Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supporting Information

for

Norbornane-based covalent organic frameworks for gas separation

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Table of Contents

Section S1: Synthetic Procedures

Synthesis of CANAL(Me)$_2$. To a dry glass pressure flask (15 ml), 4-bromo-3-methylaniline (353.4 mg, 1.9 mmol), PPh_3 (20 mg, 0.076 mmol), $Pd(OAc)_2$ (8.55 mg, 0.038 mmol), Cs_2CO_3 (618 mg, 1.9 mmol), norbornadiene (430 mg, 4.56 mmol), and 2 mL of 1,4-dioxane were added under inert atmosphere. The flask was sealed with a Teflon cap, and the mixture was stirred at 150 °C for 24 h. The mixture was then cooled to room temperature, passed through Celite to remove inorganic solvents. The filtered solution was then concentrated by rotavap, and the obtained crude product was washed three times with methanol prior to silica column purification (dichloromethane/hexane: 1/1). The obtained solid was dried under vacuum to obtain CANAL(Me)$_2$ (275 mg, 72% yield). ^{1}H NMR (400 MHz, DMSO-d$_6$, δ): 0.65 (s, 2H), 1.98 (m, 6H), 3.0 (m, 4H), 4.73 (br s, 4H), 6.06 (s, 2H), 6.17 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d$_6$, δ): 17.1, 24.6, 36.6, 36.7, 47.4, 48, 105.7, 114.5, 131.9, 132.1, 146, 146.2, 149.1, 149.2. ESI-MS m/z Calcd for $[C_{21}H_{23}N_2]^+$ [M+H$^+$]: 303.1783; found: 303.2027.

Synthesis of CANAL(Me)$_4$. To a dry glass pressure flask (15 ml), 4-bromo-2,5-dimethylaniline (200 mg, 1.0 mmol), PPh_3 (10 mg, 0.04 mmol), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), norbornadiene (0.05 ml, 0.5 mmol), and 1 mL of 1,4-dioxane were added under inert atmosphere. The flask was sealed with a Teflon cap, and the mixture was stirred at 150 °C for 24 h. The mixture was then cooled to room temperature, passed through Celite to remove inorganic solvents. The filtered solution was then concentrated by rotavap, and the obtained crude product was washed three times with methanol prior to silica column purification (dichloromethane/hexane: 1/1). The obtained solid was dried under vacuum to obtain CANAL(Me)$_4$ (140 mg, 75% yield). ^{1}H NMR (400 MHz, DMSO-d$_6$, δ): 0.60 (s, 2H), 1.91 (s, 6H), 2.02 (s, 6H), 2.13-2.21 (m, 2H), 3.02 (m, 4H), 4.26 (br s, 4H), 6.46 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d$_6$, δ): 12.5, 12.6, 19, 26.4, 36, 36.9, 37.9, 47.5, 47.6, 47.7, 47.9, 11.6, 120.65, 121.4, 132.9, 142.8, 142.9, 143.9. ESI-MS m/z Calcd for $[C_{23}H_{27}N_2]^+$ [M+H$^+$]: 331.2130; found: 331.2082.

General procedure for the synthesis of covalent organic frameworks (COFs). The COFs were synthesized following method reported in the literature.[2] In a typical synthesis, a pyrex tube (outer diameter x inner diameter = 20 mm x 18 mm, and length 25 cm) is charged with the 0.3 mmol of **Tp**, 0.45 mmol of corresponding diamine in 3 mL of mixture of mesitylene and 1,4-dioxane (1:1, v/v), and 0.4 mL of acetic acid. After sonication for 15 minutes, the mixture was subjected to three consecutive freeze-pump-thaw cycles under liquid nitrogen (77K). The pyrex tube was sealed under 1 mbar vacuum and heated in an oven maintained at 120 °C for 72 h. The resulted solid material was then purified by immersing in hot water followed by solvent exchange hot N,N-dimethylacetamide for several days. After washing with water and acetone, the obtained COFs were dried at 100 °C in a vacuum oven to isolate crystalline porous COFs.

Section S2: NMR characterizations of diamines

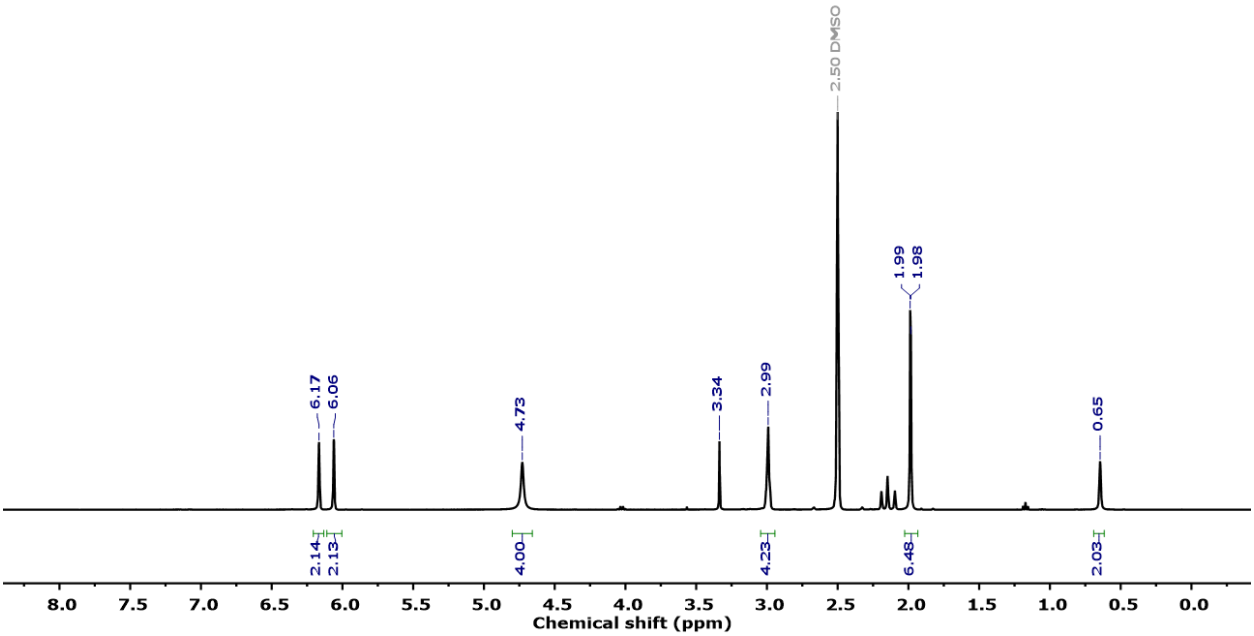

Figure S1. ^{1}H NMR spectrum of CANAL(Me)$_2$ recorded in DMSO-d$_6$.

