Supporting Information

Noninterpenetrated Three-dimensional Covalent Organic Framework with dia Topology for Au Ions Capture

Minghao Liu, Hui-Yuan Kong, Shuai Bi, Xuesong Ding, George Zheng Chen, Jun He, Qing Xu, Bao-Hang Han*, Gaofeng Zeng**

M. Liu, Prof. Q. Xu, Prof. G. Zeng,
CAS Key Laboratory of Low-Carbon Conversion Science and Engineering
Shanghai Advanced Research Institute (SARI), Chinese Academy of Sciences (CAS)
Shanghai 201210, P. R. China
E-mail: xuqing@sari.ac.cn; zenggf@sari.ac.cn

M. Liu, Prof. J. He,
Department of Chemical and Environmental Engineering
University of Nottingham Ningbo China
Ningbo, 315199, P.R. China

Prof. G. Z. Chen,
Department of Chemical and Environmental Engineering
University of Nottingham
Nottingham, NG7 2RD, UK

H.-Y. Kong, Prof. X. Ding, Prof. B.-H. Han,
CAS Key Laboratory of Nanosystem and Hierarchical Fabrication
CAS Center for Excellence in Nanoscience
National Center for Nanoscience and Technology, Beijing 100190, China
E-mail: hanbh@nanoctr.cn

S. Bi,
School of Chemistry and Chemical Engineering,
Shanghai Jiao Tong University,
Shanghai 200240, China

Experimental Procedures

Characterizations. Powder X-ray diffraction (PXRD) data were recorded on a Rigaku model RINT Ultima III diffractometer by depositing powder on glass substrate, from 2θ = 1.5° up to 60° with 0.02° increment. Nitrogen sorption isotherms were measured at 77 K with a Micromeritics Instrument Corporation model 3Flex surface characterization analyzer. The Brunauer-Emmett-Teller (BET) method was utilized to calculate the specific surface areas. By using the non-local density functional theory (NLDFT) model, the pore volume was derived from the sorption curve. TGA measurements were performed on a Mettler-Toledo model TGA/SDTA851e under N_2, by heating to 800 °C at a rate of 10 °C min^{-1}. FE-SEM images were obtained on a FEI Sirion-200 or Hitachi high technologies (SU-6600) field-emission scanning electron microscope at an electric voltage of 5 KV. EDX and elemental mapping were acquired using a HITCHI Miniscope TM3030. High-resolution transmission electron microscope images were obtained by transmission electron microscopy (TEM, FEI Tecnai G2). The metal ion concentrations were measured by PerkinElmer inductively couple plasma-optical emission spectroscopy (ICP-OES, Avio 200, USA). Elemental microanalyses (EA) were performed by using an Elementar vario MICRO cube elemental analyzer. Solution state ^{13}C NMR spectra were collected using a Bruker NEO 500 spectrometer.

Pawley refinement. The powder X-ray diffraction (PXRD) pattern simulation was performed using a software package for crystal determination from PXRD pattern, implemented in Reflex module of Materials Studio. We performed Pawley refinement to optimize the lattice parameters iteratively until the R_P and R_{WP} values converge. The pseudo-Voigt profile function was used for whole profile fitting and Finger-Cox-Jephcoat function was used for asymmetry correction during the refinement processes.

Geometry optimization. Molecular modelling of COFs was generated with the Materials Studio (ver. 7.0) suite of programs. Pawley refinement was carried out using Reflex, a software package for crystal determination from PXRD pattern. Unit cell dimension was set to the theoretical parameters. The Pawley refinement was performed to optimize the lattice parameters iteratively until the R_{wp} value converges and the overlay of the observed with refined profiles shows good agreement. The lattice models (e.g., cell parameters, atomic positions, and total energies) were then fully optimized using MS Forcite molecular dynamics module (universal force fields, Ewald summations) method.

Pore size distribution. We used the Atom Volumes & Surfaces tools implemented in Materials Studio to calculate the accessible solvent surface of the frameworks and measured the pore diameters based on the surface.

Au^{3+} sorption study. Aqueous solutions with different concentrations of gold ion were prepared at first. Then, 2 mg of BMTA-TFPM-COF was mixed with different concentrations of Au^{3+} solution (10 mL) at room temperature for 12 h. The mixtures were filtered through a 0.2 μm membrane filter. The gold concentration is determined by inductively coupled plasma-optical emission spectroscopy (ICP-OES) measurement by the collected filtrate.

The adsorption capacity (q_e, mg g^{-1}) is calculated from the following equation.

$$q_e = \frac{(C_0 - C_e)}{m} \times V$$

The linear form of the Langmuir isotherm model is used for fitting, and the linear equation is as follows.

$$\frac{C_e}{q_e} = \frac{C_e}{q_m} + \frac{1}{K_L q_m}$$

where q_e (mg g^{-1}) is the equilibrium adsorption capacity, q_m (mg g^{-1}) is the maximum adsorption capacity, C_e (mg L^{-1}) is the equilibrium concentration of Au^{3+}, and K_L (L mg^{-1}) is the constant related to the affinity between adsorbate and adsorbent.

Kinetic study of Au^{3+} sorption: Aqueous solutions containing 100 ppm gold ion were prepared at first. Then, 20 mg of BMTA-TFPM-COF was mixed with Au^{3+} solution (100 mL) for 3 h. A small amount of the mixture was taken out at the predetermined time interval and filtered with a 0.2 μm membrane. The gold concentration is determined by ICP-OES measurement.

The capture efficiency (R_e, %) is calculated from the following equation.

$$R_e = \frac{(C_0 - C_e)}{C_0} \times 100\%$$

where C_0 (mg L^{-1}) is the initial concentrations of Au^{3+}, and C_e (mg L^{-1}) is the equilibrium concentration of Au^{3+}.

Recycling experiment. Aqueous solutions with 20 ppm gold ion were prepared at first. Then, 20 mg of BMTA-TFPM-COF was mixed with Au^{3+} solution (20 mL) for 12 h. The mixture was filtered through filter paper and washed with water for three times. The recycled BMTA-TFPM-COF-Au was added to a mixed solution of 0.01 mol L^{-1} thiourea and 0.05 mol L^{-1} hydrochloric acid for 12 h, and then filtered and washed with water for three times to regenerate the adsorbents.

Ion selectivity tests. A mixture solution of Na^+, K^+, Pb^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Ni^{2+}, Al^{3+}, and Au^{3+} at the concentration of each metal ion of 10 ppm was prepared at first. Then, 10 mg of BMTA-TFPM-COF was added to the mixture solution (100 mL), and the mixture was kept stirring at room temperature for 12 h. The mixtures were filtered through a 0.2 μm membrane filter. The filtrate was collected, and the concentrations were determined by ICP-OES measurement.

Materials.

3,3',5,5'-tetra(p-aminophenyl)-bimesitylene (BMTA), and tetrahedral tetrakis(4-formylphenyl)methane (TFPM) were obtained from Alfa. Acetic acid, *o*-Dichlorobenzene (*o*-DCB) and tetrahydrofuran (THF) were obtained from Sinopharm Chemical Reagent Co.,Ltd.

Supporting Figures

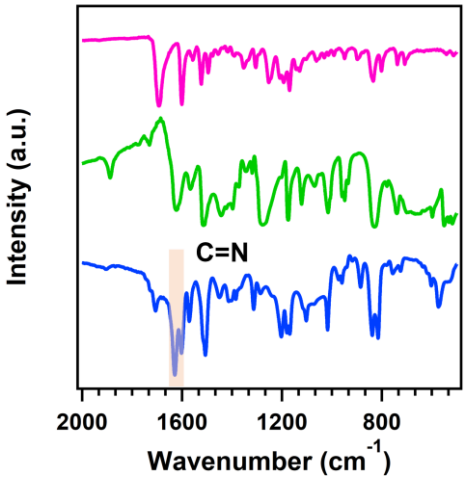

Figure S1. FT-IR spectra of BMTA-TFPM-COF (blue), BMTA (green) and TFPM (pink).

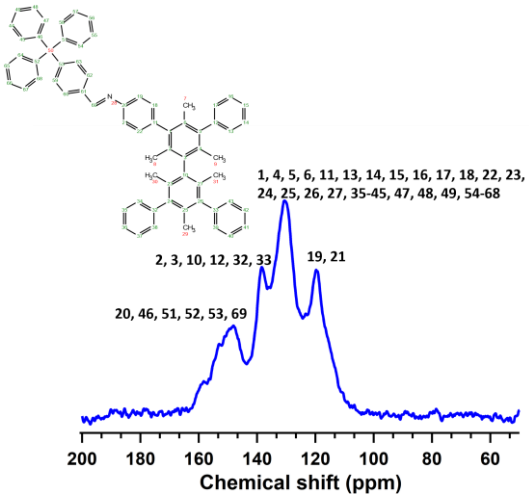

Figure S2. Solid State ^{13}C CP-MAS NMR spectrum of BMTA-TFPM-COF.

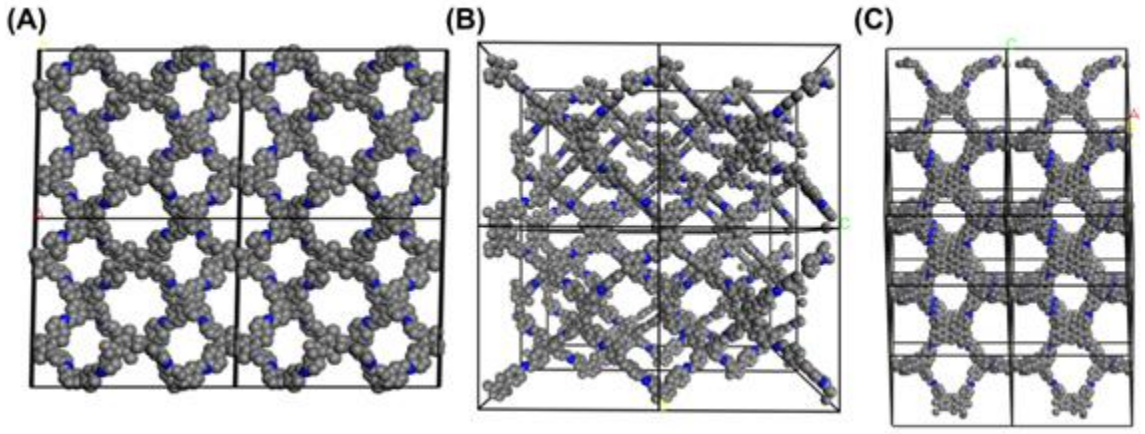

Figure S3. Structural illustration for possible 3D ***pts*** topology built from BMTA and TFPM.

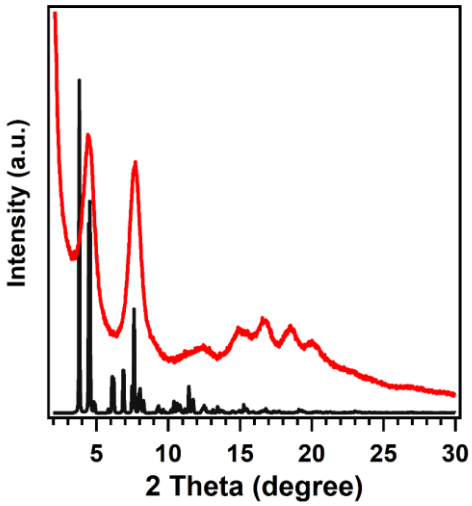

Figure S4. PXRD patterns (Cu Kα) for possible 3D structure with ***pts*** topology built from BMTA and TFPM.

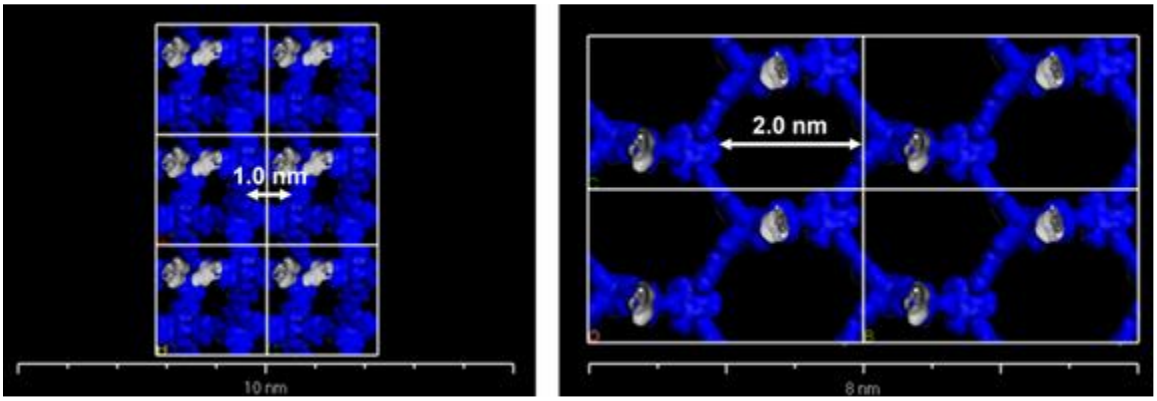

Figure S5. The theorical pore size of BMTA-TFPM-COF.

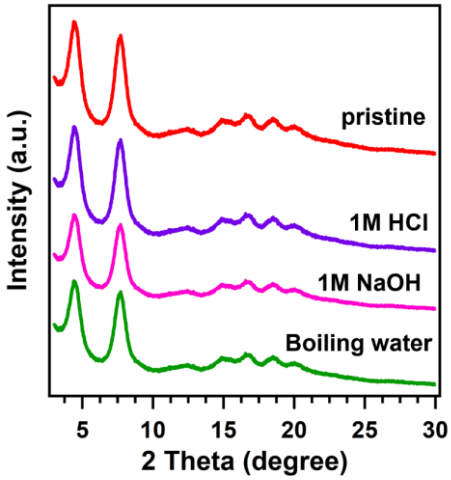

Figure S6. The PXRD patterns for BMTA-TFPM-COF under different conditions for one week.

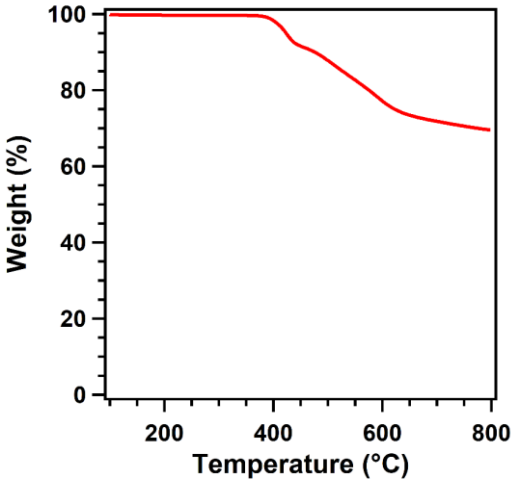

Figure S7. Thermogravimetric curve of BMTA-TFPM-COF from 100 ℃ to 800 ℃.

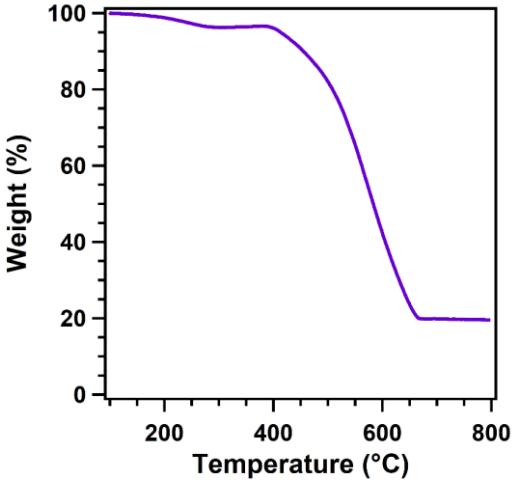

Figure S8. The TGA curve of BMTA-TFPM-COF from 100 to 800 ℃ under air.

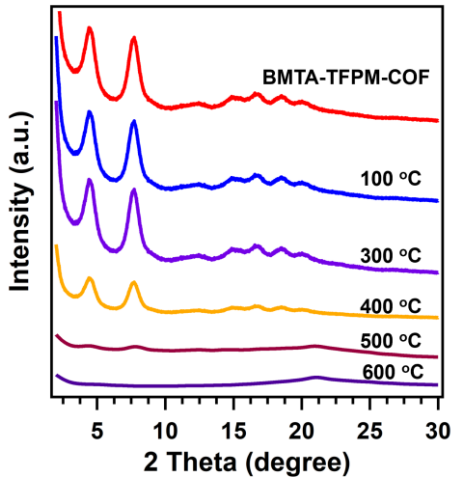

Figure S9. The PXRD patterns for BMTA-TFPM-COF with increasing the temperature from 25 to 600 °C under air.

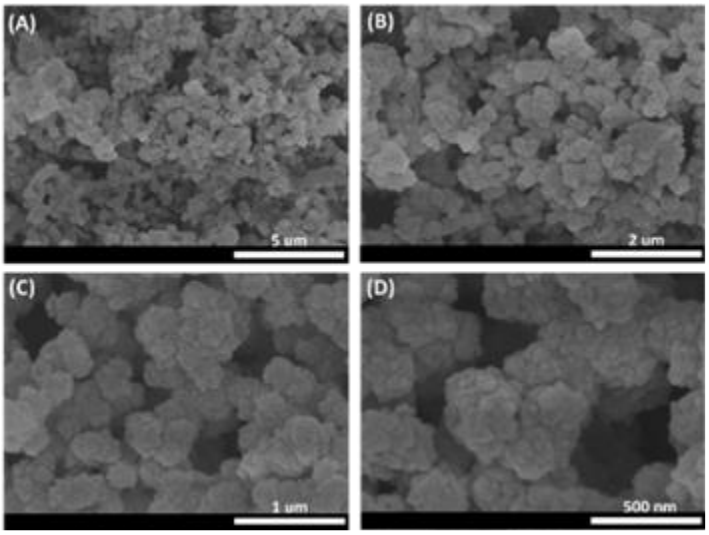

Figure S10. FE-SEM images of BMTA-TFPM-COF.

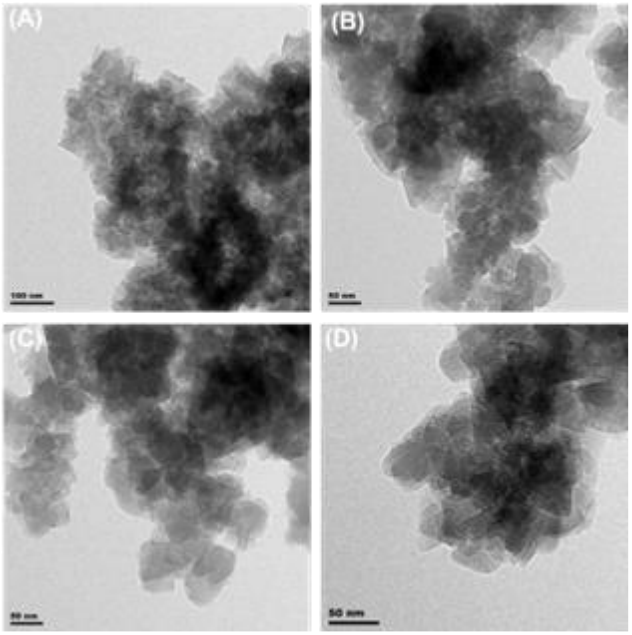

Figure S11. TEM images of BMTA-TFPM-COF.

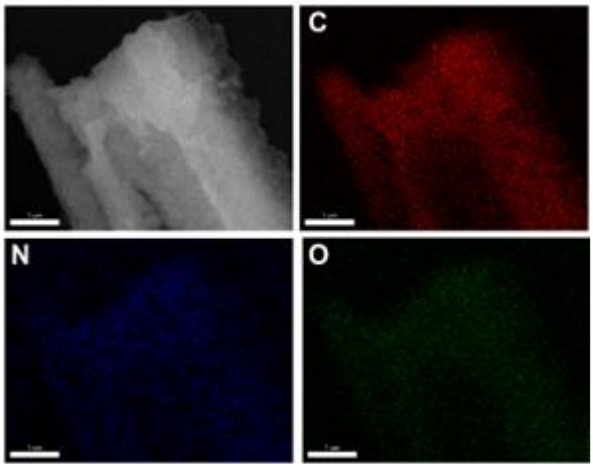

Figure S12. EDX mapping images of BMTA-TFPM-COF.

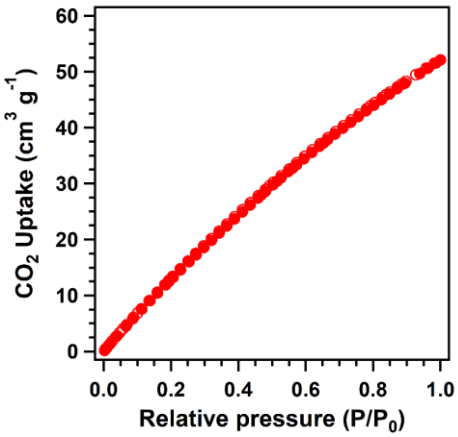

Figure S13. CO_2 uptakes of BMTA-TFPM-COF at 298 K.

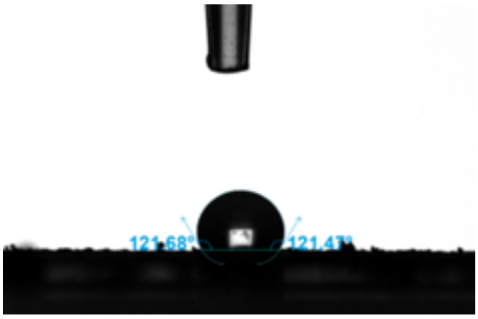

Figure S14. The contact angle of water for BMTA-TFPM-COF.

