Supporting Information

A metal-free perylene-porphyrin based covalent organic framework for electrocatalytic hydrogen evolution

Siddhartha Samanta, [a] Sahina Khatun, [a] Ishita Mukherjee, [a] Sanhita Maity, [b] Matthew A. Addicoat, [c] Anirban Pradhan, [a,*]

[a] Department of Chemistry, Birla Institute of Technology (BIT) – Mesra, Ranchi, Jharkhand, 835215, India, Email: anirbanpradhan@bitmesra.ac.in

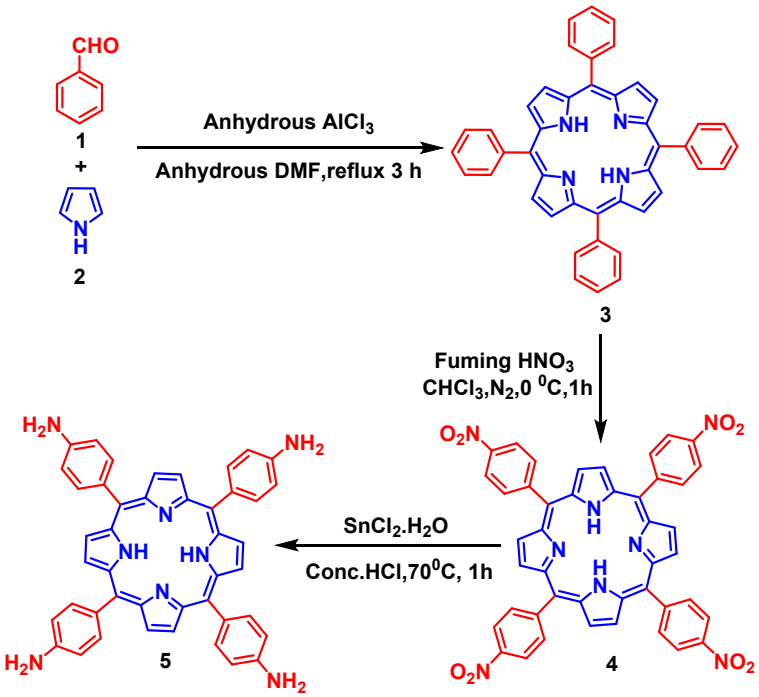
[b] Department of Applied Sciences, Amity University, Jharkhand

[c] School of Science and Technology, Nottingham Trent University, Clifton Lane, Nottingham, NG11 8NS, UK.

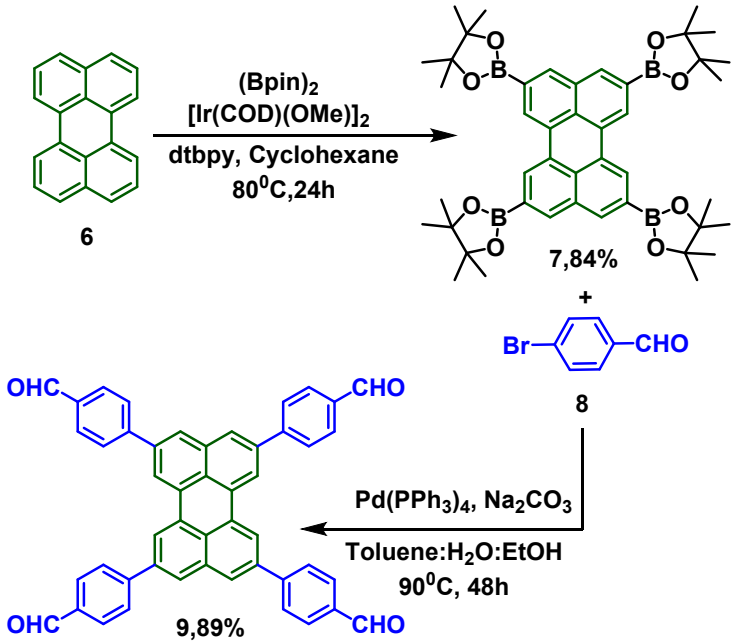
Section S1:

1. Synthetic Scheme of 5,10,15,20tetrakis (paraaminophenyl) 21H,23Hporphyrin(5):

The synthesis of tetra-amine porphyrin (5) was done using previously reported procedure.[14]



2. Synthetic Scheme of 4,4',4'',4'''-(perylene-2,5,8,11-tetrayl) tetrabenzaldehyde (9):



Section S2:

^{1}H NMR and ^{13}C NMR spectrum of synthesized compounds:

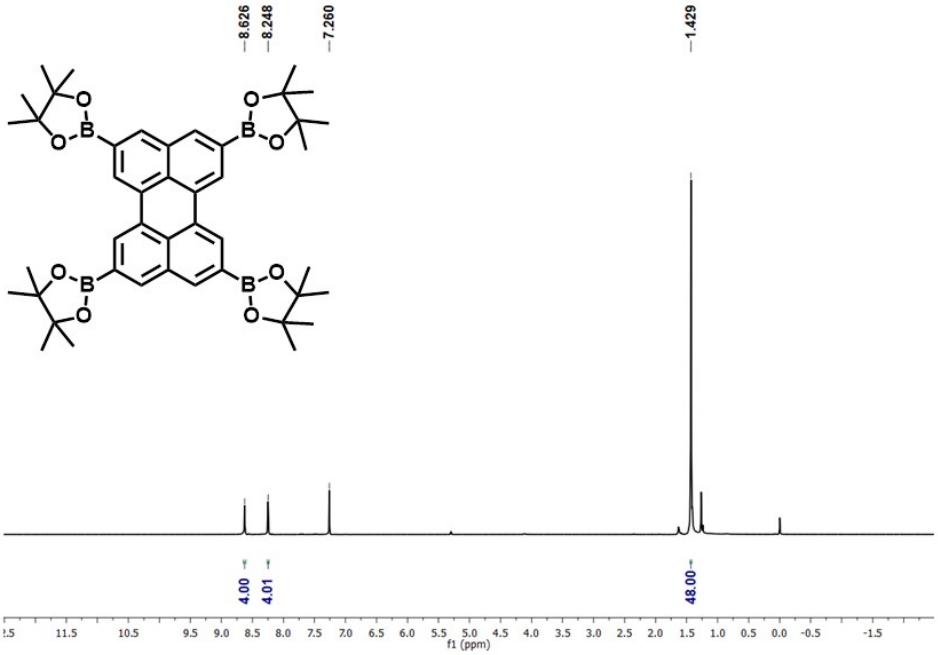


Fig. S1. ^{1}H-NMR of compound 2,5,8,11-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) perylene (**7**).

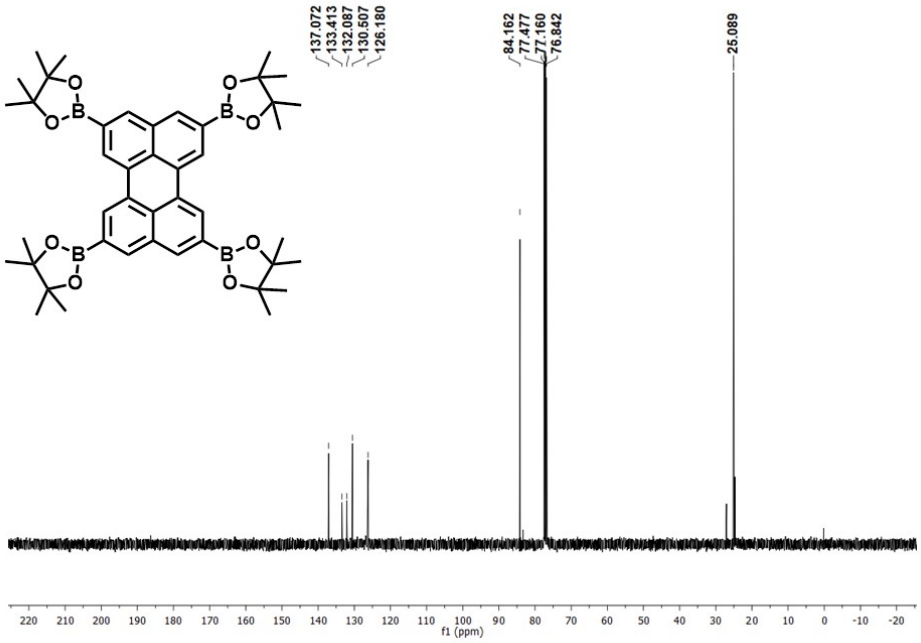


Fig. S2. ^{13}C-NMR of compound 2,5,8,11-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) perylene (**7**).

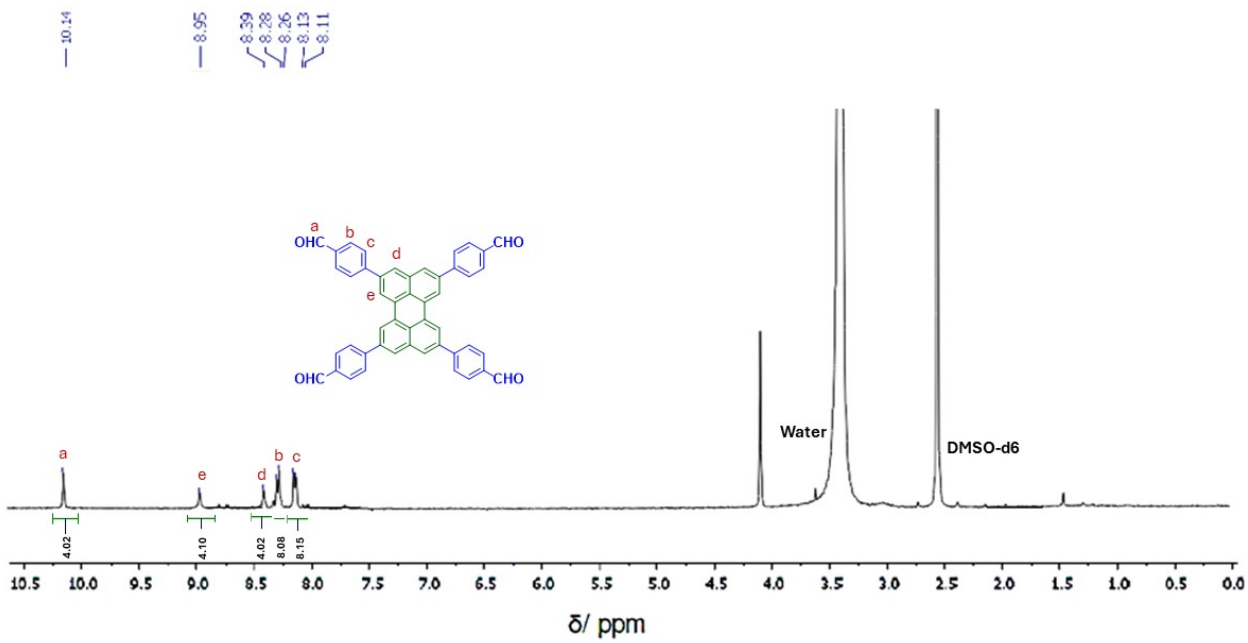


Fig. S3. [1]H-NMR of compound 4,4',4",4"'-(perylene-2,5,8,11-tetrayl) tetrabenzaldehyde (**9**):