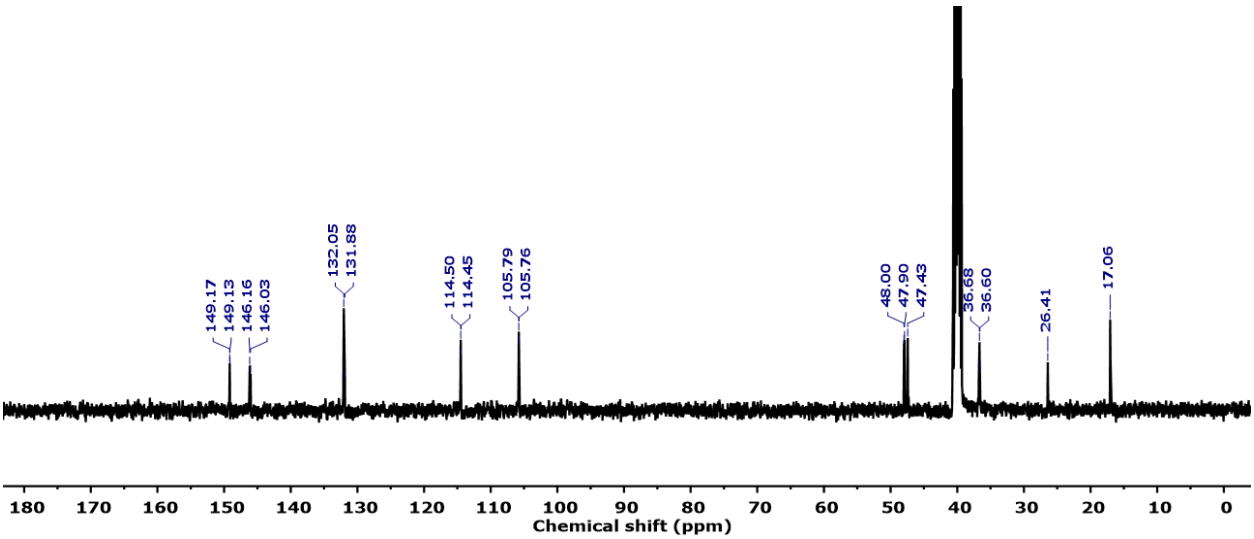

Figure S2. ^{13}C NMR spectrum of CANAL(Me)$_2$ recorded in DMSO-d$_6$.

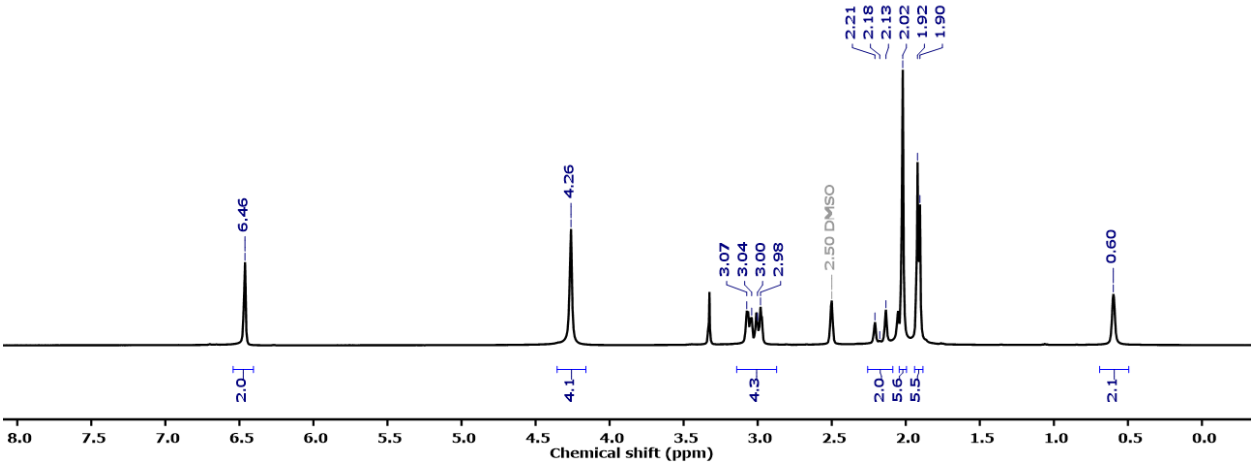

Figure S3. ^{1}H NMR spectrum of CANAL $(Me)_4$ recorded in DMSO-d_6.