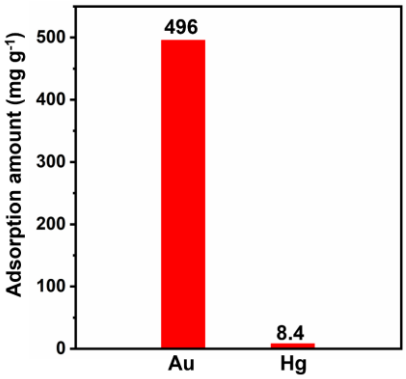

Figure S15. Au^{3+} and Hg^{2+} adsorption isotherms of BMTA-TFPM-COF.

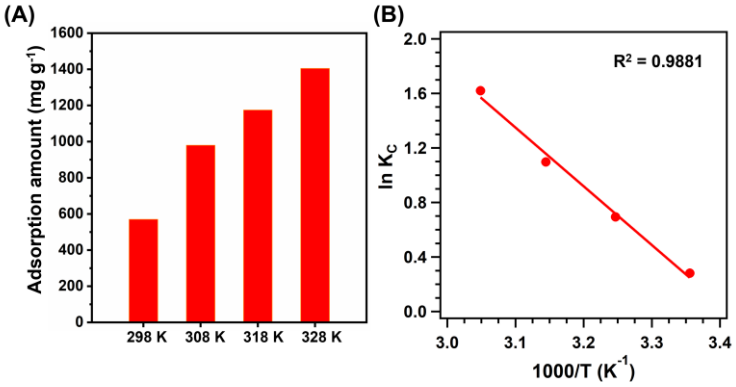

Figure S16. (A) The adsorption amount of Au(III) of BMTA-TFPM-COF at different temperatures and (B) the corresponding linear fitting model.

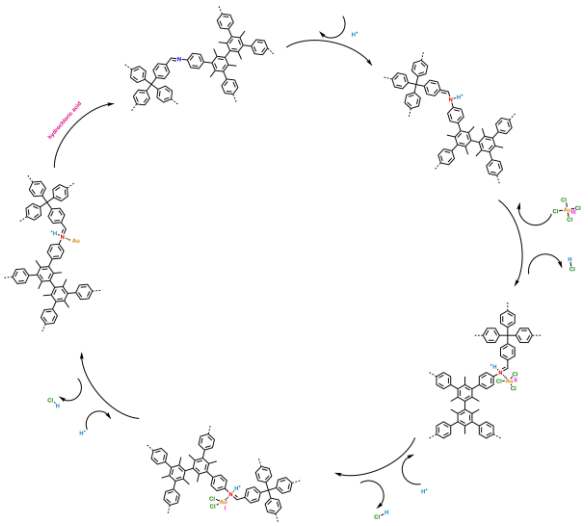

Figure S17. The proposed mechanism of Au(III) adsorption and reduction process on BMTA-TFPM-COF.

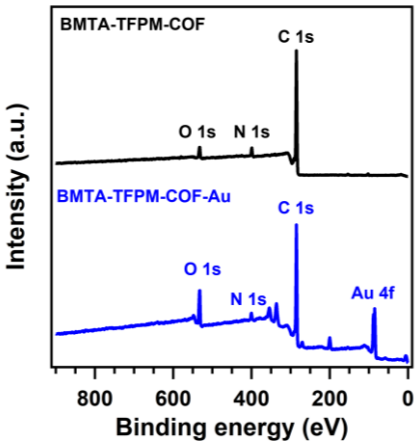

Figure S18. The XPS spectra of BMTA-TFPM-COF before and after the Au(III) capture.

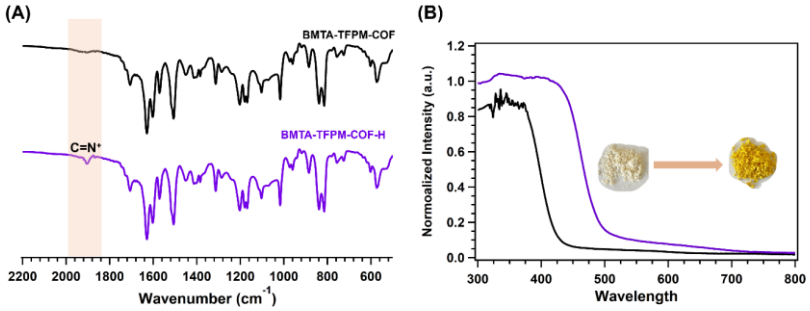

Figure S19. (A) The FT IR spectra and (B) UV-Vis spectra of BMTA-TFPM-COF (black curve) and BMTA-TFPM-COF-H (purple curve).

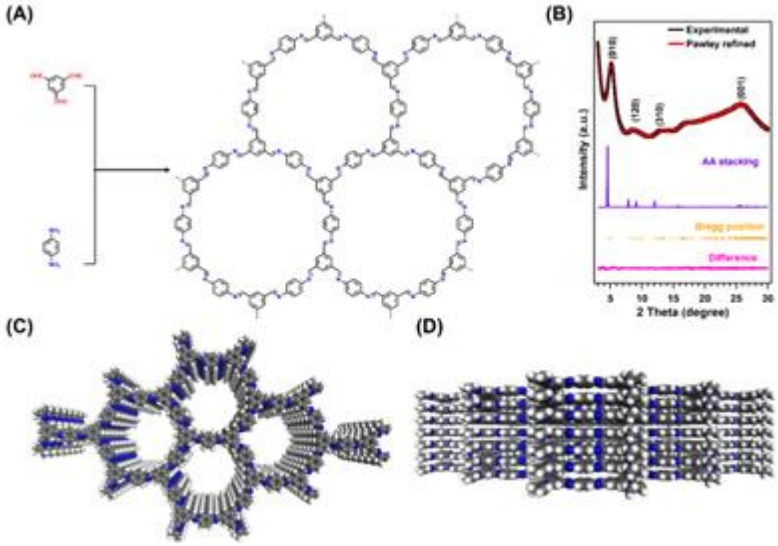

Figure S20. (A) Synthesis of catalytic COFs (BTH-DA-COF). (B) PXRD profiles of BTH-DA-COF for the experimentally observed (black), Pawley refined (red) and their difference (pink), simulated using the AA (purple) stacking modes. (C) and (D) Theoretically modelled eclipsed-AA stacking model (C-grey, N-blue, H-white).

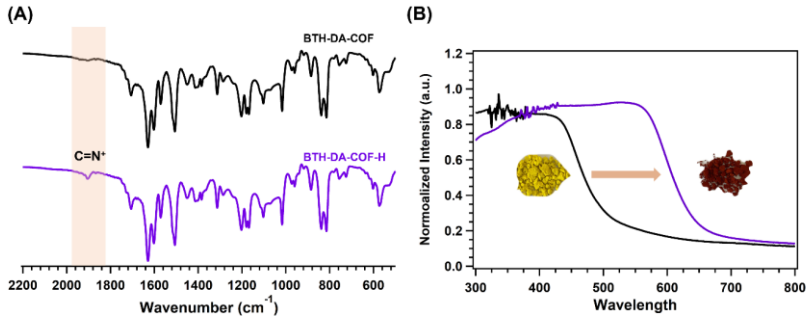

Figure S21. (A) The FT IR spectra and (B) UV-Vis spectra of BTH-DA-COF (black curve) and BTH-DA-COF-H (purple curve).

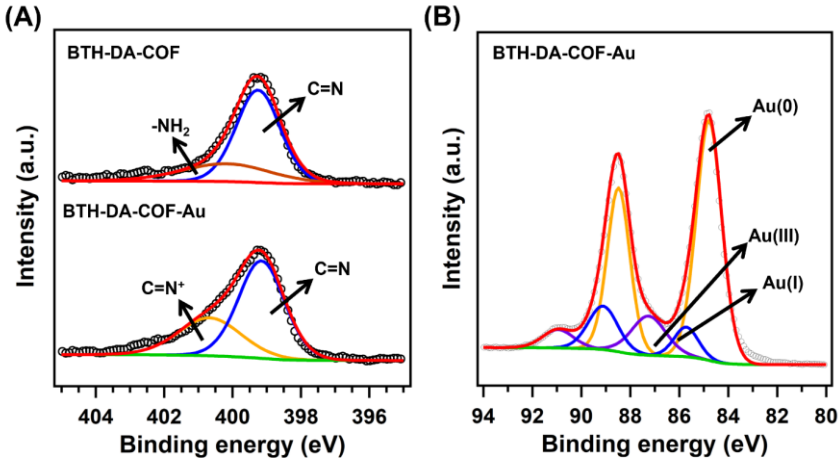

Figure S22. (A) The N 1s and (B) the Au 4f of XPS for BTH-DA-COF and BTH-DA-COF-Au.

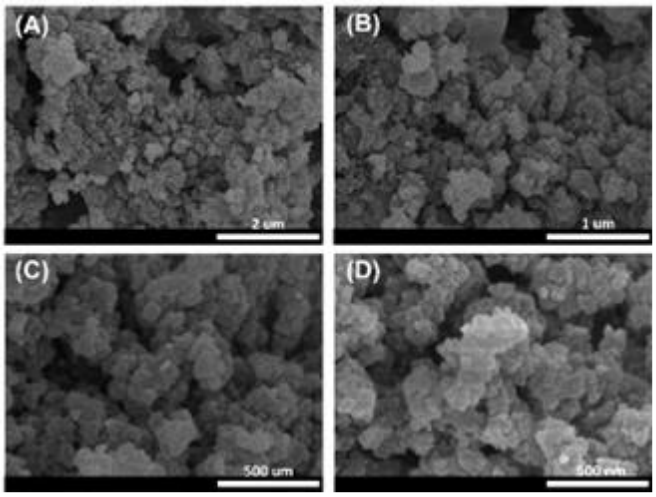

Figure S23. FE-SEM images of BMTA-TFPM-COF after the Au^{3+} adsorption.

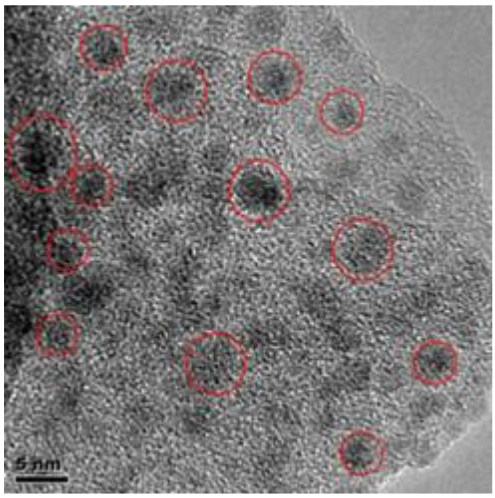

Figure S24. The HR-TEM image of BMTA-TFPM-COF after the Au capture.

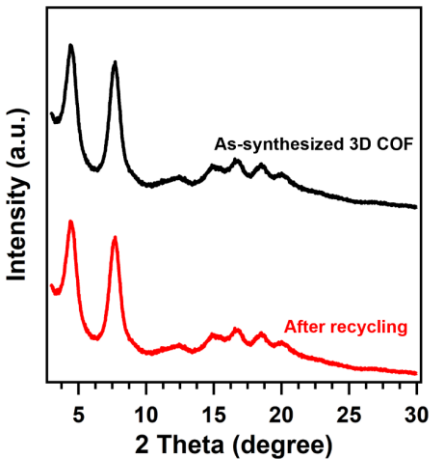

Figure S25. The PXRD patterns of BMTA-TFPM-COF after the Au^{3+} adsorption.

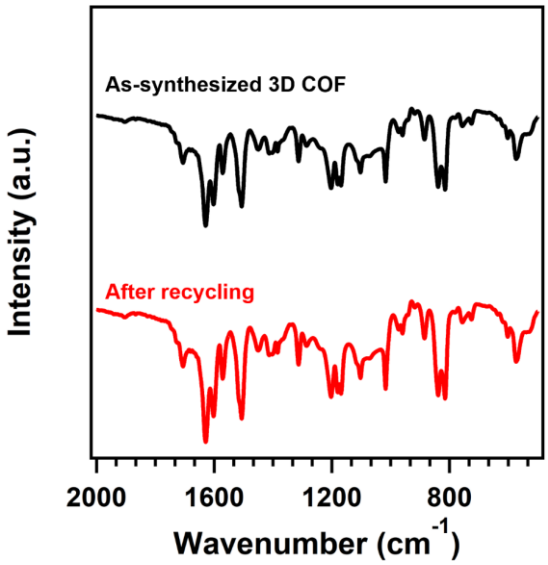

Figure S26. The FT IR spectra of BMTA-TFPM-COF after recycling 5 times for adsorption of Au^{3+} in aqueous solution.

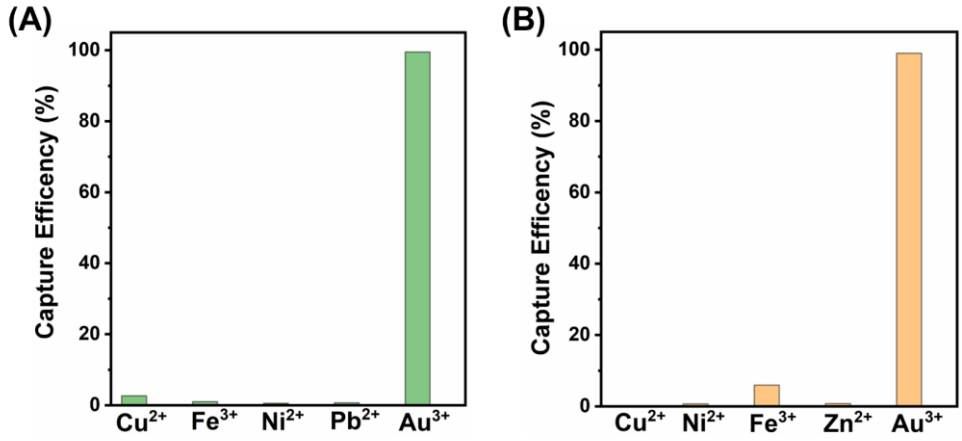

Figure S27. The capture efficiency of metals using BMTA-TFPM-COF from (A) mobile motherboard and (B) CPUs.

Table S1. The review of 3D COFs with different topologies and interpenetrations.

COFs	interpenetration	topology	BET surface area	Ref.
BMTA-TFPM-COF	**non**	**dia**	**1924**	
LZU-301	9-fold	**dia**	654	[S1]
3D-ceq-COF	2-fold	ceq	1148.6	[S2]
FCOF-5	6-fold	pts	-	[S3]
3D-Py-COF	2-fold	pts	1290	[S4]
TUS-84	2-fold	scu-c	679	[S5]
BUCT-COF-4	9-fold	**dia**	477.7	[S6]
COF-300	5-fold	**dia**	1360	[S7]
CCOF 5	4-fold	**dia**	655	[S8]
CCOF 6	4-fold	**dia**	613	[S8]
PI-COF-4	**non**	**dia**	1085	[S9]
PI-COF-5	4-fold	**dia**	699	[S9]
3D-ionic-COF-1	3-fold	**dia**	966	[S10]
3D-ionic-COF-2	3-fold	**dia**	880 m/g	[S10]
COF-320	9-fold	**dia**	2400 (Langmuir)	[S11]
JUC-570	10-fold	**dia**	1227	[S12]
JUC-571	10-fold	**dia**	254	[S12]
JUC-590	5-fold	**dia**	1521.5	[S13]
JUC-591	7-fold	**dia**	328.8	[S13]
JUC-508	**non**	**dia**	1513	[S14]
JUC-509	**non**	**dia**	1443	[S14]
COF-1	**non**	tbo	-	[S15]
COF-2	**non**	tbo	-	[S15]
3D-TPB-COF-OMe	5-fold	pts	880	[S16]
3D-TPB-COF-Ph	self-penetrated	ljh	1430	[S16]
3D-BMTA-COF	7-fold	pts	1650	[S17]
3D-Por-COF	2-fold	pts	1398	[S18]
3D-Por-COF-Cu	2-fold	pts	1335	[S18]
3D-TPE-COF	7-fold	pts	1084	[S19]
SiCOF-5	2-fold	srs-c	370	[S20]
3D-ETTA-TFPB	-	ffc	1174	[S21]

3D-ETTA-TFPA	-	ffc	1202	[S21]
COF-790	-	fjh	2650	[S22]
COF-791	-	fjh	1920	[S22]
COF-792	-	fjh	2250	[S22]
SPB-COF-DBA	**non**	nbo	1726	[S23]
COF-102	-	ctn	3472	[S24]
COF-103	-	bor	4210	[S24]
JUC-568	**non**	ceq	1433	[S25]
JUC-569	**non**	acs	1254	[S25]
CD-COFs	-	rra	760	[S26]
JUC-596	**non**	hea	2629	[S27]
JUC-597	**non**	hea	1857	[S27]
Marta-COF-3	6-fold	pcu	778	[S28]
Marta-COF-4	6-fold	pcu	723	[S28]
BP-COF	-	bcu	519	[S29]
JUC-518	**non**	pts	3018	[S30]
JUC-519	2-fold	pts	1513	[S30]
COF-202	-	ctn	2690	[S31]
NPN-1	4-fold	**dia**	-	[S32]
NPN-2	4-fold	**dia**	-	[S32]
CAF-2	7-fold	**dia**	354	[S33]
3D CTF-TPM	-	ctn	2002	[S34]
3D CTF-TPA	-	ctn	1804	[S34]
BF-COF-1	-	ctn	1028	[S35]
BF-COF-2	-	ctn	974	[S35]
3D-IL-COF-1	5-fold	**dia**	517	[S36]
3D-IL-COF-2	9-fold	**dia**	653	[S36]
3D-IL-COF-3	11-fold	**dia**	870	[S36]
JUC-575	10-fold	**dia**	343	[S37]
JUC-576	10-fold	**dia**	246	[S37]
JUC-565	10-fold	**dia**	313	[S38]
JUC-566	10-fold	**dia**	482	[S38]
JUC-556	2-fold	**dia**	634	[S39]

JUC-530	15-fold	**dia**	962	[S40]
JUC-531	17-fold	**dia**	1579	[S40]
COF-505	10-fold	**dia**	-	[S41]
3D-BMTA-COF	7-fold	pts	1680	[S42]
JUC-525	3-fold	**dia**	372.9	[S43]
JUC-526	3-fold	**dia**	386.9	[S43]
DL-COF-1	-	ctn	2259	[S44]
DL-COF-2	-	ctn	2071	[S44]
3D-OH-COF	9-fold	**dia**	1077	[S45]
3D-COOH-COF	9-fold	**dia**	540	[S46]
SP-3D-COF 1	6-fold	**dia**	641	[S47]
SP-3D-COF 2	7-fold	**dia**	1582	[S47]
TAPM-PZI	8-fold	**dia**	598.3	[S48]
TFPM-PZI	5-fold	**dia**	501.6	[S48]
CoPc-PI-COF-3	3-fold	pts	217	[S49]
H_2Pc-PI-COF-3	3-fold	pts	258	[S49]
LZU-306	**non**	pts	2059	[S50]

Table S2. Elemental analysis of BMTA-TFPM-COF.

Material	C (wt.%)	N (wt.%)	H (wt.%)
BMTA-TFPM-COF	89.45	4.89	5.66

Table S3. Atomistic coordinates for the refined unit cell parameters for BMTA-TFPM-COF via Pawley refinement.

Space group: *P1;*

a = 22.2968 Å, b = 40.1278 Å, c = 22.3912 Å;

$\alpha = \beta = \gamma = 90^{\circ}$.