Section S3

Experimental Section:

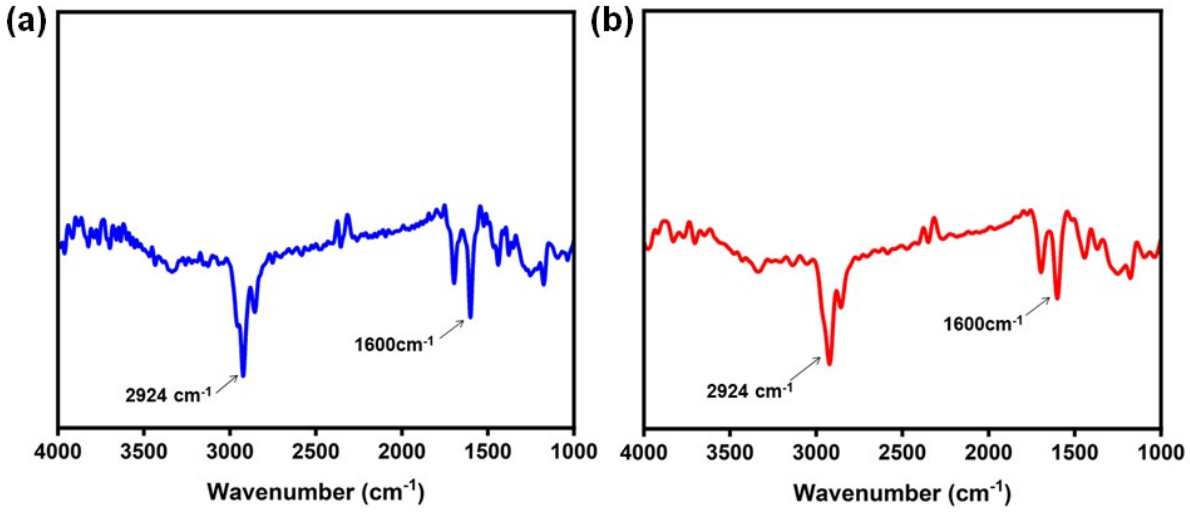


Fig. S4. FTIR Spectra of the **PETA-PAM-COF** after immersion in acidic (a) and basic medium (b).

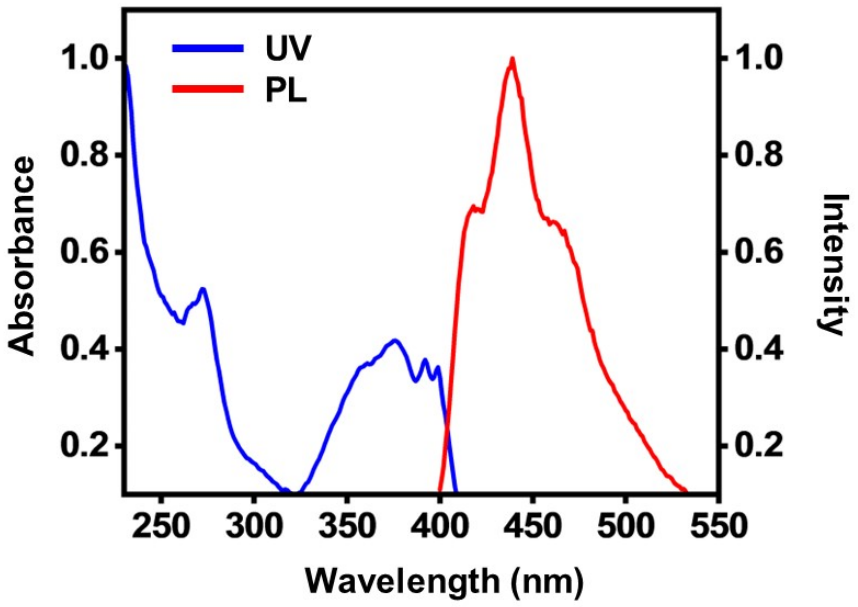


Fig. S5. Solid-state UV and photoluminescence spectra of **PETA-PAM-COF**.

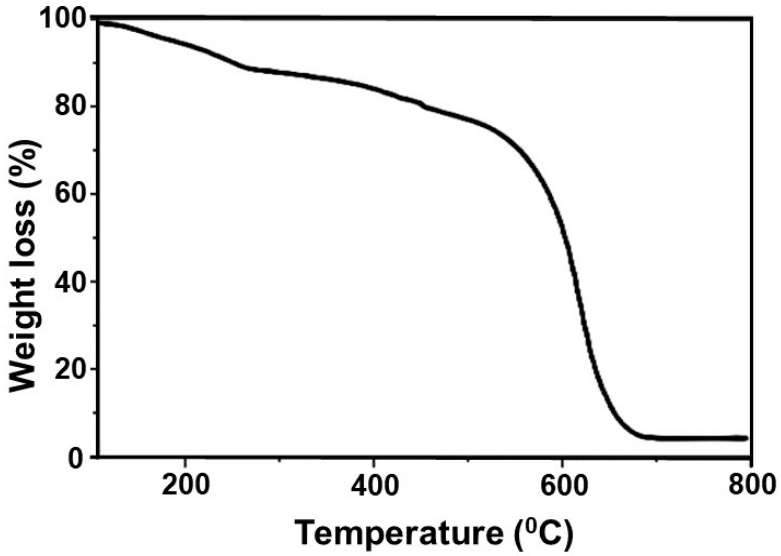


Fig. S6. Thermogravimetric Analysis (TGA) graph of **PETA-PAM-COF**.