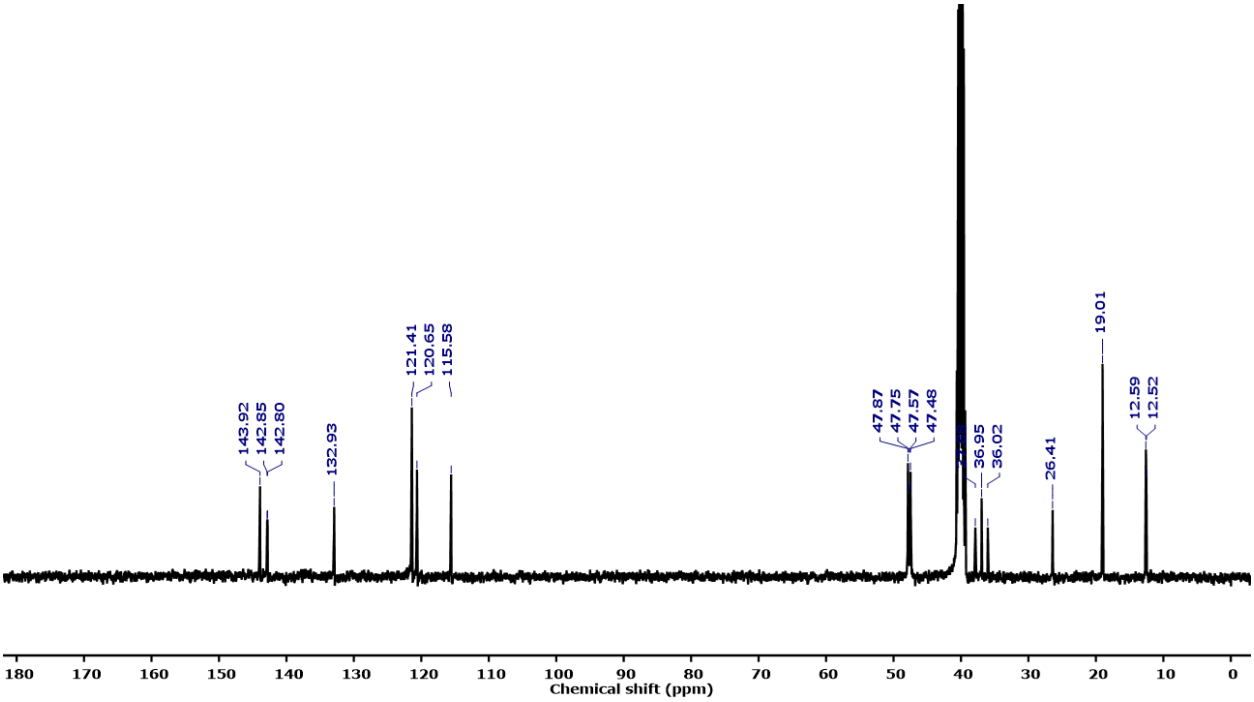

Figure S4. ^{13}C NMR spectrum of CANAL$(Me)_4$ recorded in DMSO-d_6.

Section S3: PXRD simulation, Pawley refinement and fractional atomic coordinates of the as-synthesized COFs

For each COF, the monolayer structures were optimized using DFTB+ version 19.1 [10.1021/jp070186p] using the Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) method, including Lennard-Jones dispersion. C, N, O and H atoms were described using the mio-0-1 parameter set [DOI: 10.1103/PhysRevB.58.7260]. From the optimized monolayers, AA (eclipsed), AB (staggered) and ABC structures were generated as bilayers of each monolayer.

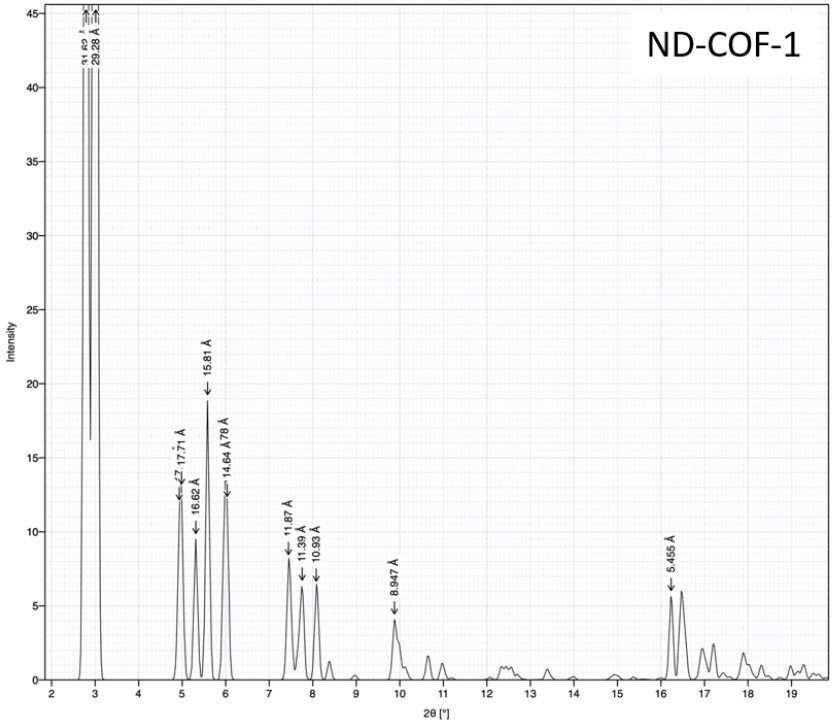

Figure S5. Simulated PXRD pattern of **ND-COF-1** showing *d*-spacing for AA stacking model.

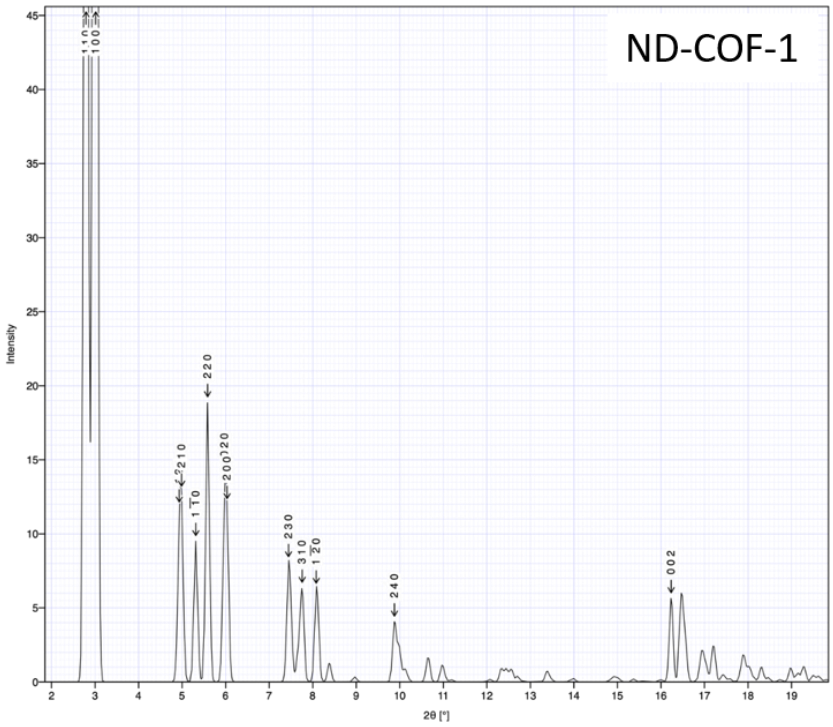

Figure S6. Simulated PXRD pattern of **ND-COF-1** showing *hkl* values for AA stacking model.

