1.59296	0.19796
C145	0.75374	-0.62197	-0.79353	H292	0.14425	1.62778	0.13387
C146	0.88543	-0.82095	-0.84276	Ni293	0.24789	0.72378	-1.06958
C147	0.92208	-0.82893	-0.83375	Ni294	0.73907	1.23445	-0.54496

Table S6. Fractional atomic coordinates for the unit cell of COF-BATA-TAPP-Zn with AA stacking.

P1							
a = 37.59969 Å, b = 37.16598 Å, c = 4.91175 Å, $\alpha = \beta = \gamma = 90^{o}$							
C1	0.72102	-0.23288	-1.04502	C148	0.93585	-0.81145	-0.62
C2	0.69483	-0.20608	-1.00873	C149	0.92074	-0.78494	-0.45067
C3	0.67094	-0.20701	-0.78707	C150	0.88405	-0.77707	-0.46211
C4	0.67339	-0.2369	-0.61093	C151	0.58097	-0.75865	-1.04873
C5	0.6992	-0.26393	-0.64902	C152	0.54451	-0.75013	-1.02083
C6	0.72432	-0.26256	-0.86461	C153	0.53229	-0.72758	-0.80958
N7	0.6481	-0.17871	-0.74212	C154	0.5581	-0.71276	-0.63228
C8	0.75171	-0.28904	-0.89177	C155	0.59434	-0.72196	-0.65505
C9	0.78531	-0.28091	-1.00842	C156	0.68486	-0.91041	-0.37367
C10	0.8128	-0.30665	-1.02386	C157	0.67778	-0.94758	-0.35199
C11	0.80907	-0.34185	-0.91619	C158	0.6944	-0.97252	-0.52649

C12	0.77529	-0.35011	-0.80404	C159	0.71906	-0.95936	-0.71969
C13	0.74733	-0.32487	-0.79724	C160	0.72565	-0.92214	-0.74552
N14	0.83695	-0.36628	-0.91407	N161	0.79189	-0.53558	-1.09855
C15	0.61283	-0.18497	-0.79978	N162	0.49654	-0.72179	-0.78942
C16	0.66092	-0.14475	-0.671	C163	0.80358	-0.51476	-0.88958
C17	0.8305	-0.40277	-0.92443	C164	0.47771	-0.70544	-0.58798
C18	0.87157	-0.35468	-0.88345	C165	0.14554	1.76594	-0.04298
C19	0.84603	-0.42638	-0.73218	C166	0.1634	1.79772	-0.05526
C20	0.8376	-0.46327	-0.72638	C167	0.19873	1.792	0.01847
C21	0.81321	-0.47822	-0.91409	N168	0.20083	1.75639	0.10553
C22	0.79866	-0.4552	-1.11436	C169	0.1683	1.73955	0.05783
C23	0.80722	-0.41817	-1.11893	C170	0.22381	1.82094	-0.00599
C24	0.89952	-0.36745	-1.05067	C171	0.2606	1.81461	-0.03337
C25	0.93492	-0.3556	-1.01546	C172	0.28844	1.83872	-0.08118
C26	0.94384	-0.33038	-0.81056	C173	0.31987	1.82004	-0.04371
C27	0.91595	-0.31761	-0.64268	C174	0.31069	1.78479	0.02541
C28	0.88073	-0.32969	-0.67783	N175	0.27558	1.78262	0.00234
C29	0.59652	-0.16801	-1.02529	C176	0.33203	1.75633	0.11907
C30	0.56014	-0.17312	-1.0859	C177	0.31795	1.72199	0.19901
C31	0.53874	-0.19626	-0.9264	C178	0.34182	1.69444	0.25942
C32	0.5549	-0.21345	-0.70173	C179	0.32318	1.66367	0.30695
C33	0.59108	-0.20773	-0.63968	C180	0.287	1.67049	0.27091
C34	0.63845	-0.11425	-0.63427	N181	0.28415	1.70767	0.24206
C35	0.65184	-0.07913	-0.59305	C182	0.26254	1.64071	0.27577
C36	0.68882	-0.07254	-0.58395	C183	0.22594	1.64451	0.22099
C37	0.71154	-0.10272	-0.59533	C184	0.19803	1.61968	0.237
C38	0.69784	-0.13763	-0.63302	C185	0.16669	1.63821	0.19359
N39	0.68472	-0.00768	-0.50727	C186	0.17583	1.67387	0.13907
C40	0.70348	-0.03754	-0.57462	N187	0.21112	1.67524	0.14301