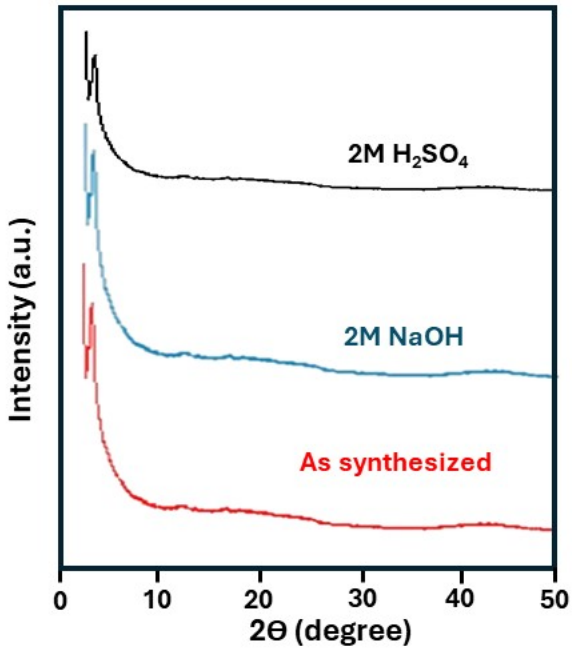


Fig. S7. XRD pattern of **PETA-PAM-COF** after treating in different conditions; 2M H_2SO_4 and 2M NaOH.

Fig. S8. XRD pattern of **PETA-PAM-COF** after and before HER was performed.

Section S4

Table S1: A Comparison table for the metal free HER activity of **PETA-PAM-COF** with other different materials which are previously reported in literature:

Material	**Over potential @ 10 mAcm^{-2} (mV)**	**Tafel slope (mV/decade)**	**Exchange current density (i_0)**	**Experiment condition**	**Reference**
Pt electrode	58	30	2.7×10^{-3} A cm^{-2}	0.5 M H_2SO_4	1-3
C3N4@NG	240	51.5	3.5×10^{-7}A cm^{-2}	4 M AgCl/KCl	4
CoP-2ph-CMP-800	360	121	-	1 M KOH	5
Cu-MOF	209	84	-	0.5 M H_2SO_4	6
N,P-graphene	420	91	2.4×10^{-7} A cm^{-2}	0.5 M H_2SO_4	7
P-doped graphene	553	133	9×10^{-3} µF cm^{-2}	0.5 M H_2SO_4	7
N-doped graphene	490	116	7×10^{-2} µF cm^{-2}	0.5 M H_2SO_4	7
NS co-doped Nano-porous Graphene 5000C	276	81	6.5×10^{-5} mA cm^{-2}	0.5 M H_2SO_4	8
C3N4/FTO	100	120	-	0.1M KOH	9
p-MWCNTs-ao-cp	220	71.3	16×10^{-3} mA cm^{-2}	0.5 M H_2SO_4	10
g-C3N4 nanoribbon-G	207	54	3.98×10^{-3} mA cm^{-2}	0.5 M H_2SO_4	11
THTNi 2DSP	333	80.5	6×10^{-4} mA cm^{-2}	0.5 M H_2SO_4	12
Cu-CMP850	350	135	-	1 M KOH	13
TpPAM	250	106	2.4×10^{-4} A cm^{-2}	0.5 M H_2SO_4	14
Ru@COF	212	79	-	1.5 M H_2SO_4	15

SB-PORPy COF	380 @ 5 mA.cm^{-2}	116	5 mA cm^{-2}	0.5 M H_2SO_4	16
CoP nanosheets	100	76	0.67 mA cm^{-2}	1.0 M KOH	17
MoCx	142	53	0.023 mA cm^{-2}	0.5 M H_2SO_4	18
Mo_2C@NPC	260	126.4	1.9×10^{-3} A cm^{-2}	0.5 M H_2SO_4	19
NU-1000_Ni-S	238	111	-	0.5 M H_2SO_4	20
Co-(MOFs)	324	33	-	1 M KOH	21
C-Fe, Co-COF	260	150	6.1 mA cm^{-2}	0.1 M KOH	22
Cu-CMP850	350	135	-	1.0 M KOH	23
TFPB-PAM	185	68.5	4.9×10^{-4} A cm^{-2}	0.5 M H_2SO_4	24
NENU-500	237	96	0.139 mA cm^{-2}	0.5 M H_2SO_4	25
PETA-PAM-COF	261	122	3.7×10^{-4} A cm^{-2}	0.5 M H_2SO_4	**This work**

Section S5

Computational Method:

The theoretical calculations from the powder X-ray diffraction (PXRD) pattern for the PETA-PAM-COF: The positions of atoms of the PETA-PAM-COF were optimized using the Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) method as implemented in the DFTB+ version 19.1. All pair wise atomic interactions (C, H) were treated using the mio-0-1 parameter set 3 and dispersion was accounted for using UFF dispersion. It is known that the layer stacking is affected by the Coulomb repulsion between the partial atomic charges in adjacent layers. Hence, several simulated stacking possibilities were considered for the COF by shifting adjacent layers with respect to each other in different directions. Every one of the starting geometry was fully optimized without any constraints (P1 space group). The predicted AA stacking structure has the lowest energy, and is in good agreement with the experimental PXRD pattern.