	Atom	***x/a***	***y/b***	***z/c***
C1	C	0.24732	-0.42936	0.7457
C2	C	0.15761	-0.39926	0.79658
C3	C	0.10877	-0.37742	0.79431
C4	C	0.09179	-0.36252	0.74015
C5	C	0.12501	-0.36952	0.6886
C6	C	0.1739	-0.39122	0.69085
C7	C	0.19001	-0.40758	0.74436
C8	C	0.30819	-0.4537	0.83429
C9	C	0.31313	-0.47413	0.88441
C10	C	0.26408	-0.49282	0.90432
C11	C	0.20998	-0.49127	0.87236
C12	C	0.20495	-0.47075	0.82208
C13	C	0.25315	-0.45038	0.80347
C14	C	0.3029	-0.4736	0.68527
C15	C	0.3071	-0.49733	0.63999
C16	C	0.25736	-0.50474	0.60428
C17	C	0.20242	-0.48904	0.61646
C18	C	0.19804	-0.46538	0.66216
C19	C	0.24912	-0.45586	0.69544
C20	C	0.33007	-0.39854	0.6854
C21	C	0.37754	-0.37593	0.68217
C22	C	0.39391	-0.35706	0.73217
C23	C	0.35957	-0.35959	0.78449
C24	C	0.31172	-0.38197	0.78757
C25	C	0.29858	-0.40354	0.73946

C26	C	0.44776	-0.33578	0.7293
C27	C	0.04032	-0.33938	0.73637
C28	C	0.27104	-0.5138	0.95803
C29	C	0.26446	-0.52832	0.55417
C30	C	0.2279	-0.59178	0.24482
C31	C	0.22817	-0.60934	0.29965
C32	C	0.22972	-0.64455	0.30023
C33	C	0.23088	-0.66226	0.24552
C34	C	0.23077	-0.64493	0.19046
C35	C	0.22911	-0.60967	0.19037
C36	C	0.17416	-0.71621	0.24568
C37	C	0.17303	-0.75143	0.24649
C38	C	0.22715	-0.76984	0.24734
C39	C	0.28286	-0.75283	0.24819
C40	C	0.28434	-0.71753	0.24734
C41	C	0.22989	-0.69943	0.24553
C42	C	0.232	-0.6646	0.13248
C43	C	0.22969	-0.66264	0.35981
C44	C	0.11657	-0.69594	0.2461
C45	C	0.34321	-0.69855	0.24971
C46	C	0.28326	-0.5826	0.10579
C47	C	0.28345	-0.56353	0.05358
C48	C	0.22902	-0.55231	0.02852
C49	C	0.17483	-0.56178	0.05529
C50	C	0.17469	-0.58089	0.10749
C51	C	0.22896	-0.591	0.13334
C52	C	0.28069	-0.58143	0.38438
C53	C	0.27976	-0.56292	0.43721
C54	C	0.22468	-0.55381	0.46359
C55	C	0.17109	-0.56334	0.43569
C56	C	0.17208	-0.58188	0.38283
C57	C	0.22692	-0.59092	0.35693

C58	C	0.08722	-0.77469	0.30436
C59	C	0.03319	-0.79221	0.30743
C60	C	0.00614	-0.80447	0.25494
C61	C	0.03437	-0.79904	0.19988
C62	C	0.08833	-0.7814	0.19684
C63	C	0.1151	-0.76935	0.24914
C64	C	0.36265	-0.78015	0.30895
C65	C	0.41388	-0.80004	0.31372
C66	C	0.44223	-0.81244	0.26197
C67	C	0.4196	-0.80343	0.20583
C68	C	0.36831	-0.78353	0.2011
C69	C	0.3393	-0.7721	0.2527
N70	N	-0.04727	-0.82447	0.25612
N71	N	0.2268	-0.53149	-0.02374
N72	N	0.22125	-0.53338	0.51628
N73	N	0.49419	-0.8337	0.26443
C74	C	0.22665	-0.55393	0.24318
C75	C	0.22408	-0.80768	0.24861
C76	C	0.73288	-0.92982	1.30991
C77	C	0.63753	-0.9071	1.36293
C78	C	0.58531	-0.88789	1.36285
C79	C	0.56653	-0.87142	1.311
C80	C	0.60105	-0.87447	1.25889
C81	C	0.65322	-0.89382	1.25881
C82	C	0.6718	-0.91137	1.31034
C83	C	0.79746	-0.95018	1.39949
C84	C	0.80596	-0.97036	1.4495
C85	C	0.76146	-0.99274	1.46768
C86	C	0.70866	-0.99534	1.43385
C87	C	0.70014	-0.97519	1.38361
C88	C	0.74313	-0.95105	1.3669
C89	C	0.79445	-0.97137	1.24926

C90	C	0.80222	-0.99472	1.20381
C91	C	0.7542	-1.0036	1.16688
C92	C	0.69754	-0.98952	1.17759
C93	C	0.6896	-0.96618	1.22341
C94	C	0.73865	-0.95548	1.25851
C95	C	0.81308	-0.89537	1.25203
C96	C	0.8568	-0.87047	1.2504
C97	C	0.86656	-0.84996	1.30022
C98	C	0.82959	-0.85353	1.35034
C99	C	0.78601	-0.87848	1.35209
C100	C	0.77934	-0.90126	1.30443
C101	C	0.91636	-0.82577	1.30176
C102	C	0.51179	-0.85069	1.31305
C103	C	0.77151	-1.013	1.52179
C104	C	0.76479	-1.02712	1.11726
C105	C	0.73897	-0.09053	1.81177
C106	C	0.73991	-0.10848	1.86621
C107	C	0.74364	-0.14365	1.86598
C108	C	0.74599	-0.16092	1.81087
C109	C	0.74532	-0.14317	1.75624
C110	C	0.74162	-0.10798	1.75695
C111	C	0.6906	-0.21526	1.80717
C112	C	0.69026	-0.25036	1.80148
C113	C	0.74498	-0.26828	1.79927
C114	C	0.80013	-0.25094	1.80343
C115	C	0.80077	-0.21579	1.80894
C116	C	0.74592	-0.19809	1.80951
C117	C	0.7479	-0.16237	1.69776
C118	C	0.74443	-0.1622	1.92506
C119	C	0.63259	-0.19546	1.81094
C120	C	0.85915	-0.19661	1.8147
C121	C	0.79267	-0.07773	1.67384

C122	C	0.79064	-0.05888	1.6214
C123	C	0.73505	-0.05087	1.59496
C124	C	0.68221	-0.0631	1.62078
C125	C	0.68429	-0.08194	1.67324
C126	C	0.73951	-0.08901	1.70029
C127	C	0.78862	-0.07925	1.95183
C128	C	0.78514	-0.06047	2.00428
C129	C	0.72887	-0.05284	2.02968
C130	C	0.67671	-0.06426	2.00139
C131	C	0.68026	-0.08304	1.94892
C132	C	0.73624	-0.09047	1.92381
C133	C	0.60489	-0.28204	1.84599
C134	C	0.55095	-0.29944	1.84001
C135	C	0.52438	-0.30354	1.78377
C136	C	0.5517	-0.28889	1.73342
C137	C	0.60559	-0.27146	1.73945
C138	C	0.63263	-0.26824	1.79562
C139	C	0.88054	-0.2861	1.8494
C140	C	0.93202	-0.30579	1.8442
C141	C	0.96078	-0.30964	1.78895
C142	C	0.93774	-0.29261	1.73877
C143	C	0.88621	-0.27297	1.74404
C144	C	0.85704	-0.2699	1.79917
N145	N	0.47024	-0.32285	1.77994
N146	N	0.73027	-0.03065	1.54213
N147	N	0.7226	-0.03206	2.08168
N148	N	1.01219	-0.33133	1.7861
C149	C	0.73494	-0.05273	1.8109
C150	C	0.74576	-0.30592	1.79164

Table S4. Atomistic coordinates for the refined unit cell parameters for BMTA-TFPM-COF with 2-fold interpenetrated dia topology via Pawley refinement.

	Atom	*x/a*	*y/b*	*z/c*
C1	C	0.24367	-0.42843	0.75406
C2	C	0.1503	-0.40338	0.80245
C3	C	0.1023	-0.38104	0.80247
C4	C	0.09225	-0.3595	0.75438
C5	C	0.13073	-0.36044	0.70653
C6	C	0.17878	-0.38279	0.70658
C7	C	0.18909	-0.40495	0.75426
C8	C	0.29612	-0.44785	0.84887
C9	C	0.29934	-0.46781	0.8995
C10	C	0.25405	-0.49052	0.9132
C11	C	0.20551	-0.4934	0.87551
C12	C	0.20234	-0.47336	0.82472
C13	C	0.24728	-0.44984	0.81091
C14	C	0.28726	-0.47844	0.69702
C15	C	0.28791	-0.50158	0.65036
C16	C	0.24284	-0.50124	0.60869
C17	C	0.19644	-0.47787	0.61451
C18	C	0.19583	-0.45469	0.66127
C19	C	0.24173	-0.4542	0.70285
C20	C	0.33791	-0.40741	0.70164
C21	C	0.38795	-0.38672	0.69912
C22	C	0.39874	-0.36276	0.74322
C23	C	0.35826	-0.35892	0.78916
C24	C	0.3081	-0.37954	0.79153
C25	C	0.29772	-0.40473	0.74852
C26	C	0.45385	-0.34331	0.74181
C27	C	0.04165	-0.33614	0.75299
C28	C	0.25856	-0.5104	0.96752
C29	C	0.2467	-0.52454	0.55839
C30	C	0.22269	-0.58763	0.25351
C31	C	0.22285	-0.60516	0.3078
C32	C	0.22738	-0.64115	0.30843
C33	C	0.23142	-0.65946	0.25523
C34	C	0.23105	-0.64186	0.20122
C35	C	0.22661	-0.60593	0.20017
C36	C	0.18058	-0.71628	0.25375
C37	C	0.1819	-0.75231	0.25367
C38	C	0.2366	-0.76949	0.25572
C39	C	0.2898	-0.75077	0.25782
C40	C	0.28804	-0.71471	0.25781
C41	C	0.23349	-0.6975	0.25585
C42	C	0.23626	-0.66152	0.14481
C43	C	0.226	-0.66022	0.36563
C44	C	0.1228	-0.6977	0.25

C45	C	0.34412	-0.69449	0.26108
C46	C	0.27146	-0.56516	0.12857
C47	C	0.26965	-0.547	0.07582
C48	C	0.22183	-0.5509	0.03716
C49	C	0.17619	-0.57333	0.05192
C50	C	0.17797	-0.59153	0.10475
C51	C	0.22554	-0.58745	0.1434
C52	C	0.26388	-0.58648	0.40469
C53	C	0.26015	-0.56711	0.45615
C54	C	0.21029	-0.54678	0.46717
C55	C	0.16426	-0.54637	0.42636
C56	C	0.16794	-0.56578	0.37495
C57	C	0.21789	-0.5858	0.36364
C58	C	0.08531	-0.76932	0.29752
C59	C	0.03343	-0.7885	0.29631
C60	C	0.02185	-0.81062	0.24909
C61	C	0.06256	-0.81314	0.2032
C62	C	0.1144	-0.79391	0.20434
C63	C	0.12619	-0.77202	0.25163
C64	C	0.36057	-0.79023	0.30764
C65	C	0.41304	-0.80887	0.30828
C66	C	0.4527	-0.80661	0.26104
C67	C	0.43934	-0.7852	0.21363
C68	C	0.38677	-0.76654	0.21295
C69	C	0.34699	-0.76907	0.25986
N70	N	-0.0295	-0.83182	0.24791
N71	N	0.21815	-0.53187	-0.01648
N72	N	0.20643	-0.52533	0.51803
N73	N	0.50594	-0.8263	0.25965
C74	C	0.21838	-0.54932	0.25242
C75	C	0.23818	-0.80787	0.25572
C76	C	0.73629	-0.92832	1.29517
C77	C	0.6392	-0.90924	1.34417
C78	C	0.58801	-0.88947	1.34528
C79	C	0.57476	-0.86766	1.29858
C80	C	0.61322	-0.86573	1.25059
C81	C	0.66445	-0.88556	1.24951
C82	C	0.67813	-0.90792	1.2961
C83	C	0.79148	-0.94534	1.38983
C84	C	0.79769	-0.96529	1.44022
C85	C	0.75627	-0.99049	1.45329
C86	C	0.70875	-0.99592	1.41515
C87	C	0.70262	-0.97593	1.3646
C88	C	0.74345	-0.94989	1.35149
C89	C	0.78709	-0.97555	1.23695
C90	C	0.79091	-0.99834	1.18992
C91	C	0.74587	-0.99991	1.14829
C92	C	0.69643	-0.97877	1.15446

C93	C	0.69264	-0.95596	1.20158
C94	C	0.73829	-0.95359	1.24323
C95	C	0.82794	-0.90248	1.24459
C96	C	0.87418	-0.879	1.24275
C97	C	0.87946	-0.85403	1.28648
C98	C	0.83755	-0.85234	1.33127
C99	C	0.79129	-0.87585	1.33307
C100	C	0.78628	-0.90176	1.29036
C101	C	0.92988	-0.83068	1.28789
C102	C	0.5205	-0.84737	1.30115
C103	C	0.7633	-1.01016	1.50759
C104	C	0.75251	-1.02296	1.09792
C105	C	0.73583	-0.08794	1.79375
C106	C	0.73562	-0.10526	1.84824
C107	C	0.73987	-0.14124	1.84937
C108	C	0.7438	-0.15979	1.79641
C109	C	0.74403	-0.14241	1.74219
C110	C	0.73982	-0.10646	1.74063
C111	C	0.68928	-0.2154	1.79551
C112	C	0.68815	-0.25142	1.79477
C113	C	0.74162	-0.26986	1.79616
C114	C	0.79607	-0.25238	1.79802
C115	C	0.7968	-0.2163	1.79854
C116	C	0.74346	-0.19785	1.79737
C117	C	0.74918	-0.16236	1.68607
C118	C	0.73795	-0.16004	1.90682
C119	C	0.63276	-0.19551	1.79239
C120	C	0.85427	-0.19742	1.80123
C121	C	0.78191	-0.06492	1.66841
C122	C	0.77865	-0.04694	1.61551
C123	C	0.73105	-0.05214	1.57702
C124	C	0.68719	-0.07566	1.59203
C125	C	0.69042	-0.09364	1.64499
C126	C	0.73769	-0.08828	1.68354
C127	C	0.77495	-0.08531	1.94513
C128	C	0.76957	-0.06585	1.99636
C129	C	0.71836	-0.04655	2.00674
C130	C	0.67271	-0.04723	1.96553
C131	C	0.67805	-0.0667	1.91436
C132	C	0.72929	-0.08571	1.9037
C133	C	0.59008	-0.26692	1.83722
C134	C	0.53639	-0.2843	1.83412
C135	C	0.52311	-0.30463	1.78536
C136	C	0.56419	-0.30737	1.73942
C137	C	0.61781	-0.28997	1.74247
C138	C	0.63114	-0.26975	1.79149
C139	C	0.86588	-0.29297	1.84646
C140	C	0.91687	-0.31298	1.84561

C141	C	0.95446	-0.31235	1.79694
C142	C	0.94079	-0.29108	1.74908
C143	C	0.88979	-0.27103	1.74992
C144	C	0.85195	-0.27199	1.79854
N145	N	0.46862	-0.32304	1.78438
N146	N	0.72553	-0.03323	1.52342
N147	N	0.71245	-0.0252	2.05752
N148	N	1.00509	-0.33421	1.79664
C149	C	0.73124	-0.04965	1.79229
C150	C	0.74057	-0.30824	1.79547
C151	C	0.21833	0.95345	0.50671
N152	N	0.21242	0.9748	0.55749
N153	N	-0.49494	0.66579	1.29662
C154	C	0.23626	0.07168	0.79514
C155	C	0.13917	0.09076	0.84415
C156	C	0.08798	0.11053	0.84526
C157	C	0.07473	0.13234	0.79856
C158	C	0.1132	0.13427	0.75056
C159	C	0.16442	0.11444	0.74949
C160	C	0.17811	0.09208	0.79608
C161	C	0.29145	0.05466	0.88981
C162	C	0.29766	0.03471	0.9402
C163	C	0.25625	0.00951	0.95327
C164	C	0.20872	0.00408	0.91513
C165	C	0.20259	0.02407	0.86457
C166	C	0.24342	0.05011	0.85146
C167	C	0.28706	0.02445	0.73693
C168	C	0.29088	0.00166	0.6899
C169	C	0.24584	0.00009	0.64827
C170	C	0.1964	0.02123	0.65443
C171	C	0.19261	0.04404	0.70156
C172	C	0.23826	0.04641	0.74321
C173	C	0.32792	0.09752	0.74457
C174	C	0.37415	0.121	0.74273
C175	C	0.37943	0.14597	0.78646
C176	C	0.33752	0.14766	0.83124
C177	C	0.29127	0.12415	0.83304
C178	C	0.28625	0.09824	0.79034
C179	C	0.42985	0.16932	0.78786
C180	C	0.02047	0.15263	0.80113
C181	C	0.25248	-0.02296	0.59789
C182	C	0.23581	0.91206	1.29373
C183	C	0.23559	0.89474	1.34821
C184	C	0.23984	0.85876	1.34934
C185	C	0.24377	0.84021	1.29639
C186	C	0.244	0.85759	1.24217
C187	C	0.23979	0.89354	1.2406
C188	C	0.18926	0.7846	1.29549

C189	C	0.18812	0.74858	1.29474
C190	C	0.24159	0.73014	1.29614
C191	C	0.29604	0.74762	1.29799
C192	C	0.29677	0.7837	1.29852
C193	C	0.24343	0.80215	1.29734
C194	C	0.24915	0.83764	1.18604
C195	C	0.23792	0.83996	1.40679
C196	C	0.13273	0.80449	1.29236
C197	C	0.35424	0.80258	1.3012
C198	C	0.28189	0.93508	1.16839
C199	C	0.27862	0.95306	1.11549
C200	C	0.23103	0.94786	1.077
C201	C	0.18717	0.92434	1.092
C202	C	0.19039	0.90636	1.14497
C203	C	0.23766	0.91172	1.18352
C204	C	0.27492	0.91469	1.44511
C205	C	0.26954	0.93415	1.49634
C206	C	0.21833	0.95345	1.50671
C207	C	0.17268	0.95277	1.46551
C208	C	0.17802	0.9333	1.41433
C209	C	0.22927	0.91429	1.40368
C210	C	0.09005	0.73308	1.3372
C211	C	0.03637	0.7157	1.3341
C212	C	0.02309	0.69537	1.28533
C213	C	0.06416	0.69263	1.23939
C214	C	0.11778	0.71003	1.24244
C215	C	0.13111	0.73025	1.29147
C216	C	0.36586	0.70703	1.34643
C217	C	0.41684	0.68702	1.34559
C218	C	0.45443	0.68765	1.29691
C219	C	0.44076	0.70892	1.24905
C220	C	0.38976	0.72897	1.2499
C221	C	0.35192	0.72801	1.29852
N222	N	-0.03141	0.67696	1.28435
N223	N	0.2255	0.96677	1.02339
N224	N	0.21242	0.9748	1.55749
C225	C	0.23122	0.95035	1.29227
C226	C	0.24054	0.69176	1.29544
C227	C	0.26327	0.98984	1.00757
C228	C	0.25248	0.97704	0.59789
C229	C	-0.25636	0.57157	1.25404
C230	C	-0.34973	0.59662	1.30242
C231	C	-0.39773	0.61896	1.30245
C232	C	-0.40778	0.6405	1.25436
C233	C	-0.36929	0.63956	1.20651
C234	C	-0.32125	0.61721	1.20655
C235	C	-0.31094	0.59505	1.25424
C236	C	-0.20391	0.55215	1.34885

C237	C	-0.20069	0.53219	1.39947
C238	C	-0.24598	0.50948	1.41318
C239	C	-0.29452	0.5066	1.37549
C240	C	-0.29769	0.52664	1.32469
C241	C	-0.25275	0.55016	1.31089
C242	C	-0.21277	0.52156	1.19699
C243	C	-0.21212	0.49842	1.15033
C244	C	-0.25719	0.49876	1.10867
C245	C	-0.30359	0.52213	1.11449
C246	C	-0.3042	0.54531	1.16125
C247	C	-0.2583	0.5458	1.20282
C248	C	-0.16212	0.59259	1.20162
C249	C	-0.11208	0.61328	1.19909
C250	C	-0.10129	0.63724	1.2432
C251	C	-0.14177	0.64108	1.28914
C252	C	-0.19193	0.62046	1.2915
C253	C	-0.20231	0.59527	1.2485
C254	C	-0.04618	0.65669	1.24179
C255	C	-0.45837	0.66386	1.25296
C256	C	-0.24147	0.4896	1.4675
C257	C	-0.25333	0.47546	1.05836
C258	C	-0.27734	0.41237	0.75349
C259	C	-0.27718	0.39484	0.80778
C260	C	-0.27265	0.35885	0.8084
C261	C	-0.26861	0.34054	0.7552
C262	C	-0.26898	0.35814	0.7012
C263	C	-0.27342	0.39407	0.70014
C264	C	-0.31945	0.28372	0.75372
C265	C	-0.31813	0.24769	0.75364
C266	C	-0.26343	0.23051	0.7557
C267	C	-0.21022	0.24923	0.75779
C268	C	-0.21199	0.28529	0.75778
C269	C	-0.26653	0.3025	0.75583
C270	C	-0.26377	0.33848	0.64478
C271	C	-0.27403	0.33978	0.86561
C272	C	-0.37723	0.3023	0.74997
C273	C	-0.15591	0.30551	0.76106
C274	C	-0.22857	0.43484	0.62855
C275	C	-0.23038	0.453	0.5758
C276	C	-0.2782	0.4491	0.53714
C277	C	-0.32384	0.42667	0.55189
C278	C	-0.32206	0.40847	0.60473
C279	C	-0.27449	0.41255	0.64337
C280	C	-0.23615	0.41352	0.90467
C281	C	-0.23988	0.43289	0.95612
C282	C	-0.28974	0.45322	0.96714
C283	C	-0.33577	0.45363	0.92634
C284	C	-0.33209	0.43422	0.87493

C285	C	-0.28213	0.4142	0.86361
C286	C	-0.41472	0.23068	0.7975
C287	C	-0.46659	0.2115	0.79629
C288	C	-0.47817	0.18938	0.74907
C289	C	-0.43746	0.18686	0.70318
C290	C	-0.38562	0.20609	0.70431
C291	C	-0.37384	0.22798	0.75161
C292	C	-0.13946	0.20977	0.80762
C293	C	-0.08699	0.19113	0.80826
C294	C	-0.04733	0.19339	0.76101
C295	C	-0.06069	0.2148	0.7136
C296	C	-0.11326	0.23346	0.71293
C297	C	-0.15303	0.23093	0.75983
N298	N	-0.2936	0.47467	1.01801
N299	N	0.00591	0.1737	0.75963
C300	C	-0.28165	0.45068	0.7524
C301	C	-0.26184	0.19213	0.75569
N302	N	0.47047	0.16818	0.74789
N303	N	-0.28188	0.46813	1.48349
loop_				

Table S5. Atomistic coordinates for the refined unit cell parameters for BMTA-TFPM-COF with 3-fold interpenetrated dia topology via Pawley refinement.