N41	1.0068	-0.32699	-0.93054	C188	0.15411	1.704	0.09297
C42	0.97897	-0.31799	-0.76784	H189	0.73768	-0.23029	-1.20819
C43	0.18929	-0.7821	-0.45281	H190	0.69347	-0.18514	-1.14317
C44	0.16262	-0.80884	-0.46943	H191	0.65707	-0.2388	-0.44636
C45	0.16469	-0.83724	-0.66116	H192	0.69991	-0.28424	-0.5088
C46	0.19437	-0.83702	-0.83946	H193	0.79065	-0.25572	-1.08092
C47	0.22132	-0.81083	-0.82196	H194	0.83623	-0.29918	-1.11227
C48	0.21927	-0.78314	-0.62654	H195	0.77069	-0.37498	-0.72285
N49	0.14023	-0.86498	-0.66721	H196	0.72352	-0.33329	-0.71981
C50	0.24666	-0.75724	-0.61054	H197	0.86329	-0.41651	-0.59008
C51	0.242	-0.72293	-0.72722	H198	0.84927	-0.47912	-0.58079
C52	0.2695	-0.69724	-0.71641	H199	0.7813	-0.46523	-1.25595
C53	0.30274	-0.70427	-0.58918	H200	0.79606	-0.4021	-1.26449
C54	0.30683	-0.73897	-0.47269	H201	0.89405	-0.38558	-1.20106
C55	0.27951	-0.76503	-0.48364	H202	0.95428	-0.36557	-1.14119
N56	0.329	-0.67821	-0.57257	H203	0.92103	-0.29941	-0.49095
C57	0.1534	-0.89954	-0.6842	H204	0.86143	-0.32026	-0.55023
C58	0.10382	-0.85938	-0.65178	H205	0.61141	-0.1515	-1.14639
C59	0.36478	-0.68651	-0.57619	H206	0.54939	-0.15976	-1.24863
C60	0.31963	-0.64256	-0.54307	H207	0.54029	-0.23036	-0.58093
C61	0.38834	-0.67062	-0.38616	H208	0.6012	-0.22004	-0.47186
C62	0.42518	-0.67712	-0.39237	H209	0.61147	-0.1171	-0.64056
C63	0.44043	-0.70025	-0.58905	H210	0.63436	-0.05814	-0.57527
C64	0.41707	-0.71702	-0.77623	H211	0.73852	-0.09956	-0.57873
C65	0.38	-0.71025	-0.76943	H212	0.71593	-0.15807	-0.63583
C66	0.33429	-0.61521	-0.70904	H213	0.72977	-0.03457	-0.62447
C67	0.32471	-0.5788	-0.67499	H214	0.98349	-0.3015	-0.60475
C68	0.29998	-0.56832	-0.47262	H215	0.18696	-0.7621	-0.3106
C69	0.28537	-0.59557	-0.30551	H216	0.14172	-0.80794	-0.33652

C70	0.29511	-0.63185	-0.34071	H217	0.19671	-0.85654	-0.9838
C71	0.14083	-0.92437	-0.88023	H218	0.24243	-0.8121	-0.95342
C72	0.15409	-0.95986	-0.89356	H219	0.21858	-0.71646	-0.82178
C73	0.18068	-0.97178	-0.71077	H220	0.2648	-0.67272	-0.80183
C74	0.19361	-0.94692	-0.51642	H221	0.32998	-0.74544	-0.37539
C75	0.18017	-0.91165	-0.50398	H222	0.28369	-0.78975	-0.39744
C76	0.08093	-0.88504	-0.52793	H223	0.37857	-0.65384	-0.23978
C77	0.04372	-0.88101	-0.52324	H224	0.44082	-0.66458	-0.2502
C78	0.0273	-0.85036	-0.63735	H225	0.42704	-0.73422	-0.92001
C79	0.04959	-0.82373	-0.75212	H226	0.36394	-0.72244	-0.9097
C80	0.08694	-0.82843	-0.76165	H227	0.3521	-0.62184	-0.85738
N81	-0.02842	-0.81691	-0.60609	H228	0.33591	-0.55989	-0.80013
C82	-0.01017	-0.84806	-0.63978	H229	0.26744	-0.5893	-0.15584
C83	0.21391	-0.14201	-0.98992	H230	0.28423	-0.65084	-0.21676
C84	0.36905	-0.23579	-0.86612	H231	0.12174	-0.91645	-1.01496
C85	0.27387	-0.39539	-0.67642	H232	0.14417	-0.97705	-1.03771
C86	0.11677	-0.30284	-0.91561	H233	0.2129	-0.95428	-0.37999
C87	0.22809	-0.12109	-0.77446	H234	0.18999	-0.89459	-0.36007
C88	0.22019	-0.0843	-0.74661	H235	0.09133	-0.90759	-0.44042
C89	0.19634	-0.06704	-0.92624	H236	0.02867	-0.90078	-0.43462
C90	0.18232	-0.08745	-1.14272	H237	0.03856	-0.80102	-0.83463
C91	0.19162	-0.12398	-1.17804	H238	0.10195	-0.80902	-0.8537
C92	0.39371	-0.25002	-1.05539	H239	-0.02424	-0.8715	-0.6609
C93	0.43025	-0.24142	-1.03814	H240	0.24469	-0.13261	-0.6336
C94	0.44308	-0.21838	-0.83168	H241	0.23184	-0.07055	-0.59088
C95	0.41858	-0.20421	-0.64326	H242	0.16533	-0.07551	-1.27806
C96	0.38212	-0.21273	-0.65993	H243	0.18199	-0.13723	-1.34479
C97	0.10147	-0.32594	-1.11284	H244	0.38513	-0.26678	-1.20736
C98	0.06469	-0.33347	-1.11177	H245	0.44762	-0.25223	-1.17567