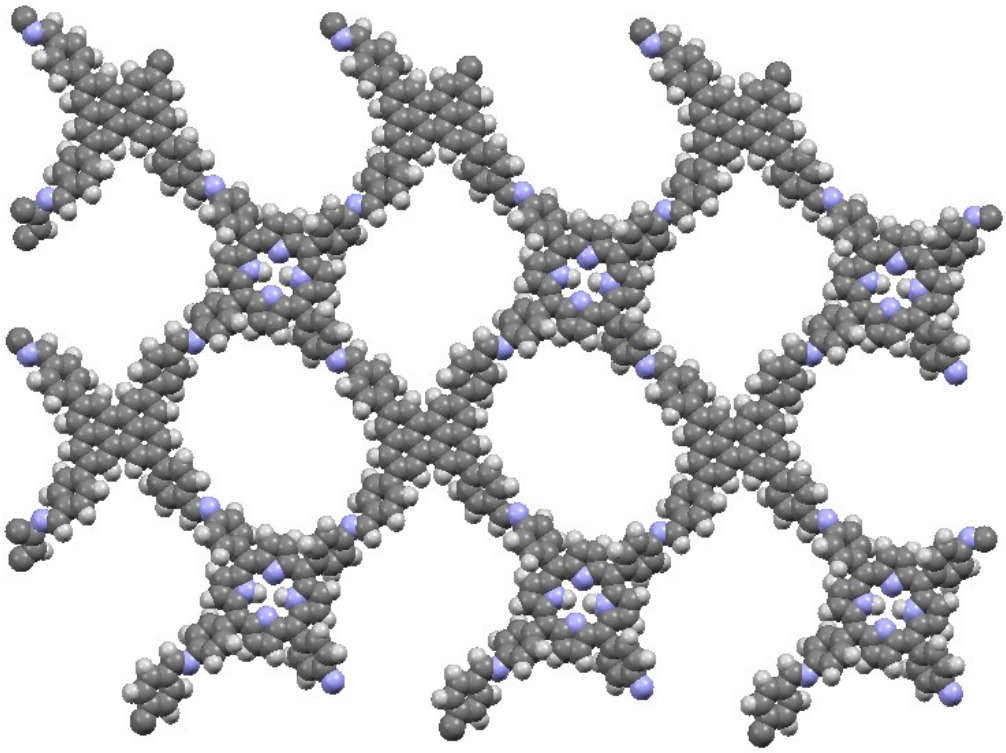


Fig. S9. Simulated AA stacking structure of **PETA-PAM-COF.**

Table S2. Energies, stabilization energies, interlayer distance and the HOMO-LUMO gap of the optimized **PETA-PAM-COF** structures.

Stacking mode	**c (Å)** **Interlayer distance**	**Total DFTB Energy (a.u.)**	**LJ energy (a.u.)**	**Per layer stabilization (kcal mol^{-1})**	**HOMO-LUMO gap (eV)**
Monolayer		-196.789961	0.8600		1.304
Slip AA	3.66	-393.866047	1.4385	-89.77	0.803
AA	3.83	-393.821260	1.4298	-75.72	1.151
AB	3.13	-393.7863914	1.5347	-64.78	1.220

Unit cell structure and parameters:

PETA-PAM-COF

Lattice type: Triclinic

Space Group: P1

a=26.8849; **b**=27.9821; **c**=7.65738

α=90.1737; **β**=89.7679; **γ**=89.7558

Table S3. Fractional atomic coordinates for the unit cell of the **PETA-PAM-COF.**

Number	Atomic Number	Label	X-axis	Y-axis	Z-axis	Element
1	6	C1	0.57114	0.95467	0.02193	C
2	6	C2	0.59122	0.90760	0.01806	C
3	6	C3	0.64401	0.90077	0.01645	C
4	6	C4	0.67572	0.94180	0.01828	C
5	6	C5	0.65426	0.98738	0.02807	C
6	6	C6	0.60196	0.99463	0.02968	C
7	6	C7	0.66369	0.85307	0.01387	C
8	6	C8	0.72990	0.93466	0.01298	C
9	6	C9	0.74958	0.88699	0.01546	C
10	6	C10	0.71791	0.84591	0.01792	C
11	6	C11	0.80239	0.88030	0.01598	C
12	6	C12	0.83448	0.92059	0.01629	C
13	6	C13	0.81534	0.96697	0.01192	C
14	6	C14	0.76288	0.97311	0.00709	C

15	1	H1	0.53042	0.95892	0.01748	H
16	1	H2	0.87489	0.91432	0.02380	H
17	6	C15	0.55907	0.86737	0.01847	C
18	6	C16	0.57813	0.82094	0.01383	C
19	6	C17	0.63061	0.81467	0.00888	C
20	1	H3	0.51865	0.87371	0.02629	H
21	6	C18	0.73949	0.80037	0.02641	C
22	6	C19	0.82255	0.83330	0.01863	C
23	1	H4	0.86328	0.82915	0.01295	H
24	6	C20	0.79184	0.79326	0.02622	C
25	1	H5	0.74811	1.00972	-0.00206	H
26	1	H6	0.71555	0.76868	0.03522	H
27	1	H7	0.64532	0.77801	0.00020	H
28	1	H8	0.67828	1.01901	0.03684	H
29	6	C21	0.54498	0.77875	0.01845	C
30	6	C22	0.49618	0.78066	-0.04928	C
31	6	C23	0.56123	0.73533	0.09316	C
32	6	C24	0.46486	0.74118	-0.04113	C
33	1	H9	0.48251	0.81337	-0.11291	H
34	6	C25	0.53019	0.69563	0.09926	C
35	1	H10	0.59845	0.73252	0.15184	H
36	6	C26	0.48131	0.69788	0.03345	C
37	1	H11	0.42707	0.74348	-0.09535	H
38	1	H12	0.54382	0.66241	0.15976	H
39	6	C27	0.58018	0.04338	0.03755	C
40	6	C28	0.53300	0.05070	0.11546	C