	Atom	*x/a*	*y/b*	*z/c*
C1	C	0.24367	-0.42843	0.75406
C2	C	0.1503	-0.40338	0.80245
C3	C	0.1023	-0.38104	0.80247
C4	C	0.09225	-0.3595	0.75438
C5	C	0.13073	-0.36044	0.70653
C6	C	0.17878	-0.38279	0.70658
C7	C	0.18909	-0.40495	0.75426
C8	C	0.29612	-0.44785	0.84887
C9	C	0.29934	-0.46781	0.8995
C10	C	0.25405	-0.49052	0.9132
C11	C	0.20551	-0.4934	0.87551
C12	C	0.20234	-0.47336	0.82472
C13	C	0.24728	-0.44984	0.81091
C14	C	0.28726	-0.47844	0.69702
C15	C	0.28791	-0.50158	0.65036
C16	C	0.24284	-0.50124	0.60869
C17	C	0.19644	-0.47787	0.61451
C18	C	0.19583	-0.45469	0.66127
C19	C	0.24173	-0.4542	0.70285
C20	C	0.33791	-0.40741	0.70164
C21	C	0.38795	-0.38672	0.69912
C22	C	0.39874	-0.36276	0.74322
C23	C	0.35826	-0.35892	0.78916
C24	C	0.3081	-0.37954	0.79153
C25	C	0.29772	-0.40473	0.74852
C26	C	0.45385	-0.34331	0.74181
C27	C	0.04165	-0.33614	0.75299
C28	C	0.25856	-0.5104	0.96752
C29	C	0.2467	-0.52454	0.55839
C30	C	0.22269	-0.58763	0.25351
C31	C	0.22285	-0.60516	0.3078
C32	C	0.22738	-0.64115	0.30843
C33	C	0.23142	-0.65946	0.25523
C34	C	0.23105	-0.64186	0.20122
C35	C	0.22661	-0.60593	0.20017
C36	C	0.18058	-0.71628	0.25375
C37	C	0.1819	-0.75231	0.25367
C38	C	0.2366	-0.76949	0.25572
C39	C	0.2898	-0.75077	0.25782
C40	C	0.28804	-0.71471	0.25781
C41	C	0.23349	-0.6975	0.25585
C42	C	0.23626	-0.66152	0.14481
C43	C	0.226	-0.66022	0.36563
C44	C	0.1228	-0.6977	0.25

C45	C	0.34412	-0.69449	0.26108
C46	C	0.27146	-0.56516	0.12857
C47	C	0.26965	-0.547	0.07582
C48	C	0.22183	-0.5509	0.03716
C49	C	0.17619	-0.57333	0.05192
C50	C	0.17797	-0.59153	0.10475
C51	C	0.22554	-0.58745	0.1434
C52	C	0.26388	-0.58648	0.40469
C53	C	0.26015	-0.56711	0.45615
C54	C	0.21029	-0.54678	0.46717
C55	C	0.16426	-0.54637	0.42636
C56	C	0.16794	-0.56578	0.37495
C57	C	0.21789	-0.5858	0.36364
C58	C	0.08531	-0.76932	0.29752
C59	C	0.03343	-0.7885	0.29631
C60	C	0.02185	-0.81062	0.24909
C61	C	0.06256	-0.81314	0.2032
C62	C	0.1144	-0.79391	0.20434
C63	C	0.12619	-0.77202	0.25163
C64	C	0.36057	-0.79023	0.30764
C65	C	0.41304	-0.80887	0.30828
C66	C	0.4527	-0.80661	0.26104
C67	C	0.43934	-0.7852	0.21363
C68	C	0.38677	-0.76654	0.21295
C69	C	0.34699	-0.76907	0.25986
N70	N	-0.0295	-0.83182	0.24791
N71	N	0.21815	-0.53187	-0.01648
N72	N	0.20643	-0.52533	0.51803
N73	N	0.50594	-0.8263	0.25965
C74	C	0.21838	-0.54932	0.25242
C75	C	0.23818	-0.80787	0.25572
C76	C	0.73629	-0.92832	1.29517
C77	C	0.6392	-0.90924	1.34417
C78	C	0.58801	-0.88947	1.34528
C79	C	0.57476	-0.86766	1.29858
C80	C	0.61322	-0.86573	1.25059
C81	C	0.66445	-0.88556	1.24951
C82	C	0.67813	-0.90792	1.2961
C83	C	0.79148	-0.94534	1.38983
C84	C	0.79769	-0.96529	1.44022
C85	C	0.75627	-0.99049	1.45329
C86	C	0.70875	-0.99592	1.41515
C87	C	0.70262	-0.97593	1.3646
C88	C	0.74345	-0.94989	1.35149
C89	C	0.78709	-0.97555	1.23695
C90	C	0.79091	-0.99834	1.18992
C91	C	0.74587	-0.99991	1.14829
C92	C	0.69643	-0.97877	1.15446

C93	C	0.69264	-0.95596	1.20158
C94	C	0.73829	-0.95359	1.24323
C95	C	0.82794	-0.90248	1.24459
C96	C	0.87418	-0.879	1.24275
C97	C	0.87946	-0.85403	1.28648
C98	C	0.83755	-0.85234	1.33127
C99	C	0.79129	-0.87585	1.33307
C100	C	0.78628	-0.90176	1.29036
C101	C	0.92988	-0.83068	1.28789
C102	C	0.5205	-0.84737	1.30115
C103	C	0.7633	-1.01016	1.50759
C104	C	0.75251	-1.02296	1.09792
C105	C	0.73583	-0.08794	1.79375
C106	C	0.73562	-0.10526	1.84824
C107	C	0.73987	-0.14124	1.84937
C108	C	0.7438	-0.15979	1.79641
C109	C	0.74403	-0.14241	1.74219
C110	C	0.73982	-0.10646	1.74063
C111	C	0.68928	-0.2154	1.79551
C112	C	0.68815	-0.25142	1.79477
C113	C	0.74162	-0.26986	1.79616
C114	C	0.79607	-0.25238	1.79802
C115	C	0.7968	-0.2163	1.79854
C116	C	0.74346	-0.19785	1.79737
C117	C	0.74918	-0.16236	1.68607
C118	C	0.73795	-0.16004	1.90682
C119	C	0.63276	-0.19551	1.79239
C120	C	0.85427	-0.19742	1.80123
C121	C	0.78191	-0.06492	1.66841
C122	C	0.77865	-0.04694	1.61551
C123	C	0.73105	-0.05214	1.57702
C124	C	0.68719	-0.07566	1.59203
C125	C	0.69042	-0.09364	1.64499
C126	C	0.73769	-0.08828	1.68354
C127	C	0.77495	-0.08531	1.94513
C128	C	0.76957	-0.06585	1.99636
C129	C	0.71836	-0.04655	2.00674
C130	C	0.67271	-0.04723	1.96553
C131	C	0.67805	-0.0667	1.91436
C132	C	0.72929	-0.08571	1.9037
C133	C	0.59008	-0.26692	1.83722
C134	C	0.53639	-0.2843	1.83412
C135	C	0.52311	-0.30463	1.78536
C136	C	0.56419	-0.30737	1.73942
C137	C	0.61781	-0.28997	1.74247
C138	C	0.63114	-0.26975	1.79149
C139	C	0.86588	-0.29297	1.84646
C140	C	0.91687	-0.31298	1.84561

C141	C	0.95446	-0.31235	1.79694
C142	C	0.94079	-0.29108	1.74908
C143	C	0.88979	-0.27103	1.74992
C144	C	0.85195	-0.27199	1.79854
N145	N	0.46862	-0.32304	1.78438
N146	N	0.72553	-0.03323	1.52342
N147	N	0.71245	-0.0252	2.05752
N148	N	1.00509	-0.33421	1.79664
C149	C	0.73124	-0.04965	1.79229
C150	C	0.74057	-0.30824	1.79547
C151	C	0.38486	0.95345	0.3402
N152	N	0.37895	0.9748	0.39098
N153	N	-0.32841	0.66579	1.13011
C154	C	0.40279	0.07168	0.62863
C155	C	0.3057	0.09076	0.67764
C156	C	0.25451	0.11053	0.67874
C157	C	0.24126	0.13234	0.63205
C158	C	0.27972	0.13427	0.58405
C159	C	0.33095	0.11444	0.58298
C160	C	0.34463	0.09208	0.62956
C161	C	0.45798	0.05466	0.7233
C162	C	0.46419	0.03471	0.77369
C163	C	0.42277	0.00951	0.78676
C164	C	0.37525	0.00408	0.74862
C165	C	0.36912	0.02407	0.69806
C166	C	0.40995	0.05011	0.68495
C167	C	0.45359	0.02445	0.57041
C168	C	0.45741	0.00166	0.52339
C169	C	0.41237	0.00009	0.48176
C170	C	0.36293	0.02123	0.48792
C171	C	0.35914	0.04404	0.53504
C172	C	0.40479	0.04641	0.57669
C173	C	0.49445	0.09752	0.57806
C174	C	0.54068	0.121	0.57621
C175	C	0.54596	0.14597	0.61995
C176	C	0.50405	0.14766	0.66473
C177	C	0.4578	0.12415	0.66653
C178	C	0.45278	0.09824	0.62383
C179	C	0.59638	0.16932	0.62135
C180	C	0.187	0.15263	0.63462
C181	C	0.41901	-0.02296	0.43138
C182	C	0.40233	0.91206	1.12722
C183	C	0.40212	0.89474	1.1817
C184	C	0.40637	0.85876	1.18283
C185	C	0.4103	0.84021	1.12988
C186	C	0.41053	0.85759	1.07566
C187	C	0.40632	0.89354	1.07409
C188	C	0.35578	0.7846	1.12897

C189	C	0.35465	0.74858	1.12823
C190	C	0.40812	0.73014	1.12963
C191	C	0.46257	0.74762	1.13148
C192	C	0.4633	0.7837	1.13201
C193	C	0.40996	0.80215	1.13083
C194	C	0.41568	0.83764	1.01953
C195	C	0.40445	0.83996	1.24028
C196	C	0.29926	0.80449	1.12585
C197	C	0.52077	0.80258	1.13469
C198	C	0.44842	0.93508	1.00188
C199	C	0.44515	0.95306	0.94898
C200	C	0.39756	0.94786	0.91048
C201	C	0.3537	0.92434	0.92549
C202	C	0.35692	0.90636	0.97846
C203	C	0.40419	0.91172	1.01701
C204	C	0.44145	0.91469	1.2786
C205	C	0.43607	0.93415	1.32983
C206	C	0.38486	0.95345	1.3402
C207	C	0.33921	0.95277	1.299
C208	C	0.34455	0.9333	1.24782
C209	C	0.39579	0.91429	1.23717
C210	C	0.25658	0.73308	1.17069
C211	C	0.20289	0.7157	1.16759
C212	C	0.18961	0.69537	1.11882
C213	C	0.23069	0.69263	1.07288
C214	C	0.28431	0.71003	1.07593
C215	C	0.29764	0.73025	1.12496
C216	C	0.53238	0.70703	1.17992
C217	C	0.58337	0.68702	1.17907
C218	C	0.62096	0.68765	1.1304
C219	C	0.60729	0.70892	1.08254
C220	C	0.55629	0.72897	1.08339
C221	C	0.51845	0.72801	1.13201
N222	N	0.13512	0.67696	1.11784
N223	N	0.39203	0.96677	0.85688
N224	N	0.37895	0.9748	1.39098
C225	C	0.39775	0.95035	1.12575
C226	C	0.40707	0.69176	1.12893
C227	C	0.4298	0.98984	0.84106
C228	C	0.41901	0.97704	0.43138
C229	C	-0.08983	0.57157	1.08753
C230	C	-0.1832	0.59662	1.13591
C231	C	-0.2312	0.61896	1.13593
C232	C	-0.24125	0.6405	1.08784
C233	C	-0.20276	0.63956	1.04
C234	C	-0.15472	0.61721	1.04004
C235	C	-0.14441	0.59505	1.08773
C236	C	-0.03738	0.55215	1.18233

C237	C	-0.03416	0.53219	1.23296
C238	C	-0.07945	0.50948	1.24666
C239	C	-0.12799	0.5066	1.20898
C240	C	-0.13116	0.52664	1.15818
C241	C	-0.08622	0.55016	1.14438
C242	C	-0.04624	0.52156	1.03048
C243	C	-0.04559	0.49842	0.98382
C244	C	-0.09066	0.49876	0.94215
C245	C	-0.13706	0.52213	0.94798
C246	C	-0.13767	0.54531	0.99474
C247	C	-0.09177	0.5458	1.03631
C248	C	0.00441	0.59259	1.0351
C249	C	0.05445	0.61328	1.03258
C250	C	0.06524	0.63724	1.07669
C251	C	0.02476	0.64108	1.12262
C252	C	-0.0254	0.62046	1.12499
C253	C	-0.03578	0.59527	1.08199
C254	C	0.12035	0.65669	1.07527
C255	C	-0.29185	0.66386	1.08645
C256	C	-0.07494	0.4896	1.30099
C257	C	-0.0868	0.47546	0.89185
C258	C	-0.11081	0.41237	0.58697
C259	C	-0.11065	0.39484	0.64127
C260	C	-0.10612	0.35885	0.64189
C261	C	-0.10208	0.34054	0.58869
C262	C	-0.10245	0.35814	0.53469
C263	C	-0.10689	0.39407	0.53363
C264	C	-0.15292	0.28372	0.58721
C265	C	-0.1516	0.24769	0.58713
C266	C	-0.0969	0.23051	0.58918
C267	C	-0.0437	0.24923	0.59128
C268	C	-0.04546	0.28529	0.59127
C269	C	-0.1	0.3025	0.58931
C270	C	-0.09724	0.33848	0.47827
C271	C	-0.1075	0.33978	0.6991
C272	C	-0.2107	0.3023	0.58346
C273	C	0.01062	0.30551	0.59455
C274	C	-0.06204	0.43484	0.46204
C275	C	-0.06385	0.453	0.40928
C276	C	-0.11167	0.4491	0.37063
C277	C	-0.15731	0.42667	0.38538
C278	C	-0.15553	0.40847	0.43822
C279	C	-0.10796	0.41255	0.47686
C280	C	-0.06962	0.41352	0.73815
C281	C	-0.07335	0.43289	0.78961
C282	C	-0.12321	0.45322	0.80063
C283	C	-0.16924	0.45363	0.75982
C284	C	-0.16556	0.43422	0.70841

C285	C	-0.11561	0.4142	0.6971
C286	C	-0.24819	0.23068	0.63098
C287	C	-0.30006	0.2115	0.62978
C288	C	-0.31164	0.18938	0.58255
C289	C	-0.27093	0.18686	0.53666
C290	C	-0.21909	0.20609	0.5378
C291	C	-0.20731	0.22798	0.5851
C292	C	0.02707	0.20977	0.6411
C293	C	0.07954	0.19113	0.64174
C294	C	0.1192	0.19339	0.5945
C295	C	0.10584	0.2148	0.54709
C296	C	0.05327	0.23346	0.54641
C297	C	0.01349	0.23093	0.59332
N298	N	-0.12707	0.47467	0.85149
N299	N	0.17244	0.1737	0.59312
C300	C	-0.11512	0.45068	0.58588
C301	C	-0.09531	0.19213	0.58918
N302	N	0.637	0.16818	0.58138
N303	N	-0.11535	0.46813	1.31698
C304	C	1.05274	0.95345	-0.32585
N305	N	1.04683	0.9748	-0.27507
N306	N	0.33947	0.66579	0.46406
C307	C	1.07067	0.07168	-0.03742
C308	C	0.97358	0.09076	0.01159
C309	C	0.92239	0.11053	0.01269
C310	C	0.90914	0.13234	-0.034
C311	C	0.9476	0.13427	-0.082
C312	C	0.99883	0.11444	-0.08307
C313	C	1.01251	0.09208	-0.03649
C314	C	1.12586	0.05466	0.05725
C315	C	1.13207	0.03471	0.10764
C316	C	1.09065	0.00951	0.12071
C317	C	1.04313	0.00408	0.08257
C318	C	1.037	0.02407	0.03201
C319	C	1.07783	0.05011	0.0189
C320	C	1.12147	0.02445	-0.09563
C321	C	1.12529	0.00166	-0.14266
C322	C	1.08025	0.00009	-0.18429
C323	C	1.03081	0.02123	-0.17813
C324	C	1.02702	0.04404	-0.13101
C325	C	1.07267	0.04641	-0.08935
C326	C	1.16232	0.09752	-0.08799
C327	C	1.20856	0.121	-0.08983
C328	C	1.21384	0.14597	-0.0461
C329	C	1.17193	0.14766	-0.00132
C330	C	1.12567	0.12415	0.00048
C331	C	1.12066	0.09824	-0.04222
C332	C	1.26426	0.16932	-0.0447

C333	C	0.85488	0.15263	-0.03143
C334	C	1.08689	-0.02296	-0.23467
C335	C	1.07021	0.91206	0.46117
C336	C	1.07	0.89474	0.51565
C337	C	1.07425	0.85876	0.51678
C338	C	1.07818	0.84021	0.46383
C339	C	1.07841	0.85759	0.40961
C340	C	1.0742	0.89354	0.40804
C341	C	1.02366	0.7846	0.46293
C342	C	1.02253	0.74858	0.46218
C343	C	1.076	0.73014	0.46358
C344	C	1.13045	0.74762	0.46543
C345	C	1.13118	0.7837	0.46596
C346	C	1.07784	0.80215	0.46478
C347	C	1.08356	0.83764	0.35348
C348	C	1.07233	0.83996	0.57423
C349	C	0.96714	0.80449	0.4598
C350	C	1.18865	0.80258	0.46864
C351	C	1.11629	0.93508	0.33583
C352	C	1.11303	0.95306	0.28293
C353	C	1.06543	0.94786	0.24444
C354	C	1.02157	0.92434	0.25944
C355	C	1.0248	0.90636	0.31241
C356	C	1.07207	0.91172	0.35096
C357	C	1.10933	0.91469	0.61255
C358	C	1.10395	0.93415	0.66378
C359	C	1.05274	0.95345	0.67415
C360	C	1.00709	0.95277	0.63295
C361	C	1.01243	0.9333	0.58177
C362	C	1.06367	0.91429	0.57112
C363	C	0.92446	0.73308	0.50464
C364	C	0.87077	0.7157	0.50154
C365	C	0.85749	0.69537	0.45277
C366	C	0.89857	0.69263	0.40683
C367	C	0.95219	0.71003	0.40988
C368	C	0.96552	0.73025	0.45891
C369	C	1.20026	0.70703	0.51387
C370	C	1.25125	0.68702	0.51302
C371	C	1.28884	0.68765	0.46435
C372	C	1.27517	0.70892	0.41649
C373	C	1.22417	0.72897	0.41734
C374	C	1.18633	0.72801	0.46596
N375	N	0.803	0.67696	0.45179
N376	N	1.05991	0.96677	0.19083
N377	N	1.04683	0.9748	0.72493
C378	C	1.06562	0.95035	0.45971
C379	C	1.07495	0.69176	0.46288
C380	C	1.09768	0.98984	0.17501

C381	C	1.08689	0.97704	-0.23467
C382	C	0.57805	0.57157	0.42148
C383	C	0.48468	0.59662	0.46986
C384	C	0.43668	0.61896	0.46989
C385	C	0.42663	0.6405	0.4218
C386	C	0.46511	0.63956	0.37395
C387	C	0.51316	0.61721	0.37399
C388	C	0.52347	0.59505	0.42168
C389	C	0.6305	0.55215	0.51629
C390	C	0.63372	0.53219	0.56691
C391	C	0.58843	0.50948	0.58062
C392	C	0.53989	0.5066	0.54293
C393	C	0.53672	0.52664	0.49213
C394	C	0.58166	0.55016	0.47833
C395	C	0.62164	0.52156	0.36443
C396	C	0.62229	0.49842	0.31777
C397	C	0.57722	0.49876	0.27611
C398	C	0.53082	0.52213	0.28193
C399	C	0.53021	0.54531	0.32869
C400	C	0.57611	0.5458	0.37026
C401	C	0.67229	0.59259	0.36906
C402	C	0.72233	0.61328	0.36653
C403	C	0.73312	0.63724	0.41064
C404	C	0.69264	0.64108	0.45658
C405	C	0.64248	0.62046	0.45894
C406	C	0.6321	0.59527	0.41594
C407	C	0.78823	0.65669	0.40922
C408	C	0.37603	0.66386	0.4204
C409	C	0.59294	0.4896	0.63494
C410	C	0.58108	0.47546	0.2258
C411	C	0.55707	0.41237	-0.07907
C412	C	0.55723	0.39484	-0.02478
C413	C	0.56176	0.35885	-0.02416
C414	C	0.5658	0.34054	-0.07736
C415	C	0.56543	0.35814	-0.13136
C416	C	0.56099	0.39407	-0.13242
C417	C	0.51496	0.28372	-0.07884
C418	C	0.51628	0.24769	-0.07892
C419	C	0.57098	0.23051	-0.07686
C420	C	0.62418	0.24923	-0.07477
C421	C	0.62242	0.28529	-0.07478
C422	C	0.56787	0.3025	-0.07673
C423	C	0.57064	0.33848	-0.18778
C424	C	0.56038	0.33978	0.03305
C425	C	0.45718	0.3023	-0.08259
C426	C	0.6785	0.30551	-0.0715
C427	C	0.60584	0.43484	-0.20401
C428	C	0.60403	0.453	-0.25676

C429	C	0.55621	0.4491	-0.29542
C430	C	0.51057	0.42667	-0.28067
C431	C	0.51235	0.40847	-0.22783
C432	C	0.55992	0.41255	-0.18919
C433	C	0.59826	0.41352	0.0721
C434	C	0.59453	0.43289	0.12356
C435	C	0.54467	0.45322	0.13458
C436	C	0.49864	0.45363	0.09378
C437	C	0.50232	0.43422	0.04237
C438	C	0.55227	0.4142	0.03105
C439	C	0.41969	0.23068	-0.03506
C440	C	0.36781	0.2115	-0.03627
C441	C	0.35623	0.18938	-0.08349
C442	C	0.39694	0.18686	-0.12938
C443	C	0.44878	0.20609	-0.12825
C444	C	0.46057	0.22798	-0.08095
C445	C	0.69495	0.20977	-0.02495
C446	C	0.74742	0.19113	-0.0243
C447	C	0.78708	0.19339	-0.07155
C448	C	0.77372	0.2148	-0.11896
C449	C	0.72115	0.23346	-0.11964
C450	C	0.68137	0.23093	-0.07273
N451	N	0.54081	0.47467	0.18545
N452	N	0.84032	0.1737	-0.07293
C453	C	0.55276	0.45068	-0.08016
C454	C	0.57257	0.19213	-0.07687
N455	N	1.30488	0.16818	-0.08467
N456	N	0.55253	0.46813	0.65093

Table S6. Atomistic coordinates for the refined unit cell parameters for BMTA-TFPM-COF with 4-fold interpenetrated dia topology via Pawley refinement.