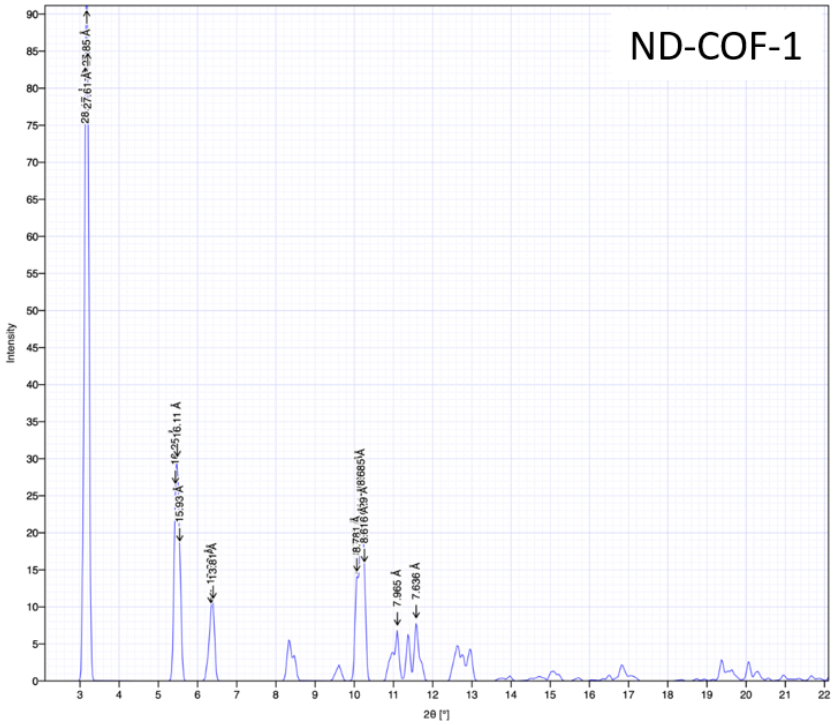

Figure S7. Simulated PXRD pattern of **ND-COF-1** showing *d*-spacing values for the AB model.

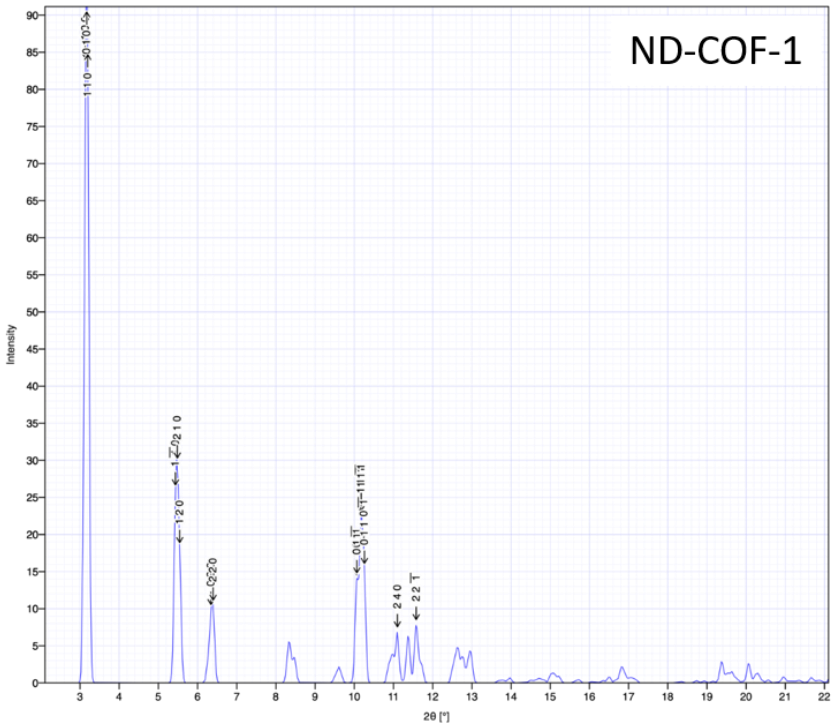

Figure S8. Simulated PXRD pattern of **ND-COF-1** showing *hkl* values for AB model.

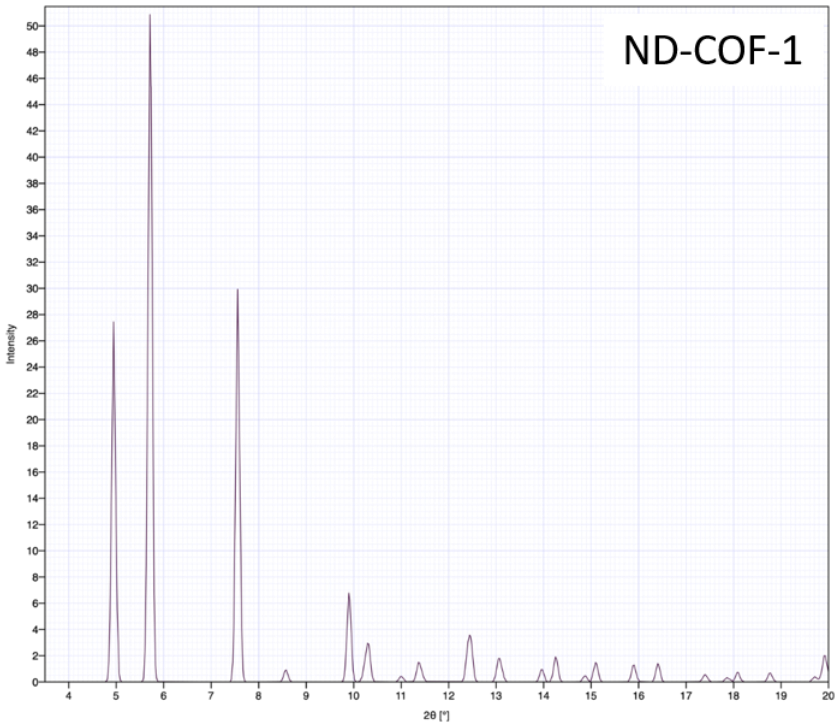

Figure S9. Full image of PXRD pattern simulated for the **ND-COF-1** where linkers can point up or down relative to the connectors.