41	6	C29	0.60451	0.08339	-0.03489	C
42	6	C30	0.51010	0.09531	0.11239	C
43	1	H13	0.51378	0.02106	0.18110	H
44	6	C31	0.58178	0.12835	-0.03615	C
45	1	H14	0.64117	0.07929	-0.09800	H
46	6	C32	0.53358	0.13480	0.03340	C
47	1	H15	0.47300	0.10021	0.17133	H
48	1	H16	0.60114	0.15855	-0.09813	H
49	6	C33	0.84829	1.00929	0.01747	C
50	6	C34	0.89728	1.00758	-0.05004	C
51	6	C35	0.83165	1.05259	0.09342	C
52	6	C36	0.92847	1.04711	-0.03983	C
53	1	H17	0.91122	0.97497	-0.11486	H
54	6	C37	0.86256	1.09236	0.10150	C
55	1	H18	0.79421	1.05525	0.15161	H
56	6	C38	0.91169	1.09024	0.03658	C
57	1	H19	0.96644	1.04498	-0.09367	H
58	1	H20	0.84862	1.12548	0.16303	H
59	6	C39	0.81411	0.74469	0.03065	C
60	6	C40	0.86165	0.73774	0.10488	C
61	6	C41	0.79018	0.70459	-0.04291	C
62	6	C42	0.88533	0.69354	0.09651	C
63	1	H21	0.88056	0.76737	0.17183	H
64	6	C43	0.81364	0.65999	-0.04904	C
65	1	H22	0.75321	0.70835	-0.10293	H
66	6	C44	0.86224	0.65403	0.01608	C

67	1	H23	0.92269	0.68903	0.15262	H
68	1	H24	0.79454	0.62972	-0.11172	H
69	6	C45	0.44889	0.65588	0.04370	C
70	1	H25	0.46678	0.62181	0.09058	H
71	6	C46	0.89066	0.60926	-0.00557	C
72	1	H26	0.87059	0.57671	-0.05508	H
73	7	N1	0.40240	0.65826	0.00539	N
74	7	N2	-0.06235	0.61000	0.02337	N
75	6	C47	0.37198	0.61764	0.01024	C
76	6	C48	0.38449	0.57565	-0.08290	C
77	6	C49	0.32655	0.61927	0.10273	C
78	6	C50	0.35177	0.53711	-0.08573	C
79	1	H27	0.41857	0.57427	-0.16302	H
80	6	C51	0.29668	0.57874	0.11283	C
81	1	H28	0.31668	0.65130	0.17915	H
82	6	C52	0.30767	0.53678	0.01585	C
83	1	H29	0.36057	0.50712	-0.17377	H
84	1	H30	0.26483	0.57966	0.20335	H
85	6	C53	0.27464	0.49413	0.02025	C
86	6	C54	0.29834	0.44854	0.03203	C
87	6	C55	0.22220	0.50125	0.01379	C
88	6	C56	0.35090	0.43953	0.03838	C
89	7	N3	0.27584	0.40433	0.03174	N
90	7	N4	0.18585	0.46695	0.02173	N
91	6	C57	0.19886	0.54849	0.00785	C
92	6	C58	0.35844	0.39091	0.03040	C

93	1	H31	0.38070	0.46584	0.04924	H
94	6	C59	0.31077	0.36808	0.03232	C
95	1	H32	0.23776	0.39908	0.02987	H
96	6	C60	0.14077	0.49012	0.02609	C
97	6	C61	0.14916	0.54178	0.02796	C
98	1	H33	0.21645	0.58340	-0.00936	H
99	1	H34	0.39497	0.37372	0.02283	H
100	6	C62	0.30173	0.31796	0.03945	C
101	6	C63	0.09250	0.46912	0.02060	C
102	1	H35	0.12206	0.57080	0.04450	H
103	6	C64	0.25352	0.29694	0.04553	C
104	6	C65	0.34552	0.28512	0.03532	C
105	6	C66	0.08349	0.41894	0.02251	C
106	6	C67	0.04897	0.50215	0.01097	C
107	6	C68	0.24520	0.24531	0.05077	C
108	7	N5	0.20843	0.32000	0.03651	N
109	6	C69	0.34395	0.24286	-0.06697	C
110	6	C70	0.38928	0.29297	0.13333	C
111	7	N6	0.11851	0.38280	0.02876	N
112	6	C71	0.03589	0.39600	0.02655	C
113	6	C72	0.00453	0.49571	0.10781	C
114	6	C73	0.05171	0.54373	-0.09403	C
115	6	C74	0.19569	0.23837	0.02734	C
116	1	H36	0.27231	0.21651	0.07091	H
117	6	C75	0.17222	0.28559	0.02864	C
118	6	C76	0.38117	0.20831	-0.05782	C

119	1	H37	0.31295	0.23674	-0.15729	H
120	6	C77	0.42923	0.26081	0.12937	C
121	1	H38	0.39193	0.32371	0.22271	H
122	6	C78	0.09613	0.33861	0.03832	C
123	1	H39	0.15657	0.38811	0.02439	H
124	6	C79	0.04355	0.34764	0.04497	C
125	1	H40	-0.00071	0.41287	0.01601	H
126	6	C80	-0.03469	0.52860	0.10083	C
127	1	H41	0.00076	0.46572	0.19940	H
128	6	C81	0.01528	0.57913	-0.08748	C
129	1	H42	0.08323	0.54866	-0.18389	H
130	1	H43	0.17835	0.20332	0.01036	H
131	6	C82	0.11974	0.29285	0.03202	C
132	6	C83	0.42489	0.21711	0.03838	C
133	1	H44	0.37800	0.17518	-0.13448	H
134	1	H45	0.46230	0.26783	0.20962	H
135	1	H46	0.01384	0.32155	0.06386	H
136	6	C84	-0.02898	0.57184	0.00850	C
137	1	H47	-0.06823	0.52269	0.18072	H
138	1	H48	0.01959	0.61172	-0.16585	H
139	6	C85	0.08649	0.25039	0.02822	C
140	6	C86	0.09685	0.20837	0.12457	C
141	6	C87	0.04260	0.25030	-0.07342	C
142	6	C88	0.06671	0.16804	0.11331	C
143	1	H49	0.12834	0.20723	0.21566	H
144	6	C89	0.00951	0.21208	-0.07120	C