	Atom	*x/a*	*y/b*	*z/c*
C1	C	0.24367	-0.42843	0.75406
C2	C	0.1503	-0.40338	0.80245
C3	C	0.1023	-0.38104	0.80247
C4	C	0.09225	-0.3595	0.75438
C5	C	0.13073	-0.36044	0.70653
C6	C	0.17878	-0.38279	0.70658
C7	C	0.18909	-0.40495	0.75426
C8	C	0.29612	-0.44785	0.84887
C9	C	0.29934	-0.46781	0.8995
C10	C	0.25405	-0.49052	0.9132
C11	C	0.20551	-0.4934	0.87551
C12	C	0.20234	-0.47336	0.82472
C13	C	0.24728	-0.44984	0.81091
C14	C	0.28726	-0.47844	0.69702
C15	C	0.28791	-0.50158	0.65036
C16	C	0.24284	-0.50124	0.60869
C17	C	0.19644	-0.47787	0.61451
C18	C	0.19583	-0.45469	0.66127
C19	C	0.24173	-0.4542	0.70285
C20	C	0.33791	-0.40741	0.70164
C21	C	0.38795	-0.38672	0.69912
C22	C	0.39874	-0.36276	0.74322
C23	C	0.35826	-0.35892	0.78916
C24	C	0.3081	-0.37954	0.79153
C25	C	0.29772	-0.40473	0.74852
C26	C	0.45385	-0.34331	0.74181
C27	C	0.04165	-0.33614	0.75299
C28	C	0.25856	-0.5104	0.96752
C29	C	0.2467	-0.52454	0.55839
C30	C	0.22269	-0.58763	0.25351
C31	C	0.22285	-0.60516	0.3078
C32	C	0.22738	-0.64115	0.30843
C33	C	0.23142	-0.65946	0.25523
C34	C	0.23105	-0.64186	0.20122
C35	C	0.22661	-0.60593	0.20017
C36	C	0.18058	-0.71628	0.25375
C37	C	0.1819	-0.75231	0.25367
C38	C	0.2366	-0.76949	0.25572
C39	C	0.2898	-0.75077	0.25782
C40	C	0.28804	-0.71471	0.25781
C41	C	0.23349	-0.6975	0.25585
C42	C	0.23626	-0.66152	0.14481
C43	C	0.226	-0.66022	0.36563
C44	C	0.1228	-0.6977	0.25

C45	C	0.34412	-0.69449	0.26108
C46	C	0.27146	-0.56516	0.12857
C47	C	0.26965	-0.547	0.07582
C48	C	0.22183	-0.5509	0.03716
C49	C	0.17619	-0.57333	0.05192
C50	C	0.17797	-0.59153	0.10475
C51	C	0.22554	-0.58745	0.1434
C52	C	0.26388	-0.58648	0.40469
C53	C	0.26015	-0.56711	0.45615
C54	C	0.21029	-0.54678	0.46717
C55	C	0.16426	-0.54637	0.42636
C56	C	0.16794	-0.56578	0.37495
C57	C	0.21789	-0.5858	0.36364
C58	C	0.08531	-0.76932	0.29752
C59	C	0.03343	-0.7885	0.29631
C60	C	0.02185	-0.81062	0.24909
C61	C	0.06256	-0.81314	0.2032
C62	C	0.1144	-0.79391	0.20434
C63	C	0.12619	-0.77202	0.25163
C64	C	0.36057	-0.79023	0.30764
C65	C	0.41304	-0.80887	0.30828
C66	C	0.4527	-0.80661	0.26104
C67	C	0.43934	-0.7852	0.21363
C68	C	0.38677	-0.76654	0.21295
C69	C	0.34699	-0.76907	0.25986
N70	N	-0.0295	-0.83182	0.24791
N71	N	0.21815	-0.53187	-0.01648
N72	N	0.20643	-0.52533	0.51803
N73	N	0.50594	-0.8263	0.25965
C74	C	0.21838	-0.54932	0.25242
C75	C	0.23818	-0.80787	0.25572
C76	C	0.73629	-0.92832	1.29517
C77	C	0.6392	-0.90924	1.34417
C78	C	0.58801	-0.88947	1.34528
C79	C	0.57476	-0.86766	1.29858
C80	C	0.61322	-0.86573	1.25059
C81	C	0.66445	-0.88556	1.24951
C82	C	0.67813	-0.90792	1.2961
C83	C	0.79148	-0.94534	1.38983
C84	C	0.79769	-0.96529	1.44022
C85	C	0.75627	-0.99049	1.45329
C86	C	0.70875	-0.99592	1.41515
C87	C	0.70262	-0.97593	1.3646
C88	C	0.74345	-0.94989	1.35149
C89	C	0.78709	-0.97555	1.23695
C90	C	0.79091	-0.99834	1.18992
C91	C	0.74587	-0.99991	1.14829
C92	C	0.69643	-0.97877	1.15446

C93	C	0.69264	-0.95596	1.20158
C94	C	0.73829	-0.95359	1.24323
C95	C	0.82794	-0.90248	1.24459
C96	C	0.87418	-0.879	1.24275
C97	C	0.87946	-0.85403	1.28648
C98	C	0.83755	-0.85234	1.33127
C99	C	0.79129	-0.87585	1.33307
C100	C	0.78628	-0.90176	1.29036
C101	C	0.92988	-0.83068	1.28789
C102	C	0.5205	-0.84737	1.30115
C103	C	0.7633	-1.01016	1.50759
C104	C	0.75251	-1.02296	1.09792
C105	C	0.73583	-0.08794	1.79375
C106	C	0.73562	-0.10526	1.84824
C107	C	0.73987	-0.14124	1.84937
C108	C	0.7438	-0.15979	1.79641
C109	C	0.74403	-0.14241	1.74219
C110	C	0.73982	-0.10646	1.74063
C111	C	0.68928	-0.2154	1.79551
C112	C	0.68815	-0.25142	1.79477
C113	C	0.74162	-0.26986	1.79616
C114	C	0.79607	-0.25238	1.79802
C115	C	0.7968	-0.2163	1.79854
C116	C	0.74346	-0.19785	1.79737
C117	C	0.74918	-0.16236	1.68607
C118	C	0.73795	-0.16004	1.90682
C119	C	0.63276	-0.19551	1.79239
C120	C	0.85427	-0.19742	1.80123
C121	C	0.78191	-0.06492	1.66841
C122	C	0.77865	-0.04694	1.61551
C123	C	0.73105	-0.05214	1.57702
C124	C	0.68719	-0.07566	1.59203
C125	C	0.69042	-0.09364	1.64499
C126	C	0.73769	-0.08828	1.68354
C127	C	0.77495	-0.08531	1.94513
C128	C	0.76957	-0.06585	1.99636
C129	C	0.71836	-0.04655	2.00674
C130	C	0.67271	-0.04723	1.96553
C131	C	0.67805	-0.0667	1.91436
C132	C	0.72929	-0.08571	1.9037
C133	C	0.59008	-0.26692	1.83722
C134	C	0.53639	-0.2843	1.83412
C135	C	0.52311	-0.30463	1.78536
C136	C	0.56419	-0.30737	1.73942
C137	C	0.61781	-0.28997	1.74247
C138	C	0.63114	-0.26975	1.79149
C139	C	0.86588	-0.29297	1.84646
C140	C	0.91687	-0.31298	1.84561

C141	C	0.95446	-0.31235	1.79694
C142	C	0.94079	-0.29108	1.74908
C143	C	0.88979	-0.27103	1.74992
C144	C	0.85195	-0.27199	1.79854
N145	N	0.46862	-0.32304	1.78438
N146	N	0.72553	-0.03323	1.52342
N147	N	0.71245	-0.0252	2.05752
N148	N	1.00509	-0.33421	1.79664
C149	C	0.73124	-0.04965	1.79229
C150	C	0.74057	-0.30824	1.79547
C151	C	-0.03102	0.95345	0.7567
N152	N	-0.03693	0.9748	0.80748
N153	N	-0.74429	0.66579	1.54661
C154	C	-0.01309	0.07168	1.04513
C155	C	-0.11019	0.09076	1.09414
C156	C	-0.16138	0.11053	1.09524
C157	C	-0.17462	0.13234	1.04855
C158	C	-0.13616	0.13427	1.00055
C159	C	-0.08493	0.11444	0.99948
C160	C	-0.07125	0.09208	1.04606
C161	C	0.0421	0.05466	1.1398
C162	C	0.04831	0.03471	1.19019
C163	C	0.00689	0.00951	1.20326
C164	C	-0.04063	0.00408	1.16512
C165	C	-0.04676	0.02407	1.11456
C166	C	-0.00593	0.05011	1.10145
C167	C	0.03771	0.02445	0.98691
C168	C	0.04153	0.00166	0.93989
C169	C	-0.00352	0.00009	0.89826
C170	C	-0.05295	0.02123	0.90442
C171	C	-0.05674	0.04404	0.95154
C172	C	-0.01109	0.04641	0.99319
C173	C	0.07856	0.09752	0.99456
C174	C	0.1248	0.121	0.99271
C175	C	0.13007	0.14597	1.03645
C176	C	0.08817	0.14766	1.08123
C177	C	0.04191	0.12415	1.08303
C178	C	0.03689	0.09824	1.04033
C179	C	0.1805	0.16932	1.03785
C180	C	-0.22889	0.15263	1.05112
C181	C	0.00313	-0.02296	0.84788
C182	C	-0.01355	0.91206	1.54372
C183	C	-0.01377	0.89474	1.5982
C184	C	-0.00951	0.85876	1.59933
C185	C	-0.00559	0.84021	1.54638
C186	C	-0.00535	0.85759	1.49216
C187	C	-0.00956	0.89354	1.49059
C188	C	-0.0601	0.7846	1.54547

C189	C	-0.06123	0.74858	1.54473
C190	C	-0.00776	0.73014	1.54613
C191	C	0.04669	0.74762	1.54798
C192	C	0.04741	0.7837	1.54851
C193	C	-0.00593	0.80215	1.54733
C194	C	-0.0002	0.83764	1.43603
C195	C	-0.01143	0.83996	1.65678
C196	C	-0.11662	0.80449	1.54235
C197	C	0.10488	0.80258	1.55119
C198	C	0.03253	0.93508	1.41838
C199	C	0.02926	0.95306	1.36548
C200	C	-0.01833	0.94786	1.32698
C201	C	-0.06219	0.92434	1.34199
C202	C	-0.05897	0.90636	1.39496
C203	C	-0.0117	0.91172	1.43351
C204	C	0.02557	0.91469	1.6951
C205	C	0.02018	0.93415	1.74633
C206	C	-0.03102	0.95345	1.7567
C207	C	-0.07668	0.95277	1.7155
C208	C	-0.07133	0.9333	1.66432
C209	C	-0.02009	0.91429	1.65367
C210	C	-0.1593	0.73308	1.58719
C211	C	-0.21299	0.7157	1.58409
C212	C	-0.22627	0.69537	1.53532
C213	C	-0.18519	0.69263	1.48938
C214	C	-0.13157	0.71003	1.49243
C215	C	-0.11824	0.73025	1.54146
C216	C	0.1165	0.70703	1.59642
C217	C	0.16749	0.68702	1.59557
C218	C	0.20507	0.68765	1.5469
C219	C	0.19141	0.70892	1.49904
C220	C	0.14041	0.72897	1.49989
C221	C	0.10256	0.72801	1.54851
N222	N	-0.28076	0.67696	1.53434
N223	N	-0.02385	0.96677	1.27338
N224	N	-0.03693	0.9748	1.80748
C225	C	-0.01814	0.95035	1.54225
C226	C	-0.00881	0.69176	1.54543
C227	C	0.01391	0.98984	1.25756
C228	C	0.00313	0.97704	0.84788
C229	C	-0.50572	0.57157	1.50403
C230	C	-0.59908	0.59662	1.55241
C231	C	-0.64708	0.61896	1.55243
C232	C	-0.65714	0.6405	1.50434
C233	C	-0.61865	0.63956	1.4565
C234	C	-0.57061	0.61721	1.45654
C235	C	-0.56029	0.59505	1.50423
C236	C	-0.45326	0.55215	1.59883

C237	C	-0.45004	0.53219	1.64946
C238	C	-0.49533	0.50948	1.66316
C239	C	-0.54387	0.5066	1.62548
C240	C	-0.54704	0.52664	1.57468
C241	C	-0.5021	0.55016	1.56088
C242	C	-0.46212	0.52156	1.44698
C243	C	-0.46147	0.49842	1.40032
C244	C	-0.50654	0.49876	1.35865
C245	C	-0.55295	0.52213	1.36448
C246	C	-0.55355	0.54531	1.41124
C247	C	-0.50765	0.5458	1.45281
C248	C	-0.41147	0.59259	1.4516
C249	C	-0.36143	0.61328	1.44908
C250	C	-0.35065	0.63724	1.49319
C251	C	-0.39113	0.64108	1.53913
C252	C	-0.44129	0.62046	1.54149
C253	C	-0.45166	0.59527	1.49849
C254	C	-0.29554	0.65669	1.49177
C255	C	-0.70773	0.66386	1.50295
C256	C	-0.49082	0.4896	1.71749
C257	C	-0.50268	0.47546	1.30835
C258	C	-0.52669	0.41237	1.00347
C259	C	-0.52653	0.39484	1.05777
C260	C	-0.522	0.35885	1.05839
C261	C	-0.51797	0.34054	1.00519
C262	C	-0.51833	0.35814	0.95119
C263	C	-0.52277	0.39407	0.95013
C264	C	-0.5688	0.28372	1.00371
C265	C	-0.56748	0.24769	1.00363
C266	C	-0.51279	0.23051	1.00568
C267	C	-0.45958	0.24923	1.00778
C268	C	-0.46134	0.28529	1.00777
C269	C	-0.51589	0.3025	1.00581
C270	C	-0.51312	0.33848	0.89477
C271	C	-0.52338	0.33978	1.1156
C272	C	-0.62658	0.3023	0.99996
C273	C	-0.40526	0.30551	1.01105
C274	C	-0.47792	0.43484	0.87854
C275	C	-0.47973	0.453	0.82578
C276	C	-0.52755	0.4491	0.78713
C277	C	-0.5732	0.42667	0.80188
C278	C	-0.57141	0.40847	0.85472
C279	C	-0.52385	0.41255	0.89336
C280	C	-0.4855	0.41352	1.15465
C281	C	-0.48923	0.43289	1.20611
C282	C	-0.53909	0.45322	1.21713
C283	C	-0.58513	0.45363	1.17632
C284	C	-0.58145	0.43422	1.12491

C285	C	-0.53149	0.4142	1.1136
C286	C	-0.66408	0.23068	1.04748
C287	C	-0.71595	0.2115	1.04628
C288	C	-0.72753	0.18938	0.99906
C289	C	-0.68682	0.18686	0.95317
C290	C	-0.63498	0.20609	0.9543
C291	C	-0.62319	0.22798	1.0016
C292	C	-0.38881	0.20977	1.0576
C293	C	-0.33634	0.19113	1.05824
C294	C	-0.29668	0.19339	1.011
C295	C	-0.31004	0.2148	0.96359
C296	C	-0.36261	0.23346	0.96291
C297	C	-0.40239	0.23093	1.00982
N298	N	-0.54295	0.47467	1.26799
N299	N	-0.24345	0.1737	1.00962
C300	C	-0.53101	0.45068	1.00238
C301	C	-0.5112	0.19213	1.00568
N302	N	0.22112	0.16818	0.99788
N303	N	-0.53123	0.46813	1.73348
C304	C	0.21877	0.95345	0.50671
N305	N	0.21286	0.9748	0.55749
N306	N	-0.49449	0.66579	1.29662
C307	C	0.2367	0.07168	0.79514
C308	C	0.13961	0.09076	0.84415
C309	C	0.08842	0.11053	0.84526
C310	C	0.07517	0.13234	0.79856
C311	C	0.11364	0.13427	0.75056
C312	C	0.16486	0.11444	0.74949
C313	C	0.17855	0.09208	0.79608
C314	C	0.29189	0.05466	0.88981
C315	C	0.2981	0.03471	0.9402
C316	C	0.25669	0.00951	0.95327
C317	C	0.20916	0.00408	0.91513
C318	C	0.20303	0.02407	0.86457
C319	C	0.24386	0.05011	0.85146
C320	C	0.2875	0.02445	0.73693
C321	C	0.29132	0.00166	0.6899
C322	C	0.24628	0.00009	0.64827
C323	C	0.19684	0.02123	0.65443
C324	C	0.19305	0.04404	0.70156
C325	C	0.2387	0.04641	0.74321
C326	C	0.32836	0.09752	0.74457
C327	C	0.37459	0.121	0.74273
C328	C	0.37987	0.14597	0.78646
C329	C	0.33796	0.14766	0.83124
C330	C	0.29171	0.12415	0.83304
C331	C	0.28669	0.09824	0.79034
C332	C	0.43029	0.16932	0.78786

C333	C	0.02091	0.15263	0.80113
C334	C	0.25292	-0.02296	0.59789
C335	C	0.23625	0.91206	1.29373
C336	C	0.23603	0.89474	1.34821
C337	C	0.24028	0.85876	1.34934
C338	C	0.24421	0.84021	1.29639
C339	C	0.24444	0.85759	1.24217
C340	C	0.24023	0.89354	1.2406
C341	C	0.1897	0.7846	1.29549
C342	C	0.18856	0.74858	1.29474
C343	C	0.24203	0.73014	1.29614
C344	C	0.29648	0.74762	1.29799
C345	C	0.29721	0.7837	1.29852
C346	C	0.24387	0.80215	1.29734
C347	C	0.24959	0.83764	1.18604
C348	C	0.23836	0.83996	1.40679
C349	C	0.13317	0.80449	1.29236
C350	C	0.35468	0.80258	1.3012
C351	C	0.28233	0.93508	1.16839
C352	C	0.27906	0.95306	1.11549
C353	C	0.23147	0.94786	1.077
C354	C	0.18761	0.92434	1.092
C355	C	0.19083	0.90636	1.14497
C356	C	0.2381	0.91172	1.18352
C357	C	0.27536	0.91469	1.44511
C358	C	0.26998	0.93415	1.49634
C359	C	0.21877	0.95345	1.50671
C360	C	0.17312	0.95277	1.46551
C361	C	0.17846	0.9333	1.41433
C362	C	0.22971	0.91429	1.40368
C363	C	0.09049	0.73308	1.3372
C364	C	0.03681	0.7157	1.3341
C365	C	0.02353	0.69537	1.28533
C366	C	0.0646	0.69263	1.23939
C367	C	0.11822	0.71003	1.24244
C368	C	0.13155	0.73025	1.29147
C369	C	0.3663	0.70703	1.34643
C370	C	0.41728	0.68702	1.34559
C371	C	0.45487	0.68765	1.29691
C372	C	0.4412	0.70892	1.24905
C373	C	0.3902	0.72897	1.2499
C374	C	0.35236	0.72801	1.29852
N375	N	-0.03097	0.67696	1.28435
N376	N	0.22594	0.96677	1.02339
N377	N	0.21286	0.9748	1.55749
C378	C	0.23166	0.95035	1.29227
C379	C	0.24098	0.69176	1.29544
C380	C	0.26371	0.98984	1.00757