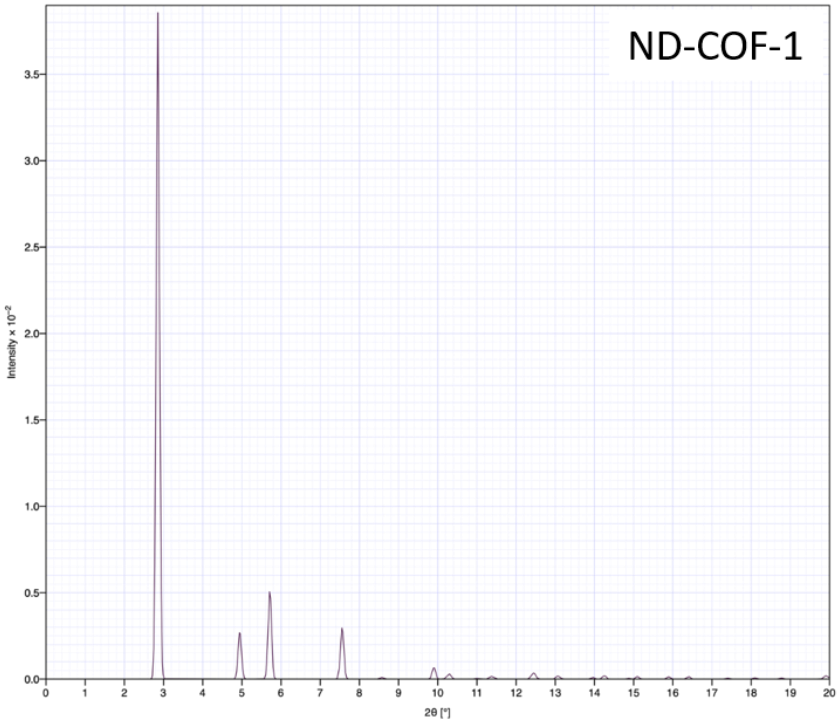

Figure S10. Magnified image of the PXRD pattern simulated for the **ND-COF-1** with layer-mismatch stacking.

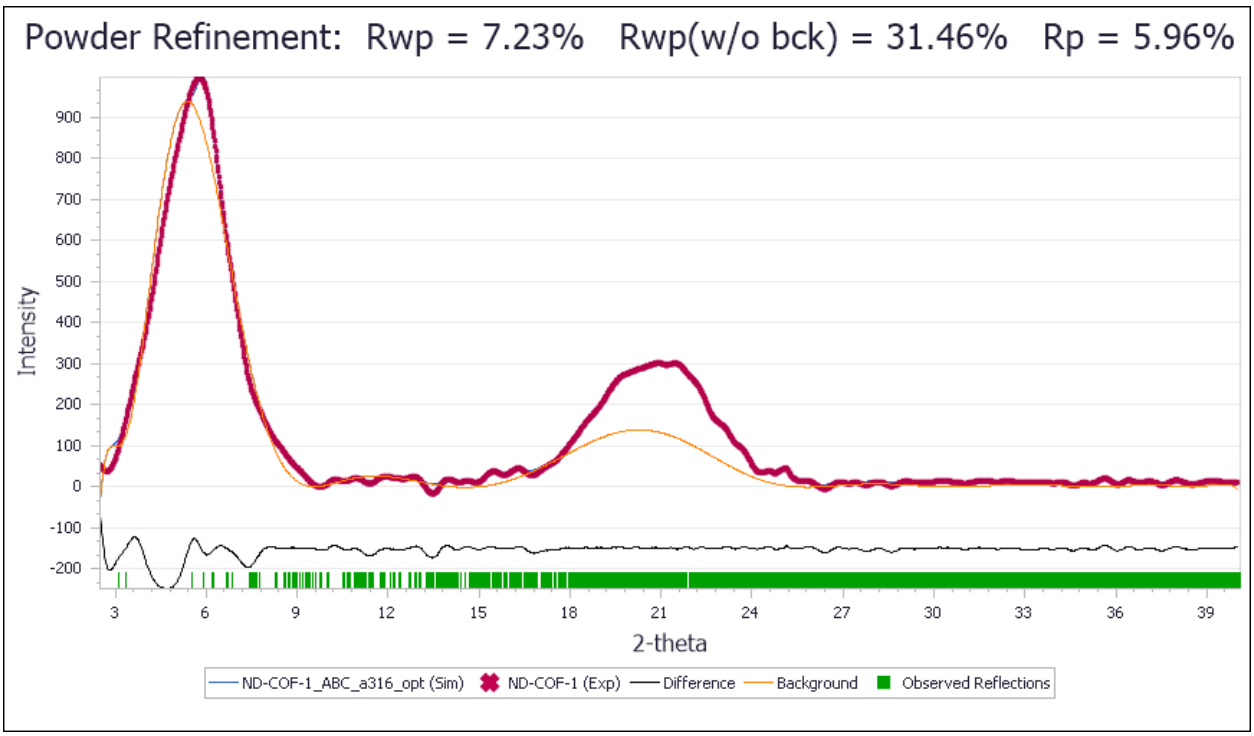

Figure S11. Pawley refinement for ND-COF-1. Pawley refinement suggests that the simulated (blue) and experimental (red) PXRD patterns are in good agreement. The black line denotes the refinement difference, and green lines denote observed reflections.

Table S1. Fractional atomic coordinates for the unit cell of ND-COF-1.