145	1	H50	0.03429	0.28029	-0.16120	H
146	6	C90	0.02151	0.16997	0.02081	C
147	1	H51	0.07615	0.13594	0.18900	H
148	1	H52	-0.02435	0.21370	-0.15142	H
149	6	C91	0.50546	0.17984	0.01566	C
150	1	H53	0.52507	0.21184	-0.04030	H
151	6	C92	0.94414	1.13215	0.04975	C
152	1	H54	0.92609	1.16628	0.09649	H
153	7	N7	0.45896	0.17959	0.05375	N
154	7	N8	0.99089	1.12954	0.01412	N
155	6	C6	0.60196	-0.00537	0.02968	C
156	6	C27	0.58018	1.04338	0.03755	C
157	6	C46	-0.10934	0.60926	-0.00557	C
158	7	N2	0.93765	0.61000	0.02337	N
159	6	C90	1.02151	1.16997	0.02081	C
160	7	N8	-0.00911	0.12954	0.01412	N
161	6	C93	0.57114	0.95467	0.52193	C
162	6	C94	0.59122	0.90760	0.51806	C
163	6	C95	0.64401	0.90077	0.51645	C
164	6	C96	0.67572	0.94180	0.51828	C
165	6	C97	0.65426	0.98738	0.52807	C
166	6	C98	0.60196	0.99463	0.52968	C
167	6	C99	0.66369	0.85307	0.51387	C
168	6	C100	0.72990	0.93466	0.51298	C
169	6	C101	0.74958	0.88699	0.51546	C
170	6	C102	0.71791	0.84591	0.51792	C

171	6	C103	0.80239	0.88030	0.51598	C
172	6	C104	0.83448	0.92059	0.51629	C
173	6	C105	0.81534	0.96697	0.51192	C
174	6	C106	0.76288	0.97311	0.50709	C
175	1	H55	0.53042	0.95892	0.51748	H
176	1	H56	0.87489	0.91432	0.52380	H
177	6	C107	0.55907	0.86737	0.51847	C
178	6	C108	0.57813	0.82094	0.51383	C
179	6	C109	0.63061	0.81467	0.50888	C
180	1	H57	0.51865	0.87371	0.52629	H
181	6	C110	0.73949	0.80037	0.52641	C
182	6	C111	0.82255	0.83330	0.51863	C
183	1	H58	0.86328	0.82915	0.51295	H
184	6	C112	0.79184	0.79326	0.52622	C
185	1	H59	0.74811	1.00972	0.49794	H
186	1	H60	0.71555	0.76868	0.53522	H
187	1	H61	0.64532	0.77801	0.50020	H
188	1	H62	0.67828	1.01901	0.53684	H
189	6	C113	0.54498	0.77875	0.51845	C
190	6	C114	0.49618	0.78066	0.45072	C
191	6	C115	0.56123	0.73533	0.59316	C
192	6	C116	0.46486	0.74118	0.45887	C
193	1	H63	0.48251	0.81337	0.38709	H
194	6	C117	0.53019	0.69563	0.59926	C
195	1	H64	0.59845	0.73252	0.65184	H
196	6	C118	0.48131	0.69788	0.53345	C

197	1	H65	0.42707	0.74348	0.40465	H
198	1	H66	0.54382	0.66241	0.65976	H
199	6	C119	0.58018	0.04338	0.53755	C
200	6	C120	0.53300	0.05070	0.61546	C
201	6	C121	0.60451	0.08339	0.46511	C
202	6	C122	0.51010	0.09531	0.61239	C
203	1	H67	0.51378	0.02106	0.68110	H
204	6	C123	0.58178	0.12835	0.46385	C
205	1	H68	0.64117	0.07929	0.40200	H
206	6	C124	0.53358	0.13480	0.53340	C
207	1	H69	0.47300	0.10021	0.67133	H
208	1	H70	0.60114	0.15855	0.40187	H
209	6	C125	0.84829	1.00929	0.51747	C
210	6	C126	0.89728	1.00758	0.44996	C
211	6	C127	0.83165	1.05259	0.59342	C
212	6	C128	0.92847	1.04711	0.46017	C
213	1	H71	0.91122	0.97497	0.38514	H
214	6	C129	0.86256	1.09236	0.60150	C
215	1	H72	0.79421	1.05525	0.65161	H
216	6	C130	0.91169	1.09024	0.53658	C
217	1	H73	0.96644	1.04498	0.40633	H
218	1	H74	0.84862	1.12548	0.66303	H
219	6	C131	0.81411	0.74469	0.53065	C
220	6	C132	0.86165	0.73774	0.60488	C
221	6	C133	0.79018	0.70459	0.45709	C
222	6	C134	0.88533	0.69354	0.59651	C