C381	C	0.25292	0.97704	0.59789
C382	C	-0.25592	0.57157	1.25404
C383	C	-0.34929	0.59662	1.30242
C384	C	-0.39729	0.61896	1.30245
C385	C	-0.40734	0.6405	1.25436
C386	C	-0.36885	0.63956	1.20651
C387	C	-0.32081	0.61721	1.20655
C388	C	-0.3105	0.59505	1.25424
C389	C	-0.20347	0.55215	1.34885
C390	C	-0.20025	0.53219	1.39947
C391	C	-0.24554	0.50948	1.41318
C392	C	-0.29408	0.5066	1.37549
C393	C	-0.29725	0.52664	1.32469
C394	C	-0.25231	0.55016	1.31089
C395	C	-0.21233	0.52156	1.19699
C396	C	-0.21168	0.49842	1.15033
C397	C	-0.25675	0.49876	1.10867
C398	C	-0.30315	0.52213	1.11449
C399	C	-0.30376	0.54531	1.16125
C400	C	-0.25786	0.5458	1.20282
C401	C	-0.16168	0.59259	1.20162
C402	C	-0.11164	0.61328	1.19909
C403	C	-0.10085	0.63724	1.2432
C404	C	-0.14133	0.64108	1.28914
C405	C	-0.19149	0.62046	1.2915
C406	C	-0.20187	0.59527	1.2485
C407	C	-0.04574	0.65669	1.24179
C408	C	-0.45793	0.66386	1.25296
C409	C	-0.24102	0.4896	1.4675
C410	C	-0.25289	0.47546	1.05836
C411	C	-0.2769	0.41237	0.75349
C412	C	-0.27674	0.39484	0.80778
C413	C	-0.27221	0.35885	0.8084
C414	C	-0.26817	0.34054	0.7552
C415	C	-0.26854	0.35814	0.7012
C416	C	-0.27298	0.39407	0.70014
C417	C	-0.31901	0.28372	0.75372
C418	C	-0.31769	0.24769	0.75364
C419	C	-0.26299	0.23051	0.7557
C420	C	-0.20978	0.24923	0.75779
C421	C	-0.21155	0.28529	0.75778
C422	C	-0.26609	0.3025	0.75583
C423	C	-0.26333	0.33848	0.64478
C424	C	-0.27359	0.33978	0.86561
C425	C	-0.37679	0.3023	0.74997
C426	C	-0.15547	0.30551	0.76106
C427	C	-0.22813	0.43484	0.62855
C428	C	-0.22994	0.453	0.5758

C429	C	-0.27776	0.4491	0.53714
C430	C	-0.3234	0.42667	0.55189
C431	C	-0.32162	0.40847	0.60473
C432	C	-0.27405	0.41255	0.64337
C433	C	-0.23571	0.41352	0.90467
C434	C	-0.23944	0.43289	0.95612
C435	C	-0.2893	0.45322	0.96714
C436	C	-0.33533	0.45363	0.92634
C437	C	-0.33165	0.43422	0.87493
C438	C	-0.28169	0.4142	0.86361
C439	C	-0.41428	0.23068	0.7975
C440	C	-0.46615	0.2115	0.79629
C441	C	-0.47773	0.18938	0.74907
C442	C	-0.43702	0.18686	0.70318
C443	C	-0.38518	0.20609	0.70431
C444	C	-0.3734	0.22798	0.75161
C445	C	-0.13901	0.20977	0.80762
C446	C	-0.08655	0.19113	0.80826
C447	C	-0.04689	0.19339	0.76101
C448	C	-0.06025	0.2148	0.7136
C449	C	-0.11282	0.23346	0.71293
C450	C	-0.15259	0.23093	0.75983
N451	N	-0.29316	0.47467	1.01801
N452	N	0.00635	0.1737	0.75963
C453	C	-0.28121	0.45068	0.7524
C454	C	-0.2614	0.19213	0.75569
N455	N	0.47091	0.16818	0.74789
N456	N	-0.28144	0.46813	1.48349
C457	C	0.46857	0.95345	0.25672
N458	N	0.46265	0.9748	0.30751
N459	N	-0.2447	0.66579	1.04663
C460	C	0.4865	0.07168	0.54515
C461	C	0.3894	0.09076	0.59416
C462	C	0.33821	0.11053	0.59527
C463	C	0.32497	0.13234	0.54857
C464	C	0.36343	0.13427	0.50058
C465	C	0.41466	0.11444	0.4995
C466	C	0.42834	0.09208	0.54609
C467	C	0.54169	0.05466	0.63982
C468	C	0.54789	0.03471	0.69021
C469	C	0.50648	0.00951	0.70328
C470	C	0.45896	0.00408	0.66514
C471	C	0.45283	0.02407	0.61458
C472	C	0.49366	0.05011	0.60147
C473	C	0.53729	0.02445	0.48694
C474	C	0.54111	0.00166	0.43991
C475	C	0.49607	0.00009	0.39828
C476	C	0.44663	0.02123	0.40444

C477	C	0.44284	0.04404	0.45157
C478	C	0.4885	0.04641	0.49322
C479	C	0.57815	0.09752	0.49458
C480	C	0.62438	0.121	0.49274
C481	C	0.62966	0.14597	0.53647
C482	C	0.58775	0.14766	0.58126
C483	C	0.5415	0.12415	0.58306
C484	C	0.53648	0.09824	0.54035
C485	C	0.68009	0.16932	0.53787
C486	C	0.2707	0.15263	0.55114
C487	C	0.50272	-0.02296	0.34791
C488	C	0.48604	0.91206	1.04374
C489	C	0.48582	0.89474	1.09823
C490	C	0.49008	0.85876	1.09935
C491	C	0.494	0.84021	1.0464
C492	C	0.49423	0.85759	0.99218
C493	C	0.49003	0.89354	0.99061
C494	C	0.43949	0.7846	1.0455
C495	C	0.43835	0.74858	1.04475
C496	C	0.49183	0.73014	1.04615
C497	C	0.54627	0.74762	1.04801
C498	C	0.547	0.7837	1.04853
C499	C	0.49366	0.80215	1.04735
C500	C	0.49939	0.83764	0.93606
C501	C	0.48816	0.83996	1.15681
C502	C	0.38297	0.80449	1.04238
C503	C	0.60447	0.80258	1.05122
C504	C	0.53212	0.93508	0.9184
C505	C	0.52885	0.95306	0.8655
C506	C	0.48126	0.94786	0.82701
C507	C	0.4374	0.92434	0.84202
C508	C	0.44062	0.90636	0.89498
C509	C	0.48789	0.91172	0.93353
C510	C	0.52515	0.91469	1.19512
C511	C	0.51977	0.93415	1.24635
C512	C	0.46857	0.95345	1.25672
C513	C	0.42291	0.95277	1.21552
C514	C	0.42826	0.9333	1.16434
C515	C	0.4795	0.91429	1.15369
C516	C	0.34029	0.73308	1.08721
C517	C	0.2866	0.7157	1.08411
C518	C	0.27332	0.69537	1.03534
C519	C	0.3144	0.69263	0.98941
C520	C	0.36802	0.71003	0.99246
C521	C	0.38134	0.73025	1.04148
C522	C	0.61609	0.70703	1.09644
C523	C	0.66708	0.68702	1.0956
C524	C	0.70466	0.68765	1.04692

C525	C	0.69099	0.70892	0.99907
C526	C	0.64	0.72897	0.99991
C527	C	0.60215	0.72801	1.04853
N528	N	0.21883	0.67696	1.03436
N529	N	0.47574	0.96677	0.77341
N530	N	0.46265	0.9748	1.30751
C531	C	0.48145	0.95035	1.04228
C532	C	0.49078	0.69176	1.04545
C533	C	0.5135	0.98984	0.75758
C534	C	0.50272	0.97704	0.34791
C535	C	-0.00613	0.57157	1.00405
C536	C	-0.09949	0.59662	1.05243
C537	C	-0.1475	0.61896	1.05246
C538	C	-0.15755	0.6405	1.00437
C539	C	-0.11906	0.63956	0.95652
C540	C	-0.07102	0.61721	0.95656
C541	C	-0.0607	0.59505	1.00425
C542	C	0.04632	0.55215	1.09886
C543	C	0.04955	0.53219	1.14949
C544	C	0.00426	0.50948	1.16319
C545	C	-0.04429	0.5066	1.1255
C546	C	-0.04745	0.52664	1.0747
C547	C	-0.00251	0.55016	1.0609
C548	C	0.03746	0.52156	0.947
C549	C	0.03812	0.49842	0.90035
C550	C	-0.00696	0.49876	0.85868
C551	C	-0.05336	0.52213	0.8645
C552	C	-0.05397	0.54531	0.91126
C553	C	-0.00806	0.5458	0.95284
C554	C	0.08812	0.59259	0.95163
C555	C	0.13816	0.61328	0.9491
C556	C	0.14894	0.63724	0.99321
C557	C	0.10846	0.64108	1.03915
C558	C	0.0583	0.62046	1.04151
C559	C	0.04793	0.59527	0.99851
C560	C	0.20405	0.65669	0.9918
C561	C	-0.20814	0.66386	1.00297
C562	C	0.00877	0.4896	1.21751
C563	C	-0.0031	0.47546	0.80838
C564	C	-0.0271	0.41237	0.5035
C565	C	-0.02695	0.39484	0.55779
C566	C	-0.02241	0.35885	0.55842
C567	C	-0.01838	0.34054	0.50522
C568	C	-0.01874	0.35814	0.45121
C569	C	-0.02318	0.39407	0.45016
C570	C	-0.06922	0.28372	0.50374
C571	C	-0.06789	0.24769	0.50365
C572	C	-0.0132	0.23051	0.50571

C573	C	0.04001	0.24923	0.50781
C574	C	0.03824	0.28529	0.5078
C575	C	-0.0163	0.3025	0.50584
C576	C	-0.01354	0.33848	0.3948
C577	C	-0.0238	0.33978	0.61562
C578	C	-0.127	0.3023	0.49999
C579	C	0.09432	0.30551	0.51107
C580	C	0.02166	0.43484	0.37856
C581	C	0.01986	0.453	0.32581
C582	C	-0.02797	0.4491	0.28715
C583	C	-0.07361	0.42667	0.30191
C584	C	-0.07182	0.40847	0.35474
C585	C	-0.02426	0.41255	0.39338
C586	C	0.01409	0.41352	0.65468
C587	C	0.01035	0.43289	0.70613
C588	C	-0.0395	0.45322	0.71715
C589	C	-0.08554	0.45363	0.67635
C590	C	-0.08186	0.43422	0.62494
C591	C	-0.0319	0.4142	0.61363
C592	C	-0.16449	0.23068	0.54751
C593	C	-0.21636	0.2115	0.5463
C594	C	-0.22794	0.18938	0.49908
C595	C	-0.18723	0.18686	0.45319
C596	C	-0.13539	0.20609	0.45433
C597	C	-0.12361	0.22798	0.50162
C598	C	0.11078	0.20977	0.55763
C599	C	0.16324	0.19113	0.55827
C600	C	0.2029	0.19339	0.51102
C601	C	0.18955	0.2148	0.46362
C602	C	0.13698	0.23346	0.46294
C603	C	0.0972	0.23093	0.50984
N604	N	-0.04336	0.47467	0.76802
N605	N	0.25614	0.1737	0.50964
C606	C	-0.03142	0.45068	0.50241
C607	C	-0.01161	0.19213	0.5057
N608	N	0.7207	0.16818	0.4979
N609	N	-0.03165	0.46813	1.23351

Table S7. Atomistic coordinates for the refined unit cell parameters for BMTA-TFPM-COF with 5-fold interpenetrated dia topology via Pawley refinement.

	Atom	*x/a*	*y/b*	*z/c*
C1	C	0.24367	-0.42843	0.75406
C2	C	0.1503	-0.40338	0.80245
C3	C	0.1023	-0.38104	0.80247
C4	C	0.09225	-0.3595	0.75438
C5	C	0.13073	-0.36044	0.70653
C6	C	0.17878	-0.38279	0.70658
C7	C	0.18909	-0.40495	0.75426
C8	C	0.29612	-0.44785	0.84887
C9	C	0.29934	-0.46781	0.8995
C10	C	0.25405	-0.49052	0.9132
C11	C	0.20551	-0.4934	0.87551
C12	C	0.20234	-0.47336	0.82472
C13	C	0.24728	-0.44984	0.81091
C14	C	0.28726	-0.47844	0.69702
C15	C	0.28791	-0.50158	0.65036
C16	C	0.24284	-0.50124	0.60869
C17	C	0.19644	-0.47787	0.61451
C18	C	0.19583	-0.45469	0.66127
C19	C	0.24173	-0.4542	0.70285
C20	C	0.33791	-0.40741	0.70164
C21	C	0.38795	-0.38672	0.69912
C22	C	0.39874	-0.36276	0.74322
C23	C	0.35826	-0.35892	0.78916
C24	C	0.3081	-0.37954	0.79153
C25	C	0.29772	-0.40473	0.74852
C26	C	0.45385	-0.34331	0.74181
C27	C	0.04165	-0.33614	0.75299
C28	C	0.25856	-0.5104	0.96752
C29	C	0.2467	-0.52454	0.55839
C30	C	0.22269	-0.58763	0.25351
C31	C	0.22285	-0.60516	0.3078
C32	C	0.22738	-0.64115	0.30843
C33	C	0.23142	-0.65946	0.25523
C34	C	0.23105	-0.64186	0.20122
C35	C	0.22661	-0.60593	0.20017
C36	C	0.18058	-0.71628	0.25375
C37	C	0.1819	-0.75231	0.25367
C38	C	0.2366	-0.76949	0.25572
C39	C	0.2898	-0.75077	0.25782
C40	C	0.28804	-0.71471	0.25781
C41	C	0.23349	-0.6975	0.25585
C42	C	0.23626	-0.66152	0.14481
C43	C	0.226	-0.66022	0.36563
C44	C	0.1228	-0.6977	0.25

C45	C	0.34412	-0.69449	0.26108
C46	C	0.27146	-0.56516	0.12857
C47	C	0.26965	-0.547	0.07582
C48	C	0.22183	-0.5509	0.03716
C49	C	0.17619	-0.57333	0.05192
C50	C	0.17797	-0.59153	0.10475
C51	C	0.22554	-0.58745	0.1434
C52	C	0.26388	-0.58648	0.40469
C53	C	0.26015	-0.56711	0.45615
C54	C	0.21029	-0.54678	0.46717
C55	C	0.16426	-0.54637	0.42636
C56	C	0.16794	-0.56578	0.37495
C57	C	0.21789	-0.5858	0.36364
C58	C	0.08531	-0.76932	0.29752
C59	C	0.03343	-0.7885	0.29631
C60	C	0.02185	-0.81062	0.24909
C61	C	0.06256	-0.81314	0.2032
C62	C	0.1144	-0.79391	0.20434
C63	C	0.12619	-0.77202	0.25163
C64	C	0.36057	-0.79023	0.30764
C65	C	0.41304	-0.80887	0.30828
C66	C	0.4527	-0.80661	0.26104
C67	C	0.43934	-0.7852	0.21363
C68	C	0.38677	-0.76654	0.21295
C69	C	0.34699	-0.76907	0.25986
N70	N	-0.0295	-0.83182	0.24791
N71	N	0.21815	-0.53187	-0.01648
N72	N	0.20643	-0.52533	0.51803
N73	N	0.50594	-0.8263	0.25965
C74	C	0.21838	-0.54932	0.25242
C75	C	0.23818	-0.80787	0.25572
C76	C	0.73629	-0.92832	1.29517
C77	C	0.6392	-0.90924	1.34417
C78	C	0.58801	-0.88947	1.34528
C79	C	0.57476	-0.86766	1.29858
C80	C	0.61322	-0.86573	1.25059
C81	C	0.66445	-0.88556	1.24951
C82	C	0.67813	-0.90792	1.2961
C83	C	0.79148	-0.94534	1.38983
C84	C	0.79769	-0.96529	1.44022
C85	C	0.75627	-0.99049	1.45329
C86	C	0.70875	-0.99592	1.41515
C87	C	0.70262	-0.97593	1.3646
C88	C	0.74345	-0.94989	1.35149
C89	C	0.78709	-0.97555	1.23695
C90	C	0.79091	-0.99834	1.18992
C91	C	0.74587	-0.99991	1.14829
C92	C	0.69643	-0.97877	1.15446

C93	C	0.69264	-0.95596	1.20158
C94	C	0.73829	-0.95359	1.24323
C95	C	0.82794	-0.90248	1.24459
C96	C	0.87418	-0.879	1.24275
C97	C	0.87946	-0.85403	1.28648
C98	C	0.83755	-0.85234	1.33127
C99	C	0.79129	-0.87585	1.33307
C100	C	0.78628	-0.90176	1.29036
C101	C	0.92988	-0.83068	1.28789
C102	C	0.5205	-0.84737	1.30115
C103	C	0.7633	-1.01016	1.50759
C104	C	0.75251	-1.02296	1.09792
C105	C	0.73583	-0.08794	1.79375
C106	C	0.73562	-0.10526	1.84824
C107	C	0.73987	-0.14124	1.84937
C108	C	0.7438	-0.15979	1.79641
C109	C	0.74403	-0.14241	1.74219
C110	C	0.73982	-0.10646	1.74063
C111	C	0.68928	-0.2154	1.79551
C112	C	0.68815	-0.25142	1.79477
C113	C	0.74162	-0.26986	1.79616
C114	C	0.79607	-0.25238	1.79802
C115	C	0.7968	-0.2163	1.79854
C116	C	0.74346	-0.19785	1.79737
C117	C	0.74918	-0.16236	1.68607
C118	C	0.73795	-0.16004	1.90682
C119	C	0.63276	-0.19551	1.79239
C120	C	0.85427	-0.19742	1.80123
C121	C	0.78191	-0.06492	1.66841
C122	C	0.77865	-0.04694	1.61551
C123	C	0.73105	-0.05214	1.57702
C124	C	0.68719	-0.07566	1.59203
C125	C	0.69042	-0.09364	1.64499
C126	C	0.73769	-0.08828	1.68354
C127	C	0.77495	-0.08531	1.94513
C128	C	0.76957	-0.06585	1.99636
C129	C	0.71836	-0.04655	2.00674
C130	C	0.67271	-0.04723	1.96553
C131	C	0.67805	-0.0667	1.91436
C132	C	0.72929	-0.08571	1.9037
C133	C	0.59008	-0.26692	1.83722
C134	C	0.53639	-0.2843	1.83412
C135	C	0.52311	-0.30463	1.78536
C136	C	0.56419	-0.30737	1.73942
C137	C	0.61781	-0.28997	1.74247
C138	C	0.63114	-0.26975	1.79149
C139	C	0.86588	-0.29297	1.84646
C140	C	0.91687	-0.31298	1.84561

C141	C	0.95446	-0.31235	1.79694
C142	C	0.94079	-0.29108	1.74908
C143	C	0.88979	-0.27103	1.74992
C144	C	0.85195	-0.27199	1.79854
N145	N	0.46862	-0.32304	1.78438
N146	N	0.72553	-0.03323	1.52342
N147	N	0.71245	-0.0252	2.05752
N148	N	1.00509	-0.33421	1.79664
C149	C	0.73124	-0.04965	1.79229
C150	C	0.74057	-0.30824	1.79547
C151	C	0.51835	0.95345	0.20708
N152	N	0.51244	0.9748	0.25786
N153	N	-0.19492	0.66579	0.99699
C154	C	0.53628	0.07168	0.49551
C155	C	0.43918	0.09076	0.54452
C156	C	0.38799	0.11053	0.54562
C157	C	0.37475	0.13234	0.49893
C158	C	0.41321	0.13427	0.45093
C159	C	0.46444	0.11444	0.44985
C160	C	0.47812	0.09208	0.49644
C161	C	0.59147	0.05466	0.59018
C162	C	0.59768	0.03471	0.64057
C163	C	0.55626	0.00951	0.65364
C164	C	0.50874	0.00408	0.6155
C165	C	0.50261	0.02407	0.56494
C166	C	0.54344	0.05011	0.55183
C167	C	0.58708	0.02445	0.43729
C168	C	0.5909	0.00166	0.39026
C169	C	0.54585	0.00009	0.34863
C170	C	0.49642	0.02123	0.3548
C171	C	0.49263	0.04404	0.40192
C172	C	0.53828	0.04641	0.44357
C173	C	0.62793	0.09752	0.44494
C174	C	0.67417	0.121	0.44309
C175	C	0.67944	0.14597	0.48683
C176	C	0.63754	0.14766	0.53161
C177	C	0.59128	0.12415	0.53341
C178	C	0.58626	0.09824	0.4907
C179	C	0.72987	0.16932	0.48823
C180	C	0.32048	0.15263	0.5015
C181	C	0.5525	-0.02296	0.29826
C182	C	0.53582	0.91206	0.99409
C183	C	0.5356	0.89474	1.04858
C184	C	0.53986	0.85876	1.04971
C185	C	0.54378	0.84021	0.99676
C186	C	0.54402	0.85759	0.94254
C187	C	0.53981	0.89354	0.94097
C188	C	0.48927	0.7846	0.99585