C99	0.0418	-0.31777	-0.91796	H246	0.4273	-0.18739	-0.4925
C100	0.05685	-0.29389	-0.72556	H247	0.36505	-0.20189	-0.51993
C101	0.0937	-0.28675	-0.7233	H248	0.11716	-0.33764	-1.25859
C102	0.26049	-0.41565	-0.45485	H249	0.05445	-0.35064	-1.25457
C103	0.26845	-0.45251	-0.42637	H250	0.04122	-0.28163	-0.58352
C104	0.29151	-0.46996	-0.61105	H251	0.10368	-0.26973	-0.57823
C105	0.30664	-0.44941	-0.82208	H252	0.24407	-0.40375	-0.31481
C106	0.29761	-0.4129	-0.8568	H253	0.25714	-0.46641	-0.26966
N107	0.47793	-0.20981	-0.80015	H254	0.32389	-0.46132	-0.9557
N108	0.29988	-0.50547	-0.60544	H255	0.30829	-0.3992	-1.01821
C109	0.50268	-0.2022	-0.99277	H256	0.49489	-0.19986	-1.19194
C110	0.28946	-0.53219	-0.43532	H257	0.27298	-0.52624	-0.27588
N111	0.18581	-1.03216	-0.90357	H258	0.2115	-1.01405	-0.56027
C112	0.19435	-1.00713	-0.71304	H259	0.63752	-0.68513	-1.00291
C113	0.66239	-0.69587	-0.98215	H260	0.69253	-0.64954	-1.062
C114	0.69268	-0.67626	-1.01385	H261	0.83438	-0.66838	-0.98119
C115	0.72202	-0.6984	-0.96846	H262	0.87052	-0.72388	-0.84626
N116	0.70845	-0.73319	-0.94076	H263	0.82646	-0.84567	-0.38105
C117	0.67141	-0.73134	-0.92079	H264	0.77071	-0.88248	-0.349
C118	0.75682	-0.68219	-0.96634	H265	0.63731	-0.87779	-0.72349
C119	0.7878	-0.70134	-0.89577	H266	0.59947	-0.82234	-0.83298
C120	0.82379	-0.69219	-0.91718	H267	0.79272	-0.65061	-1.37979
C121	0.84342	-0.72203	-0.8424	H268	0.80906	-0.58814	-1.42099
C122	0.81929	-0.74871	-0.76628	H269	0.74769	-0.56345	-0.73188
N123	0.78717	-0.73406	-0.78737	H270	0.73321	-0.62594	-0.67629
C124	0.82511	-0.78439	-0.68336	H271	0.86097	-0.83579	-0.95022
C125	0.79633	-0.8089	-0.63565	H272	0.92327	-0.84973	-0.92418
C126	0.80311	-0.83903	-0.47475	H273	0.93662	-0.77127	-0.31691
C127	0.7728	-0.8591	-0.45768	H274	0.87397	-0.75782	-0.33468

C128	0.74626	-0.84214	-0.60856	H275	0.58878	-0.77507	-1.20523
N129	0.76085	-0.81079	-0.71609	H276	0.5266	-0.76071	-1.15567
C130	0.71218	-0.85926	-0.62353	H277	0.55086	-0.69534	-0.48186
C131	0.68107	-0.83996	-0.68491	H278	0.61194	-0.71148	-0.51687
C132	0.64637	-0.85191	-0.73027	H279	0.67249	-0.89307	-0.24215
C133	0.62603	-0.82197	-0.79121	H280	0.66027	-0.95657	-0.20787
C134	0.6489	-0.79232	-0.79414	H281	0.73165	-0.97675	-0.84865
N135	0.68031	-0.8044	-0.71148	H282	0.74298	-0.91353	-0.89257
C136	0.64293	-0.75622	-0.86566	H283	0.80624	-0.5264	-0.70124
C137	0.76253	-0.64481	-1.01735	H284	0.4913	-0.69604	-0.42216
C138	0.86142	-0.7947	-0.65036	H285	0.11953	1.76312	-0.09995
C139	0.70791	-0.8969	-0.57789	H286	0.1514	1.82084	-0.11558
C140	0.60647	-0.74556	-0.86108	H287	0.28636	1.86544	-0.12749
C141	0.78341	-0.6326	-1.23893	H288	0.34487	1.83068	-0.05633
C142	0.79281	-0.59598	-1.26511	H289	0.36893	1.69575	0.26718
C143	0.78078	-0.57025	-1.07594	H290	0.33509	1.63992	0.35753
C144	0.75781	-0.5818	-0.86622	H291	0.19965	1.59285	0.27907
C145	0.74912	-0.61848	-0.83597	H292	0.14173	1.62746	0.20363
C146	0.87649	-0.82206	-0.81435	Zn293	1.24042	0.73693	-0.65274
C147	0.91309	-0.83035	-0.79907	Zn294	1.73711	1.2209	-0.00213