223	1	H75	0.88056	0.76737	0.67183	H
224	6	C135	0.81364	0.65999	0.45096	C
225	1	H76	0.75321	0.70835	0.39707	H
226	6	C136	0.86224	0.65403	0.51608	C
227	1	H77	0.92269	0.68903	0.65262	H
228	1	H78	0.79454	0.62972	0.38828	H
229	6	C137	0.44889	0.65588	0.54370	C
230	1	H79	0.46678	0.62181	0.59058	H
231	6	C138	0.89066	0.60926	0.49443	C
232	1	H80	0.87059	0.57671	0.44492	H
233	7	N9	0.40240	0.65826	0.50539	N
234	7	N10	0.93765	0.61000	0.52337	N
235	6	C139	0.37198	0.61764	0.51024	C
236	6	C140	0.38449	0.57565	0.41710	C
237	6	C141	0.32655	0.61927	0.60273	C
238	6	C142	0.35177	0.53711	0.41427	C
239	1	H81	0.41857	0.57427	0.33698	H
240	6	C143	0.29668	0.57874	0.61283	C
241	1	H82	0.31668	0.65130	0.67915	H
242	6	C144	0.30767	0.53678	0.51585	C
243	1	H83	0.36057	0.50712	0.32623	H
244	1	H84	0.26483	0.57966	0.70335	H
245	6	C145	0.27464	0.49413	0.52025	C
246	6	C146	0.29834	0.44854	0.53203	C
247	6	C147	0.22220	0.50125	0.51379	C
248	6	C148	0.35090	0.43953	0.53838	C

249	7	N11	0.27584	0.40433	0.53174	N
250	7	N12	0.18585	0.46695	0.52173	N
251	6	C149	0.19886	0.54849	0.50785	C
252	6	C150	0.35844	0.39091	0.53040	C
253	1	H85	0.38070	0.46584	0.54924	H
254	6	C151	0.31077	0.36808	0.53232	C
255	1	H86	0.23776	0.39908	0.52987	H
256	6	C152	0.14077	0.49012	0.52609	C
257	6	C153	0.14916	0.54178	0.52796	C
258	1	H87	0.21645	0.58340	0.49064	H
259	1	H88	0.39497	0.37372	0.52283	H
260	6	C154	0.30173	0.31796	0.53945	C
261	6	C155	0.09250	0.46912	0.52060	C
262	1	H89	0.12206	0.57080	0.54450	H
263	6	C156	0.25352	0.29694	0.54553	C
264	6	C157	0.34552	0.28512	0.53532	C
265	6	C158	0.08349	0.41894	0.52251	C
266	6	C159	0.04897	0.50215	0.51097	C
267	6	C160	0.24520	0.24531	0.55077	C
268	7	N13	0.20843	0.32000	0.53651	N
269	6	C161	0.34395	0.24286	0.43303	C
270	6	C162	0.38928	0.29297	0.63333	C
271	7	N14	0.11851	0.38280	0.52876	N
272	6	C163	0.03589	0.39600	0.52655	C
273	6	C164	0.00453	0.49571	0.60781	C
274	6	C165	0.05171	0.54373	0.40597	C

275	6	C166	0.19569	0.23837	0.52734	C
276	1	H90	0.27231	0.21651	0.57091	H
277	6	C167	0.17222	0.28559	0.52864	C
278	6	C168	0.38117	0.20831	0.44218	C
279	1	H91	0.31295	0.23674	0.34271	H
280	6	C169	0.42923	0.26081	0.62937	C
281	1	H92	0.39193	0.32371	0.72271	H
282	6	C170	0.09613	0.33861	0.53832	C
283	1	H93	0.15657	0.38811	0.52439	H
284	6	C171	0.04355	0.34764	0.54497	C
285	1	H94	-0.00071	0.41287	0.51601	H
286	6	C172	0.96531	0.52860	0.60083	C
287	1	H95	0.00076	0.46572	0.69940	H
288	6	C173	0.01528	0.57913	0.41252	C
289	1	H96	0.08323	0.54866	0.31611	H
290	1	H97	0.17835	0.20332	0.51036	H
291	6	C174	0.11974	0.29285	0.53202	C
292	6	C175	0.42489	0.21711	0.53838	C
293	1	H98	0.37800	0.17518	0.36552	H
294	1	H99	0.46230	0.26783	0.70962	H
295	1	H100	0.01384	0.32155	0.56386	H
296	6	C176	0.97102	0.57184	0.50850	C
297	1	H101	0.93177	0.52269	0.68072	H
298	1	H102	0.01959	0.61172	0.33415	H
299	6	C177	0.08649	0.25039	0.52822	C
300	6	C178	0.09685	0.20837	0.62457	C

301	6	C179	0.04260	0.25030	0.42658	C
302	6	C180	0.06671	0.16804	0.61331	C
303	1	H103	0.12834	0.20723	0.71566	H
304	6	C181	0.00951	0.21208	0.42880	C
305	1	H104	0.03429	0.28029	0.33880	H
306	6	C182	0.02151	0.16997	0.52081	C
307	1	H105	0.07615	0.13594	0.68900	H
308	1	H106	-0.02435	0.21370	0.34858	H
309	6	C183	0.50546	0.17984	0.51566	C
310	1	H107	0.52507	0.21184	0.45970	H
311	6	C184	0.94414	1.13215	0.54975	C
312	1	H108	0.92609	1.16628	0.59649	H
313	7	N15	0.45896	0.17959	0.55375	N
314	7	N16	0.99089	1.12954	0.51412	N
315	6	C98	0.60196	-0.00537	0.52968	C
316	6	C119	0.58018	1.04338	0.53755	C
317	6	C164	1.00453	0.49571	0.60781	C
318	6	C172	-0.03469	0.52860	0.60083	C
319	6	C173	1.01528	0.57913	0.41252	C
320	6	C176	-0.02898	0.57184	0.50850	C
321	6	C182	1.02151	1.16997	0.52081	C
322	7	N16	-0.00911	0.12954	0.51412	N

Section S6

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