ND-COF-1 in ABC stacking model											
a = 30.07 Å , b = 32.35 Å, c = 12.96 Å, α = 92.62°, β = 88.24°, γ = 117.73°											
Atoms	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**
C1	0.45884	0.51376	0.82922	**C47**	0.5542	1.02463	0.78146	**C7**	0.79213	0.18041	0.49658
C2	0.48503	0.94343	0.82224	**C48**	-0.02456	0.52967	0.78137	**C8**	0.81962	0.61176	0.4965
C3	0.05658	0.5416	0.82219	**C4**	0.12557	0.84727	0.16295	**C9**	0.38824	0.20777	0.49604
C10	0.45547	0.46836	0.87324	**C5**	0.15288	0.27842	0.16272	**C16**	0.78883	0.13502	0.54047
C11	0.53213	0.98591	0.87026	**C6**	0.72172	0.87444	0.16298	**C17**	0.865	0.65384	0.54043
C12	0.01415	0.54631	0.87016	**C13**	0.12222	0.80191	0.20716	**C18**	0.3462	0.21114	0.54002
C19	0.53127	0.51651	0.87181	**C14**	0.19829	0.32046	0.2067	**C25**	0.86461	0.18321	0.53881
C20	0.48257	0.01507	0.86876	**C15**	0.67968	0.87776	0.20715	**C26**	0.81681	0.68143	0.53879
C21	0.98489	0.4675	0.86862	**C22**	0.19801	0.85007	0.20556	**C27**	0.31857	0.13535	0.53866
C28	0.51306	0.54872	0.8301	**C23**	0.15012	0.34809	0.20536	**C34**	0.84634	0.21538	0.49725
C29	0.45015	0.96326	0.82291	**C24**	0.65207	0.80197	0.20543	**C35**	0.78464	0.631	0.49718
C30	0.03671	0.48689	0.82286	**C31**	0.17978	0.88223	0.16372	**C36**	0.36898	0.15355	0.49697
C37	0.49496	0.4863	0.95318	**C32**	0.11792	0.29768	0.16365	**C43**	0.82837	0.15297	0.62027
C38	0.51352	0.0082	0.95013	**C33**	0.70248	0.82023	0.16368	**C44**	0.84704	0.67541	0.62024
C39	0.99178	0.50536	0.95026	**C40**	0.16173	0.81992	0.28705	**C45**	0.32466	0.17168	0.61999
C46	0.47106	0.44582	0.78914	**C41**	0.18036	0.34199	0.28668	**C52**	0.80438	0.1125	0.45622
C47	0.5542	0.02463	0.78146	**C42**	0.65816	0.83822	0.28696	**C53**	0.88753	0.69193	0.45621
C48	0.97544	0.52967	0.78137	**C49**	0.13778	0.77928	0.12319	**C54**	0.30807	0.19554	0.45591