C189	C	0.48814	0.74858	0.99511
C190	C	0.54161	0.73014	0.99651
C191	C	0.59606	0.74762	0.99836
C192	C	0.59679	0.7837	0.99888
C193	C	0.54345	0.80215	0.99771
C194	C	0.54917	0.83764	0.88641
C195	C	0.53794	0.83996	1.10716
C196	C	0.43275	0.80449	0.99273
C197	C	0.65426	0.80258	1.00157
C198	C	0.5819	0.93508	0.86875
C199	C	0.57863	0.95306	0.81585
C200	C	0.53104	0.94786	0.77736
C201	C	0.48718	0.92434	0.79237
C202	C	0.4904	0.90636	0.84534
C203	C	0.53768	0.91172	0.88389
C204	C	0.57494	0.91469	1.14548
C205	C	0.56956	0.93415	1.19671
C206	C	0.51835	0.95345	1.20708
C207	C	0.47269	0.95277	1.16587
C208	C	0.47804	0.9333	1.1147
C209	C	0.52928	0.91429	1.10405
C210	C	0.39007	0.73308	1.03756
C211	C	0.33638	0.7157	1.03446
C212	C	0.3231	0.69537	0.9857
C213	C	0.36418	0.69263	0.93976
C214	C	0.4178	0.71003	0.94281
C215	C	0.43113	0.73025	0.99183
C216	C	0.66587	0.70703	1.0468
C217	C	0.71686	0.68702	1.04595
C218	C	0.75445	0.68765	0.99728
C219	C	0.74078	0.70892	0.94942
C220	C	0.68978	0.72897	0.95026
C221	C	0.65193	0.72801	0.99889
N222	N	0.26861	0.67696	0.98472
N223	N	0.52552	0.96677	0.72376
N224	N	0.51244	0.9748	1.25786
C225	C	0.53123	0.95035	0.99263
C226	C	0.54056	0.69176	0.99581
C227	C	0.56328	0.98984	0.70794
C228	C	0.5525	0.97704	0.29826
C229	C	0.04366	0.57157	0.9544
C230	C	-0.04971	0.59662	1.00279
C231	C	-0.09771	0.61896	1.00281
C232	C	-0.10777	0.6405	0.95472
C233	C	-0.06928	0.63956	0.90687
C234	C	-0.02124	0.61721	0.90692
C235	C	-0.01092	0.59505	0.95461
C236	C	0.09611	0.55215	1.04921

C237	C	0.09933	0.53219	1.09984
C238	C	0.05404	0.50948	1.11354
C239	C	0.0055	0.5066	1.07586
C240	C	0.00233	0.52664	1.02506
C241	C	0.04727	0.55016	1.01126
C242	C	0.08725	0.52156	0.89736
C243	C	0.0879	0.49842	0.8507
C244	C	0.04283	0.49876	0.80903
C245	C	-0.00358	0.52213	0.81486
C246	C	-0.00418	0.54531	0.86161
C247	C	0.04172	0.5458	0.90319
C248	C	0.1379	0.59259	0.90198
C249	C	0.18794	0.61328	0.89946
C250	C	0.19872	0.63724	0.94356
C251	C	0.15825	0.64108	0.9895
C252	C	0.10808	0.62046	0.99187
C253	C	0.09771	0.59527	0.94887
C254	C	0.25383	0.65669	0.94215
C255	C	-0.15836	0.66386	0.95333
C256	C	0.05855	0.4896	1.16787
C257	C	0.04669	0.47546	0.75873
C258	C	0.02268	0.41237	0.45385
C259	C	0.02284	0.39484	0.50814
C260	C	0.02737	0.35885	0.50877
C261	C	0.0314	0.34054	0.45557
C262	C	0.03104	0.35814	0.40157
C263	C	0.0266	0.39407	0.40051
C264	C	-0.01943	0.28372	0.45409
C265	C	-0.01811	0.24769	0.45401
C266	C	0.03659	0.23051	0.45606
C267	C	0.08979	0.24923	0.45816
C268	C	0.08803	0.28529	0.45815
C269	C	0.03348	0.3025	0.45619
C270	C	0.03625	0.33848	0.34515
C271	C	0.02599	0.33978	0.56598
C272	C	-0.07721	0.3023	0.45034
C273	C	0.14411	0.30551	0.46142
C274	C	0.07145	0.43484	0.32891
C275	C	0.06964	0.453	0.27616
C276	C	0.02182	0.4491	0.23751
C277	C	-0.02383	0.42667	0.25226
C278	C	-0.02204	0.40847	0.3051
C279	C	0.02552	0.41255	0.34374
C280	C	0.06387	0.41352	0.60503
C281	C	0.06014	0.43289	0.65649
C282	C	0.01028	0.45322	0.66751
C283	C	-0.03576	0.45363	0.6267
C284	C	-0.03208	0.43422	0.57529

C285	C	0.01788	0.4142	0.56398
C286	C	-0.11471	0.23068	0.49786
C287	C	-0.16658	0.2115	0.49666
C288	C	-0.17816	0.18938	0.44943
C289	C	-0.13745	0.18686	0.40354
C290	C	-0.08561	0.20609	0.40468
C291	C	-0.07382	0.22798	0.45198
C292	C	0.16056	0.20977	0.50798
C293	C	0.21303	0.19113	0.50862
C294	C	0.25269	0.19339	0.46138
C295	C	0.23933	0.2148	0.41397
C296	C	0.18676	0.23346	0.41329
C297	C	0.14698	0.23093	0.4602
N298	N	0.00642	0.47467	0.71837
N299	N	0.30592	0.1737	0.45999
C300	C	0.01836	0.45068	0.45276
C301	C	0.03817	0.19213	0.45606
N302	N	0.77049	0.16818	0.44825
N303	N	0.01814	0.46813	1.18386
C304	C	0.31834	0.95345	0.40742
N305	N	0.31243	0.9748	0.4582
N306	N	-0.39493	0.66579	1.19733
C307	C	0.33627	0.07168	0.69585
C308	C	0.23917	0.09076	0.74486
C309	C	0.18798	0.11053	0.74596
C310	C	0.17474	0.13234	0.69927
C311	C	0.2132	0.13427	0.65127
C312	C	0.26443	0.11444	0.6502
C313	C	0.27811	0.09208	0.69678
C314	C	0.39146	0.05466	0.79052
C315	C	0.39767	0.03471	0.84091
C316	C	0.35625	0.00951	0.85398
C317	C	0.30873	0.00408	0.81584
C318	C	0.3026	0.02407	0.76528
C319	C	0.34343	0.05011	0.75217
C320	C	0.38706	0.02445	0.63763
C321	C	0.39089	0.00166	0.59061
C322	C	0.34584	0.00009	0.54898
C323	C	0.29641	0.02123	0.55514
C324	C	0.29262	0.04404	0.60226
C325	C	0.33827	0.04641	0.64391
C326	C	0.42792	0.09752	0.64528
C327	C	0.47415	0.121	0.64343
C328	C	0.47943	0.14597	0.68717
C329	C	0.43753	0.14766	0.73195
C330	C	0.39127	0.12415	0.73375
C331	C	0.38625	0.09824	0.69105
C332	C	0.52986	0.16932	0.68857

C333	C	0.12047	0.15263	0.70184
C334	C	0.35249	-0.02296	0.4986
C335	C	0.33581	0.91206	1.19444
C336	C	0.33559	0.89474	1.24892
C337	C	0.33985	0.85876	1.25005
C338	C	0.34377	0.84021	1.1971
C339	C	0.34401	0.85759	1.14288
C340	C	0.3398	0.89354	1.14131
C341	C	0.28926	0.7846	1.19619
C342	C	0.28813	0.74858	1.19545
C343	C	0.3416	0.73014	1.19685
C344	C	0.39605	0.74762	1.1987
C345	C	0.39677	0.7837	1.19923
C346	C	0.34343	0.80215	1.19805
C347	C	0.34916	0.83764	1.08675
C348	C	0.33793	0.83996	1.3075
C349	C	0.23274	0.80449	1.19307
C350	C	0.45424	0.80258	1.20191
C351	C	0.38189	0.93508	1.0691
C352	C	0.37862	0.95306	1.0162
C353	C	0.33103	0.94786	0.9777
C354	C	0.28717	0.92434	0.99271
C355	C	0.29039	0.90636	1.04568
C356	C	0.33766	0.91172	1.08423
C357	C	0.37493	0.91469	1.34582
C358	C	0.36954	0.93415	1.39705
C359	C	0.31834	0.95345	1.40742
C360	C	0.27268	0.95277	1.36622
C361	C	0.27803	0.9333	1.31504
C362	C	0.32927	0.91429	1.30439
C363	C	0.19006	0.73308	1.23791
C364	C	0.13637	0.7157	1.23481
C365	C	0.12309	0.69537	1.18604
C366	C	0.16417	0.69263	1.1401
C367	C	0.21779	0.71003	1.14315
C368	C	0.23111	0.73025	1.19218
C369	C	0.46586	0.70703	1.24714
C370	C	0.51685	0.68702	1.24629
C371	C	0.55443	0.68765	1.19762
C372	C	0.54077	0.70892	1.14976
C373	C	0.48977	0.72897	1.15061
C374	C	0.45192	0.72801	1.19923
N375	N	0.0686	0.67696	1.18506
N376	N	0.32551	0.96677	0.9241
N377	N	0.31243	0.9748	1.4582
C378	C	0.33122	0.95035	1.19297
C379	C	0.34055	0.69176	1.19615
C380	C	0.36327	0.98984	0.90828

C381	C	0.35249	0.97704	0.4986
C382	C	-0.15636	0.57157	1.15474
C383	C	-0.24972	0.59662	1.20313
C384	C	-0.29772	0.61896	1.20315
C385	C	-0.30778	0.6405	1.15506
C386	C	-0.26929	0.63956	1.10722
C387	C	-0.22125	0.61721	1.10726
C388	C	-0.21093	0.59505	1.15495
C389	C	-0.1039	0.55215	1.24955
C390	C	-0.10068	0.53219	1.30018
C391	C	-0.14597	0.50948	1.31388
C392	C	-0.19451	0.5066	1.2762
C393	C	-0.19768	0.52664	1.2254
C394	C	-0.15274	0.55016	1.2116
C395	C	-0.11276	0.52156	1.0977
C396	C	-0.11211	0.49842	1.05104
C397	C	-0.15719	0.49876	1.00937
C398	C	-0.20359	0.52213	1.0152
C399	C	-0.20419	0.54531	1.06196
C400	C	-0.15829	0.5458	1.10353
C401	C	-0.06211	0.59259	1.10232
C402	C	-0.01207	0.61328	1.0998
C403	C	-0.00129	0.63724	1.14391
C404	C	-0.04177	0.64108	1.18984
C405	C	-0.09193	0.62046	1.19221
C406	C	-0.1023	0.59527	1.14921
C407	C	0.05382	0.65669	1.14249
C408	C	-0.35837	0.66386	1.15367
C409	C	-0.14146	0.4896	1.36821
C410	C	-0.15332	0.47546	0.95907
C411	C	-0.17733	0.41237	0.65419
C412	C	-0.17717	0.39484	0.70849
C413	C	-0.17264	0.35885	0.70911
C414	C	-0.16861	0.34054	0.65591
C415	C	-0.16897	0.35814	0.60191
C416	C	-0.17341	0.39407	0.60085
C417	C	-0.21944	0.28372	0.65443
C418	C	-0.21812	0.24769	0.65435
C419	C	-0.16343	0.23051	0.6564
C420	C	-0.11022	0.24923	0.6585
C421	C	-0.11199	0.28529	0.65849
C422	C	-0.16653	0.3025	0.65653
C423	C	-0.16377	0.33848	0.54549
C424	C	-0.17402	0.33978	0.76632
C425	C	-0.27723	0.3023	0.65068
C426	C	-0.05591	0.30551	0.66177
C427	C	-0.12857	0.43484	0.52926
C428	C	-0.13037	0.453	0.4765

C429	C	-0.1782	0.4491	0.43785
C430	C	-0.22384	0.42667	0.4526
C431	C	-0.22205	0.40847	0.50544
C432	C	-0.17449	0.41255	0.54408
C433	C	-0.13614	0.41352	0.80537
C434	C	-0.13987	0.43289	0.85683
C435	C	-0.18973	0.45322	0.86785
C436	C	-0.23577	0.45363	0.82704
C437	C	-0.23209	0.43422	0.77563
C438	C	-0.18213	0.4142	0.76432
C439	C	-0.31472	0.23068	0.6982
C440	C	-0.36659	0.2115	0.697
C441	C	-0.37817	0.18938	0.64977
C442	C	-0.33746	0.18686	0.60388
C443	C	-0.28562	0.20609	0.60502
C444	C	-0.27383	0.22798	0.65232
C445	C	-0.03945	0.20977	0.70832
C446	C	0.01301	0.19113	0.70896
C447	C	0.05268	0.19339	0.66172
C448	C	0.03932	0.2148	0.61431
C449	C	-0.01325	0.23346	0.61363
C450	C	-0.05303	0.23093	0.66054
N451	N	-0.19359	0.47467	0.91871
N452	N	0.10591	0.1737	0.66034
C453	C	-0.18165	0.45068	0.6531
C454	C	-0.16184	0.19213	0.6564
N455	N	0.57048	0.16818	0.6486
N456	N	-0.18187	0.46813	1.3842
C457	C	0.11833	0.95345	0.60776
N458	N	0.11241	0.9748	0.65854
N459	N	-0.59494	0.66579	1.39767
C460	C	0.13626	0.07168	0.89619
C461	C	0.03916	0.09076	0.9452
C462	C	-0.01203	0.11053	0.94631
C463	C	-0.02527	0.13234	0.89961
C464	C	0.01319	0.13427	0.85161
C465	C	0.06442	0.11444	0.85054
C466	C	0.0781	0.09208	0.89712
C467	C	0.19145	0.05466	0.99086
C468	C	0.19765	0.03471	1.04125
C469	C	0.15624	0.00951	1.05432
C470	C	0.10872	0.00408	1.01618
C471	C	0.10259	0.02407	0.96562
C472	C	0.14342	0.05011	0.95251
C473	C	0.18705	0.02445	0.83798
C474	C	0.19087	0.00166	0.79095
C475	C	0.14583	0.00009	0.74932
C476	C	0.09639	0.02123	0.75548

C477	C	0.0926	0.04404	0.80261
C478	C	0.13826	0.04641	0.84426
C479	C	0.22791	0.09752	0.84562
C480	C	0.27414	0.121	0.84378
C481	C	0.27942	0.14597	0.88751
C482	C	0.23751	0.14766	0.93229
C483	C	0.19126	0.12415	0.93409
C484	C	0.18624	0.09824	0.89139
C485	C	0.32985	0.16932	0.88891
C486	C	-0.07954	0.15263	0.90218
C487	C	0.15248	-0.02296	0.69894
C488	C	0.1358	0.91206	1.39478
C489	C	0.13558	0.89474	1.44926
C490	C	0.13984	0.85876	1.45039
C491	C	0.14376	0.84021	1.39744
C492	C	0.14399	0.85759	1.34322
C493	C	0.13979	0.89354	1.34165
C494	C	0.08925	0.7846	1.39654
C495	C	0.08811	0.74858	1.39579
C496	C	0.14159	0.73014	1.39719
C497	C	0.19603	0.74762	1.39904
C498	C	0.19676	0.7837	1.39957
C499	C	0.14342	0.80215	1.39839
C500	C	0.14915	0.83764	1.28709
C501	C	0.13792	0.83996	1.50784
C502	C	0.03273	0.80449	1.39341
C503	C	0.25423	0.80258	1.40225
C504	C	0.18188	0.93508	1.26944
C505	C	0.17861	0.95306	1.21654
C506	C	0.13102	0.94786	1.17805
C507	C	0.08716	0.92434	1.19305
C508	C	0.09038	0.90636	1.24602
C509	C	0.13765	0.91172	1.28457
C510	C	0.17491	0.91469	1.54616
C511	C	0.16953	0.93415	1.59739
C512	C	0.11833	0.95345	1.60776
C513	C	0.07267	0.95277	1.56656
C514	C	0.07802	0.9333	1.51538
C515	C	0.12926	0.91429	1.50473
C516	C	-0.00995	0.73308	1.43825
C517	C	-0.06364	0.7157	1.43515
C518	C	-0.07692	0.69537	1.38638
C519	C	-0.03584	0.69263	1.34044
C520	C	0.01778	0.71003	1.34349
C521	C	0.0311	0.73025	1.39252
C522	C	0.26585	0.70703	1.44748
C523	C	0.31684	0.68702	1.44664
C524	C	0.35442	0.68765	1.39796

C525	C	0.34075	0.70892	1.3501
C526	C	0.28976	0.72897	1.35095
C527	C	0.25191	0.72801	1.39957
N528	N	-0.13141	0.67696	1.3854
N529	N	0.1255	0.96677	1.12444
N530	N	0.11241	0.9748	1.65854
C531	C	0.13121	0.95035	1.39332
C532	C	0.14054	0.69176	1.39649
C533	C	0.16326	0.98984	1.10862
C534	C	0.15248	0.97704	0.69894
C535	C	-0.35637	0.57157	1.35509
C536	C	-0.44973	0.59662	1.40347
C537	C	-0.49774	0.61896	1.4035
C538	C	-0.50779	0.6405	1.35541
C539	C	-0.4693	0.63956	1.30756
C540	C	-0.42126	0.61721	1.3076
C541	C	-0.41094	0.59505	1.35529
C542	C	-0.30392	0.55215	1.4499
C543	C	-0.30069	0.53219	1.50052
C544	C	-0.34598	0.50948	1.51423
C545	C	-0.39453	0.5066	1.47654
C546	C	-0.39769	0.52664	1.42574
C547	C	-0.35275	0.55016	1.41194
C548	C	-0.31278	0.52156	1.29804
C549	C	-0.31212	0.49842	1.25138
C550	C	-0.3572	0.49876	1.20972
C551	C	-0.4036	0.52213	1.21554
C552	C	-0.40421	0.54531	1.2623
C553	C	-0.3583	0.5458	1.30387
C554	C	-0.26212	0.59259	1.30267
C555	C	-0.21208	0.61328	1.30014
C556	C	-0.2013	0.63724	1.34425
C557	C	-0.24178	0.64108	1.39019
C558	C	-0.29194	0.62046	1.39255
C559	C	-0.30231	0.59527	1.34955
C560	C	-0.14619	0.65669	1.34283
C561	C	-0.55838	0.66386	1.35401
C562	C	-0.34147	0.4896	1.56855
C563	C	-0.35334	0.47546	1.15941
C564	C	-0.37734	0.41237	0.85454
C565	C	-0.37719	0.39484	0.90883
C566	C	-0.37265	0.35885	0.90945
C567	C	-0.36862	0.34054	0.85625
C568	C	-0.36898	0.35814	0.80225
C569	C	-0.37342	0.39407	0.80119
C570	C	-0.41946	0.28372	0.85477
C571	C	-0.41813	0.24769	0.85469
C572	C	-0.36344	0.23051	0.85675

C573	C	-0.31023	0.24923	0.85884
C574	C	-0.312	0.28529	0.85883
C575	C	-0.36654	0.3025	0.85688
C576	C	-0.36378	0.33848	0.74583
C577	C	-0.37404	0.33978	0.96666
C578	C	-0.47724	0.3023	0.85102
C579	C	-0.25592	0.30551	0.86211
C580	C	-0.32858	0.43484	0.7296
C581	C	-0.33038	0.453	0.67685
C582	C	-0.37821	0.4491	0.63819
C583	C	-0.42385	0.42667	0.65294
C584	C	-0.42206	0.40847	0.70578
C585	C	-0.3745	0.41255	0.74442
C586	C	-0.33615	0.41352	1.00572
C587	C	-0.33989	0.43289	1.05717
C588	C	-0.38974	0.45322	1.06819
C589	C	-0.43578	0.45363	1.02739
C590	C	-0.4321	0.43422	0.97598
C591	C	-0.38214	0.4142	0.96466
C592	C	-0.51473	0.23068	0.89855
C593	C	-0.5666	0.2115	0.89734
C594	C	-0.57818	0.18938	0.85012
C595	C	-0.53747	0.18686	0.80423
C596	C	-0.48563	0.20609	0.80536
C597	C	-0.47385	0.22798	0.85266
C598	C	-0.23946	0.20977	0.90866
C599	C	-0.187	0.19113	0.90931
C600	C	-0.14734	0.19339	0.86206
C601	C	-0.16069	0.2148	0.81465
C602	C	-0.21326	0.23346	0.81397
C603	C	-0.25304	0.23093	0.86088
N604	N	-0.3936	0.47467	1.11906
N605	N	-0.0941	0.1737	0.86068
C606	C	-0.38166	0.45068	0.85345
C607	C	-0.36185	0.19213	0.85674
N608	N	0.37046	0.16818	0.84894
N609	N	-0.38189	0.46813	1.58454
C610	C	0.91837	0.95345	-0.19361
N611	N	0.91246	0.9748	-0.14282
N612	N	0.2051	0.66579	0.5963
C613	C	0.9363	0.07168	0.09482
C614	C	0.83921	0.09076	0.14383
C615	C	0.78802	0.11053	0.14494
C616	C	0.77477	0.13234	0.09824
C617	C	0.81324	0.13427	0.05025
C618	C	0.86446	0.11444	0.04917
C619	C	0.87814	0.09208	0.09576
C620	C	0.99149	0.05466	0.18949

C621	C	0.9977	0.03471	0.23988
C622	C	0.95629	0.00951	0.25295
C623	C	0.90876	0.00408	0.21481
C624	C	0.90263	0.02407	0.16425
C625	C	0.94346	0.05011	0.15114
C626	C	0.9871	0.02445	0.03661
C627	C	0.99092	0.00166	-0.01042
C628	C	0.94588	0.00009	-0.05205
C629	C	0.89644	0.02123	-0.04589
C630	C	0.89265	0.04404	0.00124
C631	C	0.9383	0.04641	0.04289
C632	C	1.02796	0.09752	0.04425
C633	C	1.07419	0.121	0.04241
C634	C	1.07947	0.14597	0.08614
C635	C	1.03756	0.14766	0.13093
C636	C	0.99131	0.12415	0.13273
C637	C	0.98629	0.09824	0.09002
C638	C	1.12989	0.16932	0.08754
C639	C	0.72051	0.15263	0.10081
C640	C	0.95252	-0.02296	-0.10242
C641	C	0.93584	0.91206	0.59341
C642	C	0.93563	0.89474	0.6479
C643	C	0.93988	0.85876	0.64902
C644	C	0.94381	0.84021	0.59607
C645	C	0.94404	0.85759	0.54185
C646	C	0.93983	0.89354	0.54028
C647	C	0.8893	0.7846	0.59517
C648	C	0.88816	0.74858	0.59442
C649	C	0.94163	0.73014	0.59582
C650	C	0.99608	0.74762	0.59768
C651	C	0.99681	0.7837	0.5982
C652	C	0.94347	0.80215	0.59702
C653	C	0.94919	0.83764	0.48573
C654	C	0.93796	0.83996	0.70648
C655	C	0.83277	0.80449	0.59205
C656	C	1.05428	0.80258	0.60089
C657	C	0.98193	0.93508	0.46807
C658	C	0.97866	0.95306	0.41517
C659	C	0.93107	0.94786	0.37668
C660	C	0.88721	0.92434	0.39169
C661	C	0.89043	0.90636	0.44465
C662	C	0.9377	0.91172	0.4832
C663	C	0.97496	0.91469	0.74479
C664	C	0.96958	0.93415	0.79602
C665	C	0.91837	0.95345	0.80639
C666	C	0.87272	0.95277	0.76519
C667	C	0.87806	0.9333	0.71401
C668	C	0.92931	0.91429	0.70336

C669	C	0.79009	0.73308	0.63688
C670	C	0.73641	0.7157	0.63378
C671	C	0.72312	0.69537	0.58501
C672	C	0.7642	0.69263	0.53908
C673	C	0.81782	0.71003	0.54213
C674	C	0.83115	0.73025	0.59115
C675	C	1.0659	0.70703	0.64611
C676	C	1.11688	0.68702	0.64527
C677	C	1.15447	0.68765	0.59659
C678	C	1.1408	0.70892	0.54874
C679	C	1.0898	0.72897	0.54958
C680	C	1.05196	0.72801	0.5982
N681	N	0.66863	0.67696	0.58403
N682	N	0.92554	0.96677	0.32308
N683	N	0.91246	0.9748	0.85718
C684	C	0.93126	0.95035	0.59195
C685	C	0.94058	0.69176	0.59512
C686	C	0.96331	0.98984	0.30725
C687	C	0.95252	0.97704	-0.10242
C688	C	0.44368	0.57157	0.55372
C689	C	0.35031	0.59662	0.60211
C690	C	0.30231	0.61896	0.60213
C691	C	0.29226	0.6405	0.55404
C692	C	0.33075	0.63956	0.50619
C693	C	0.37879	0.61721	0.50623
C694	C	0.3891	0.59505	0.55392
C695	C	0.49613	0.55215	0.64853
C696	C	0.49935	0.53219	0.69916
C697	C	0.45406	0.50948	0.71286
C698	C	0.40552	0.5066	0.67517
C699	C	0.40235	0.52664	0.62437
C700	C	0.44729	0.55016	0.61057
C701	C	0.48727	0.52156	0.49667
C702	C	0.48792	0.49842	0.45002
C703	C	0.44285	0.49876	0.40835
C704	C	0.39645	0.52213	0.41417
C705	C	0.39584	0.54531	0.46093
C706	C	0.44174	0.5458	0.50251
C707	C	0.53792	0.59259	0.5013
C708	C	0.58796	0.61328	0.49877
C709	C	0.59875	0.63724	0.54288
C710	C	0.55827	0.64108	0.58882
C711	C	0.50811	0.62046	0.59118
C712	C	0.49773	0.59527	0.54818
C713	C	0.65386	0.65669	0.54147
C714	C	0.24167	0.66386	0.55264
C715	C	0.45857	0.4896	0.76718
C716	C	0.44671	0.47546	0.35805

C717	C	0.4227	0.41237	0.05317
C718	C	0.42286	0.39484	0.10746
C719	C	0.42739	0.35885	0.10809
C720	C	0.43143	0.34054	0.05489
C721	C	0.43106	0.35814	0.00088
C722	C	0.42662	0.39407	-0.00017
C723	C	0.38059	0.28372	0.05341
C724	C	0.38191	0.24769	0.05332
C725	C	0.43661	0.23051	0.05538
C726	C	0.48981	0.24923	0.05748
C727	C	0.48805	0.28529	0.05747
C728	C	0.43351	0.3025	0.05551
C729	C	0.43627	0.33848	-0.05553
C730	C	0.42601	0.33978	0.16529
C731	C	0.32281	0.3023	0.04966
C732	C	0.54413	0.30551	0.06074
C733	C	0.47147	0.43484	-0.07177
C734	C	0.46966	0.453	-0.12452
C735	C	0.42184	0.4491	-0.16318
C736	C	0.3762	0.42667	-0.14842
C737	C	0.37798	0.40847	-0.09559
C738	C	0.42555	0.41255	-0.05695
C739	C	0.46389	0.41352	0.20435
C740	C	0.46016	0.43289	0.2558
C741	C	0.4103	0.45322	0.26682
C742	C	0.36427	0.45363	0.22602
C743	C	0.36795	0.43422	0.17461
C744	C	0.4179	0.4142	0.1633
C745	C	0.28532	0.23068	0.09718
C746	C	0.23345	0.2115	0.09597
C747	C	0.22187	0.18938	0.04875
C748	C	0.26258	0.18686	0.00286
C749	C	0.31442	0.20609	0.004
C750	C	0.3262	0.22798	0.05129
C751	C	0.56058	0.20977	0.1073
C752	C	0.61305	0.19113	0.10794
C753	C	0.65271	0.19339	0.06069
C754	C	0.63935	0.2148	0.01329
C755	C	0.58678	0.23346	0.01261
C756	C	0.54701	0.23093	0.05951
N757	N	0.40644	0.47467	0.31769
N758	N	0.70595	0.1737	0.05931
C759	C	0.41839	0.45068	0.05208
C760	C	0.4382	0.19213	0.05537
N761	N	1.17051	0.16818	0.04757
N762	N	0.41816	0.46813	0.78318

Table S8. The theoretical surface areas and pore volumes of BMTA-TFPM-COF with non-to five-interpenetrated models.

BMTA-TFPM-COF	SA (m^2/g)	PA (cm^3/g)
non-interpenetrated	7311	4.456
2-fold-interpenetrated	7293	1.605
3-fold-interpenetrated	5345	0.5585
4-fold-interpenetrated	2477	0.2964
5-fold-interpenetrated	1759	0.2114

Table S9. Comparison of the equilibrium time and adsorption capacity of various adsorbents for Au recovery.

Adsorbents	Equilibrium time (min)	q_m (mg g^{-1})	Reference
BMTA-TFPM-COF	30	570.18	This work
Thiosemicarbazide functionalized corn bract	1440	1470	[S51]
Aliquat-336 impregnated alginate capsule	1440	192	[S52]
Fe_3O_4@DMSA	480	296	[S53]
UiO-66-TA	372	240	[S54]
Methionine-MOFs	60	598	[S55]
TTB-COF	1	560	[S56]
TzTaCl	60	172	[S57]
JNU-1	0.17	1124	[S57]
UiO-66-TU	90	326	[S58]
UiO-66-BTU	240	680	[S59]

Table S10. Thermodynamic parameters for the absorption of Au(III) on BMTA-TFPM-COF.

T (K)	lnK_0	ΔG (kJ mol^{-1})	ΔH (Kj mol^{-1})	ΔS (J mol^{-1} K^{-1})
298	0.28185	–3.28	32.58	111.50
308	0.69396	–5.13		
318	1.09725	–7.92		
328	1.62017	–13.78		

Reference

[S1] Y.-X. Ma, Z.-J. Li, L. Wei, S.-Y. Ding, Y.-B. Zhang, W. Wang, *J. Am. Chem. Soc.* **2017**, *139*, 4995-4998.

[S2] Z. Li, L. Sheng, H. Wang, X. Wang, M. Li, Y. Xu, H. Cui, H. Zhang, H. Liang, H. Xu, X. He, *J. Am. Chem. Soc.* **2021**, *143*, 92-96.

[S3] X. Liu, J. Li, B. Gui, G. Lin, Q. Fu, S. Yin, X. Liu, J. Sun, C. Wang, *J. Am. Chem. Soc.* **2021**, *143*, 2123-2129.

[S4] G. Lin, H. Ding, D. Yuan, B. Wang, C. Wang, *J. Am. Chem. Soc.* **2016**, *138*, 3302-3305.

[S5] S. Das, T. Sekine, H. Mabuchi, T. Irie, J. Sakai, Y. Zhao, Q. Fang, Y. Negishi, *ACS Appl. Mater. Interfaces* **2022**, *14*, 48045-48051.

[S6] S. Wang, X.-X. Li, L. Da, Y. Wang, Z. Xiang, W. Wang, Y.-B. Zhang, D. Cao, *J. Am. Chem. Soc.* **2021**, *143*, 15562-15566.

[S7] F. J. Uribe-Romo, J. R. Hunt, H. Furukawa, C. Klöck, M. O'Keeffe, O. M. Yaghi, *J. Am. Chem. Soc.* **2009**, *131*, 4570-4571.

[S8] X. Han, J. Huang, C. Yuan, Y. Liu, Y. Cui, *J. Am. Chem. Soc.* **2018**, *140*, 892-895.

[S9] Q. Fang, J. Wang, S. Gu, R. B. Kaspar, Z. Zhuang, J. Zheng, H. Guo, S. Qiu, Y. Yan, *J. Am. Chem. Soc.* **2015**, *137*, 8352-8355.

[S10] Z. Li, H. Li, X. Guan, J. Tang, Y. Yusran, Z. Li, M. Xue, Q. Fang, Y. Yan, V. Valtchev, S. Qiu, *J. Am. Chem. Soc.* **2017**, *139*, 17771-17774.

[S11] Y.-B. Zhang, J. Su, H. Furukawa, Y. Yun, F. Gándara, A. Duong, X. Zou, O. M. Yaghi, *J. Am. Chem. Soc.* **2013**, *135*, 16336-16339.

[S12] Y. Zhang, H. Li, J. Chang, X. Guan, L. Tang, Q. Fang, V. Valtchev, Y. Yan, S. Qiu, *Small* **2021**, *17*, 2006112.

[S13] X. Yu, C. Li, J. Chang, Y. Wang, W. Xia, J. Suo, X. Guan, V. Valtchev, Y. Yan, S. Qiu, Q. Fang, *Angew. Chem. Int. Ed.* **2022**, *61*, e202200820.

[S14] S. Yan, X. Guan, H. Li, D. Li, M. Xue, Y. Yan, V. Valtchev, S. Qiu, Q. Fang, *J. Am. Chem. Soc.* **2019**, *141*, 2920-2924.

[S15] X. Kang, X. Han, C. Yuan, C. Cheng, Y. Liu, Y. Cui, *J. Am. Chem. Soc.* **2020**, *142*, 16346-16356.

[S16] Y. Xie, J. Li, C. Lin, B. Gui, C. Ji, D. Yuan, J. Sun, C. Wang, *J. Am. Chem. Soc.* **2021**, *143*, 7279-7284.

[S17] C. Gao, J. Li, S. Yin, J. Sun, C. Wang, *J. Am. Chem. Soc.* **2020**, *142*, 3718-3723.

[S18] G. Lin, H. Ding, R. Chen, Z. Peng, B. Wang, C. Wang, *J. Am. Chem. Soc.* **2017**, *139*, 8705-8709.

[S19] H. Ding, J. Li, G. Xie, G. Lin, R. Chen, Z. Peng, C. Yang, B. Wang, J. Sun, C. Wang, *Nat. Commun.* **2018**, *9*, 5234.

[S20] O. Yahiaoui, A. N. Fitch, F. Hoffmann, M. Fröba, A. Thomas, J. Roeser, *J. Am. Chem. Soc.* **2018**, *140*, 5330-5333.

[S21] Y. Lan, X. Han, M. Tong, H. Huang, Q. Yang, D. Liu, X. Zhao, C. Zhong, *Nat. Commun.* **2018**, *9*, 5274.

[S22] H. L. Nguyen, C. Gropp, Y. Ma, C. Zhu, O. M. Yaghi, *J. Am. Chem. Soc.* **2020**, *142*, 20335-20339.

[S23] X. Wang, M. Bahri, Z. Fu, M. A. Little, L. Liu, H. Niu, N. D. Browning, S. Y. Chong, L. Chen, J. W. Ward, A. I. Cooper, *J. Am. Chem. Soc.* **2021**, *143*, 15011-15016.

[S24] H. M. El-Kaderi, J. R. Hunt, J. L. Mendoza-Cortés, A. P. Côté, R. E. Taylor, M. O'Keeffe, O. M. Yaghi, *Science* **2007**, *316*, 268-272.

[S25] H. Li, F. Chen, X. Guan, J. Li, C. Li, B. Tang, V. Valtchev, Y. Yan, S. Qiu, Q. Fang, *J. Am. Chem. Soc.* **2021**, *143*, 2654-2659.

[S26] Y. Zhang, J. Duan, D. Ma, P. Li, S. Li, H. Li, J. Zhou, X. Ma, X. Feng, B. Wang, *Angew. Chem. Int. Ed.* **2017**, *56*, 16313-16317.

[S27] C. Yu, H. Li, Y. Wang, J. Suo, X. Guan, R. Wang, V. Valtchev, Y. Yan, S. Qiu, Q. Fang, *Angew. Chem. Int. Ed.* **2022**, *61*, e202117101.

[S28] M. Martínez-Abadía, K. Strutyński, B. Lerma-Berlanga, C. T. Stoppiello, A. N. Khlobystov, C. Martí-Gastaldo, A. Saeki, M. Melle-Franco, A. Mateo-Alonso, *Angew. Chem. Int. Ed.* **2021**, *60*, 9941-9946.

[S29] C. Gropp, T. Ma, N. Hanikel, O. M. Yaghi, *Science* **2020**, *370*, eabd6406.

[S30] H. Li, J. Chang, S. Li, X. Guan, D. Li, C. Li, L. Tang, M. Xue, Y. Yan, V. Valtchev, S. Qiu, Q. Fang, *J. Am. Chem. Soc.* **2019**, *141*, 13324-13329.

[S31] J. R. Hunt, C. J. Doonan, J. D. LeVangie, A. P. Côté, O. M. Yaghi, *J. Am. Chem. Soc.* **2008**, *130*, 11872-11873.

[S32] D. Beaudoin, T. Maris, J. D. Wuest, *Nat. Chem.* **2013**, *5*, 830-834.

[S33] D. Stewart, D. Antypov, M. S. Dyer, M. J. Pitcher, A. P. Katsoulidis, P. A. Chater, F. Blanc, M. J. Rosseinsky, *Nat. Commun.* **2017**, *8*, 1102.

[S34] R. Sun, X. Wang, X. Wang, B. Tan, *Angew. Chem. Int. Ed.* **2022**, *61*, e202117668.

[S35] Q. Fang, S. Gu, J. Zheng, Z. Zhuang, S. Qiu, Y. Yan, *Angew. Chem. Int. Ed.* **2014**, *53*, 2878-2882.

[S36] X. Guan, Y. Ma, H. Li, Y. Yusran, M. Xue, Q. Fang, Y. Yan, V. Valtchev, S. Qiu, *J. Am. Chem. Soc.* **2018**, *140*, 4494-4498.

[S37] M. Zhang, J. Fang, Y. Liu, Y. Wang, L. Liao, L. Tang, L. Zhu, S. Qiu, Q. Fang, *Small Struct.* **2021**, *2*, 2000108.

[S38] F. Chen, X. Guan, H. Li, J. Ding, L. Zhu, B. Tang, V. Valtchev, Y. Yan, S. Qiu, Q. Fang, *Angew. Chem. Int. Ed.* **2021**, *60*, 22230-22235.

[S39] W. Zhao, C. Yu, J. Zhao, F. Chen, X. Guan, H. Li, B. Tang, G. Yu, V. Valtchev, Y. Yan, S. Qiu, Q. Fang, *Small* **2021**, *17*, 2102630.

[S40] Y. Ma, Y. Wang, H. Li, X. Guan, B. Li, M. Xue, Y. Yan, V. Valtchev, S. Qiu, Q. Fang, *Angew. Chem. Int. Ed.* **2020**, *59*, 19633-19638.

[S41] Y. Liu, Y. Ma, Y. Zhao, X. Sun, F. Gándara, H. Furukawa, Z. Liu, H. Zhu, C. Zhu, K. Suenaga, P. Oleynikov, A. S. Alshammari, X. Zhang, O. Terasaki, O. M. Yaghi, *Science* **2016**, *351*, 365-369.

[S42] B. Gui, X. Liu, Y. Cheng, Y. Zhang, P. Chen, M. He, J. Sun, C. Wang, *Angew. Chem. Int. Ed.* **2022**, *61*, e202113852.

[S43] X. Yu, C. Li, Y. Ma, D. Li, H. Li, X. Guan, Y. Yan, V. Valtchev, S. Qiu, Q. Fang, *Microporous Mesoporous Mater.* **2020**, *299*, 110105.

[S44] H. Li, Q. Pan, Y. Ma, X. Guan, M. Xue, Q. Fang, Y. Yan, V. Valtchev, S. Qiu, *J. Am. Chem. Soc.* **2016**, *138*, 14783-14788.

[S45] Q. Lu, Y. Ma, H. Li, X. Guan, Y. Yusran, M. Xue, Q. Fang, Y. Yan, S. Qiu, V. Valtchev, *Angew. Chem. Int. Ed.* **2018**, *57*, 6042-6048.

[S46] C. Wu, Y. Liu, H. Liu, C. Duan, Q. Pan, J. Zhu, F. Hu, X. Ma, T. Jiu, Z. Li, Y. Zhao, *J. Am. Chem. Soc.* **2018**, *140*, 10016-10024.

[S47] C.-R. Zhang, W.-R. Cui, S.-M. Yi, C.-P. Niu, R.-P. Liang, J.-X. Qi, X.-J. Chen, W. Jiang, X. Liu, Q.-X. Luo, J.-D. Qiu, *Nat. Commun.* **2022**, *13*, 7621.

[S48] B. Han, Y. Jin, B. Chen, W. Zhou, B. Yu, C. Wei, H. Wang, K. Wang, Y. Chen, B. Chen, J. Jiang, *Angew. Chem. Int. Ed.* **2022**, *61*, e202114244.

[S49] L. Liang, Y. Qiu, W. D. Wang, J. Han, Y. Luo, W. Yu, G.-L. Yin, Z.-P. Wang, L. Zhang, J. Ni, J. Niu, J. Sun, T. Ma, W. Wang, *Angew. Chem. Int. Ed.* **2020**, *59*, 17991-17995.

[S50] S.-W. Ke, Y. Wang, J. Su, K. Liao, S. Lv, X. Song, T. Ma, S. Yuan, Z. Jin, J.-L. Zuo, *J. Am. Chem. Soc.* **2022**, *144*, 8267-8277.

[S51] G. Lin, S. Wang, L. Zhang, T. Hu, J. Peng, S. Cheng, L. Fu, *J. Mol. Liq.* **2018**, *258*, 235-243.

[S52] W. Wei, D. H. K. Reddy, J. K. Bediako, Y.-S. Yun, *Chem. Eng. J.* **2016**, *289*, 413-422.

[S53] O. F. Odio, L. Lartundo-Rojas, P. Santiago-Jacinto, R. Martínez, E. Reguera, *J. Phys. Chem. C* **2014**, *118*, 2776-2791.

[S54] C. Wang, G. Lin, J. Zhao, S. Wang, L. Zhang, Y. Xi, X. Li, Y. Ying, *Chem. Eng. J.* **2020**, *380*, 122511.

[S55] M. Mon, J. Ferrando-Soria, T. Grancha, F. R. Fortea-Pérez, J. Gascon, A. Leyva-Pérez, D. Armentano, E. Pardo, *J. Am. Chem. Soc.* **2016**, *138*, 7864-7867.

[S56] Z. Zhou, W. Zhong, K. Cui, Z. Zhuang, L. Li, L. Li, J. Bi, Y. Yu, *Chem. Commun.* **2018**, *54*, 9977-9980.

[S57] H.-L. Qian, F.-L. Meng, C.-X. Yang, X.-P. Yan, *Angew. Chem. Int. Ed.* **2020**, *59*, 17607-17613.

[S58] C. Wu, X. Zhu, Z. Wang, J. Yang, Y. Li, J. Gu, *Ind. Eng. Chem. Res.* **2017**, *56*, 13975-13982.

[S59] J. Guo, X. Fan, J. Wang, S. Yu, M. Laipan, X. Ren, C. Zhang, L. Zhang, Y. Li, *Chem. Eng. J.* **2021**, *425*, 130588.