C55	0.52551	0.48093	0.78682	**C50**	0.22081	0.3586	0.12259	**C61**	0.85882	0.14764	0.45378
C56	0.51924	0.04459	0.77931	**C51**	0.64153	0.86222	0.12312	**C62**	0.85238	0.71123	0.45378
C57	0.9554	0.47474	0.77922	**C58**	0.19223	0.81442	0.12075	**C63**	0.28874	0.14109	0.45365
C64	0.48084	0.40626	0.81577	**C59**	0.18569	0.37792	0.12036	**C70**	0.81426	0.07299	0.48267
C65	0.59374	0.07459	0.81398	**C60**	0.62222	0.80778	0.12057	**C71**	0.92704	0.74132	0.48269
C66	0.92553	0.51935	0.81393	**C67**	0.14764	0.73979	0.15005	**C72**	0.25871	0.18571	0.4825
C73	0.46017	0.35834	0.77845	**C68**	0.26035	0.40796	0.14919	**C79**	0.79365	0.02507	0.44529
C74	0.64191	0.10255	0.77904	**C69**	0.59217	0.85235	0.14991	**C80**	0.97495	0.76862	0.4453
C75	0.89764	0.53965	0.77903	**C76**	0.12702	0.69181	0.1131	**C81**	0.23141	0.20632	0.44511
C82	0.49236	0.34127	0.75251	**C77**	0.30825	0.43527	0.11175	**C88**	0.82589	0.00807	0.4193
C83	0.6589	0.15195	0.75487	**C78**	0.56483	0.873	0.11298	**C89**	0.99195	0.81785	0.41928
C84	0.84823	0.50732	0.75486	**C85**	0.15925	0.67476	0.08745	**C90**	0.18216	0.17409	0.41918
C91	0.54318	0.37446	0.74754	**C86**	0.32526	0.48451	0.08582	**C97**	0.8767	0.04132	0.41434
C92	0.62576	0.16963	0.74941	**C87**	0.51557	0.84079	0.08717	**C98**	0.95871	0.83542	0.41432
C93	0.83045	0.45648	0.74939	**C94**	0.21007	0.708	0.08244	**C99**	0.16457	0.12328	0.4143
C100	0.56159	0.42415	0.76953	**C95**	0.29202	0.50209	0.08101	**C106**	0.89505	0.09099	0.43638
C101	0.57592	0.13847	0.76998	**C96**	0.49799	0.78998	0.08197	**C107**	0.90904	0.8041	0.43639
C102	0.86153	0.43771	0.76994	**C103**	0.22842	0.7577	0.10407	**C108**	0.19588	0.10491	0.43642
C109	0.52974	0.43792	0.81121	**C104**	0.24236	0.47078	0.10319	**C115**	0.86315	0.10469	0.47811
C110	0.56155	0.0926	0.81057	**C105**	0.52933	0.7716	0.10359	**C116**	0.89534	0.7585	0.47813
C111	0.90743	0.46913	0.8105	**C112**	0.19652	0.77148	0.14544	**C117**	0.2415	0.13682	0.47806
C118	0.42198	0.56511	0.88767	**C113**	0.22866	0.42516	0.14479	**C124**	0.75533	0.2318	0.55544
C119	0.43438	0.85575	0.88891	**C114**	0.57497	0.80347	0.14515	**C125**	0.76823	0.52356	0.55519
C120	0.14424	0.5786	0.8889	**C121**	0.08879	0.89875	0.2213	**C126**	0.47646	0.24457	0.55457
C127	0.45509	0.54885	0.89851	**C122**	0.10145	0.19019	0.22124	**C133**	0.78845	0.21551	0.566
C128	0.45122	0.90524	0.89781	**C123**	0.80996	0.91122	0.22141	**C134**	0.7845	0.57295	0.56587
C129	0.09474	0.54596	0.8978	**C130**	0.12188	0.88245	0.23211	**C135**	0.42707	0.21149	0.56536
C136	0.50431	0.58066	0.90133	**C131**	0.11776	0.23959	0.23203	**C142**	0.83767	0.24733	0.56858
C137	0.41881	0.92331	0.89997	**C132**	0.76057	0.87812	0.23218	**C143**	0.75268	0.59035	0.56847
C138	0.07665	0.49548	0.89996	**C139**	0.1711	0.91424	0.23486	**C144**	0.40964	0.16226	0.56822
C145	0.52332	0.6312	0.89405	**C140**	0.08596	0.25702	0.23489	**C151**	0.85669	0.29787	0.56128
C146	0.36831	0.8916	0.89553	**C141**	0.74315	0.8289	0.23488	**C152**	0.70215	0.55884	0.56107
C147	0.10835	0.47667	0.89549	**C148**	0.19016	0.96478	0.22755	**C153**	0.44113	0.14321	0.56102
C154	0.49025	0.64875	0.89098	**C149**	0.03542	0.22553	0.22767	**C160**	0.82363	0.31542	0.55845
C155	0.35087	0.84101	0.89423	**C150**	0.77465	0.80986	0.22756	**C161**	0.6846	0.50822	0.55805
C156	0.15895	0.50982	0.89406	**C157**	0.15711	0.98237	0.22458	**C162**	0.49176	0.17626	0.55804
C163	0.43945	0.61548	0.8852	**C158**	0.01783	0.1749	0.22468	**C169**	0.77282	0.28217	0.55293
C164	0.38394	0.82323	0.88801	**C159**	0.82527	0.84292	0.22462	**C170**	0.71786	0.49067	0.5525
C165	0.17674	0.56066	0.88785	**C166**	0.10631	0.94913	0.21888	**C171**	0.50933	0.22706	0.55225
C172	0.57722	0.66565	0.8866	**C167**	0.05107	0.15733	0.2189	**C178**	0.91059	0.33229	0.55343
C173	0.33363	0.91079	0.88851	**C168**	0.84283	0.89372	0.21896	**C179**	0.66772	0.57831	0.55334
C174	0.08914	0.4228	0.88856	**C175**	0.24407	0.99919	0.22	**C180**	0.42164	0.0893	0.55353
C181	0.40601	0.32685	0.76577	**C176**	0.00102	0.24504	0.22013	**C187**	0.73951	-0.00646	0.43252
C182	0.67369	0.08024	0.76596	**C177**	0.75516	0.75596	0.21998	**C188**	1.00648	0.746	0.43255
C183	0.92005	0.59375	0.76599	**C184**	0.07287	0.66025	0.10054	**C189**	0.25403	0.26047	0.43231
C190	0.37997	0.66859	0.7331	**C185**	0.33979	0.41266	0.09894	**C196**	0.71351	0.33508	0.39986
C191	0.33098	0.71141	0.73456	**C186**	0.58743	0.92716	0.10061	**C197**	0.66495	0.37831	0.39966
C192	0.28823	0.61965	0.73348	**C193**	0.04688	1.00196	0.06592	**C198**	0.62171	0.2865	0.39963
C199	0.37803	0.71341	0.71279	**C194**	0.99817	1.04504	0.06604	**C205**	0.71184	0.37994	0.37823
C200	0.28626	0.66478	0.71268	**C195**	0.95508	0.95323	0.06602	**C206**	0.62008	0.33177	0.37819

C201	0.33484	0.62165	0.71105	**C202**	0.0451	1.04677	0.04446	**C207**	0.66827	0.28818	0.37829
O1	0.41551	0.75258	0.69872	**C203**	0.95334	0.99844	0.04465	**O7**	0.74942	0.41892	0.36338
O2	0.24711	0.66313	0.69865	**C204**	1.00167	0.95501	0.04446	**O8**	0.58109	0.33036	0.36337
O3	0.33644	0.58421	0.6955	**O4**	0.08264	1.0858	0.02969	**O9**	0.6697	0.25061	0.36358
C208	0.41506	0.67101	0.79695	**O5**	0.9143	0.99695	0.03002	**C214**	0.74851	0.3376	0.46417
C209	0.32826	0.74364	0.79933	**O6**	1.00317	0.91747	0.02973	**C215**	0.66246	0.4109	0.46368
C210	0.25614	0.58463	0.79832	**C211**	0.08195	1.00453	0.13006	**C216**	0.58911	0.25141	0.46361
N1	0.40511	0.63134	0.86657	**C212**	0.99563	1.07756	0.13017	**N7**	0.73852	0.29807	0.53426
N2	0.36758	0.77288	0.87013	**C213**	0.92258	0.91813	0.13011	**N8**	0.70198	0.44048	0.53376
N3	0.22708	0.59463	0.86986	**N4**	0.07202	0.96505	0.20026	**N9**	0.55954	0.26136	0.53367
C217	0.61693	0.32646	0.82117	**N5**	0.03514	0.10712	0.20028	**C223**	0.9507	-0.0069	0.48616
C218	0.67358	0.29151	0.82251	**N6**	0.89304	0.92803	0.20037	**C224**	0.0069	-0.04238	0.48614
C219	0.70851	0.38309	0.82253	**C220**	0.28408	0.65968	0.15425	**C225**	0.04239	0.0493	0.48616
C226	0.62409	0.28452	0.839	**C221**	0.34028	0.62419	0.15331	**C232**	0.95759	-0.04903	0.50345
C227	0.71544	0.34064	0.84043	**C222**	0.37579	0.71588	0.15409	**C233**	0.04903	0.00664	0.50348
C228	0.65932	0.37588	0.83916	**C229**	0.29099	0.61753	0.17101	**C234**	-0.00664	0.04241	0.50349
O10	0.58933	0.24414	0.85943	**C230**	0.38242	0.67318	0.17088	**O16**	0.92278	-0.08927	0.5246
O11	0.75578	0.34635	0.86172	**C231**	0.32677	0.70897	0.17161	**O17**	0.08927	0.01207	0.52466
O12	0.65356	0.41055	0.85968	**O13**	0.25618	0.57725	0.19197	**O18**	-0.01207	0.07722	0.52469
C235	0.57638	0.31965	0.77228	**O14**	0.42266	0.67856	0.19186	**C241**	0.90998	-0.01348	0.4385
C236	0.68058	0.25769	0.77462	**O15**	0.32136	0.74379	0.19295	**C242**	0.01349	-0.07651	0.43846
C237	0.74242	0.42369	0.77416	**C238**	0.24331	0.65316	0.10695	**C243**	0.07651	0.09001	0.43846
N10	0.57607	0.35861	0.71572	**C239**	0.34685	0.59014	0.10519	**N16**	0.90965	0.02557	0.38237
N11	0.64185	0.21843	0.71756	**C240**	0.40995	0.75668	0.10673	**N17**	0.97446	0.88412	0.38231
N12	0.78161	0.42385	0.71762	**N13**	0.24303	0.69221	0.05074	**N18**	0.11587	0.09034	0.38231
H1	0.43943	0.50798	0.7546	**N14**	0.30777	0.5508	0.04909	**H7**	0.77264	0.17462	0.42207
H2	0.4888	0.92911	0.74416	**N15**	0.44925	0.75706	0.0502	**H8**	0.82541	0.59808	0.42197
H3	0.07093	0.55969	0.74412	**H4**	0.10612	0.84144	0.08837	**H9**	0.40189	0.22718	0.42143
H10	0.41949	0.44314	0.90389	**H5**	0.15864	0.26477	0.08811	**H16**	0.75287	0.10977	0.57122
H11	0.55785	0.97494	0.90292	**H6**	0.73535	0.89391	0.08843	**H17**	0.89024	0.64312	0.57118
H12	0.02516	0.58303	0.90274	**H13**	0.08624	0.77671	0.23788	**H18**	0.35697	0.24713	0.57062
H19	0.56845	0.53715	0.90078	**H14**	0.22352	0.3097	0.23729	**H25**	0.90181	0.20387	0.56767
H20	0.46181	0.03222	0.89994	**H15**	0.69044	0.91372	0.23793	**H26**	0.79614	0.69796	0.56766
H21	0.9677	0.42958	0.89969	**H22**	0.2352	0.87074	0.23446	**H27**	0.30203	0.09818	0.56768
H28	0.5304	0.56667	0.7561	**H23**	0.12949	0.36462	0.23439	**H34**	0.86361	0.23332	0.42318
H29	0.43228	0.96101	0.74531	**H24**	0.63554	0.76477	0.23427	**H35**	0.76671	0.63034	0.42311
H30	0.03896	0.47127	0.74526	**H31**	0.1971	0.90013	0.08966	**H36**	0.36959	0.1362	0.42298
H37	0.49143	0.50521	1.02153	**H32**	0.09997	0.29708	0.08966	**H43**	0.82487	0.17187	0.68869
H38	0.49435	-0.01429	1.01807	**H33**	0.70309	0.80294	0.08961	**H44**	0.82814	0.65301	0.68864
H39	1.01431	0.50865	1.01838	**H40**	0.15822	0.83888	0.35532	**H45**	0.34709	0.17522	0.68836
H46	0.50062	0.45916	0.99343	**H41**	0.16147	0.31956	0.35504	**H52**	0.83408	0.12584	0.66042
H47	0.54093	0.04095	0.98983	**H42**	0.68061	0.84171	0.35527	**H53**	0.87416	0.70825	0.66042
H48	0.95893	0.50002	0.99002	**H49**	0.16741	0.79282	0.32742	**H54**	0.29185	0.16602	0.66022
H55	0.45085	0.43909	0.71542	**H50**	0.20751	0.3748	0.32692	**H61**	0.78413	0.10577	0.38257
H56	0.56028	0.01215	0.70328	**H51**	0.62536	0.83251	0.32729	**H62**	0.89426	0.67842	0.38256
H57	0.98793	0.54823	0.70319	**H58**	0.11755	0.77246	0.04949	**H63**	0.32154	0.21573	0.38217
H64	0.54249	0.49798	0.71189	**H59**	0.22753	0.34513	0.04885	**H70**	0.87575	0.1647	0.37882
H65	0.50359	0.04432	0.69998	**H60**	0.65497	0.8825	0.04947	**H71**	0.83533	0.71111	0.37881
H66	0.95564	0.45935	0.69988	**H67**	0.20918	0.83139	0.04574	**H72**	0.28882	0.1241	0.37874
H73	0.47815	0.30358	0.72944	**H68**	0.16862	0.37785	0.04545	**H79**	0.81172	-0.0296	0.39613

H74	0.69672	0.17565	0.73301	**H69**	0.6223	0.79087	0.04554	**H80**	1.02963	0.84135	0.39609
H75	0.82459	0.52151	0.73302	**H76**	0.14508	0.63705	0.06456	**H81**	0.15866	0.18827	0.39601
H82	0.5993	0.45119	0.75371	**H77**	0.36292	0.50801	0.06261	**H88**	0.93275	0.11806	0.42058
H83	0.54917	0.14946	0.75355	**H78**	0.49204	0.85498	0.06433	**H89**	0.88197	0.81472	0.42059
H84	0.85046	0.39994	0.75352	**H85**	0.26612	0.78475	0.08821	**H90**	0.18524	0.06721	0.42069
H91	0.38408	0.53929	0.87017	**H86**	0.21529	0.48142	0.08756	**H97**	0.7174	0.20598	0.53813
H92	0.45978	0.84318	0.87106	**H87**	0.51868	0.73392	0.08758	**H98**	0.79406	0.51146	0.53792
H93	0.15682	0.61658	0.87108	**H94**	0.05088	0.87296	0.20382	**H99**	0.48858	0.28248	0.53701
H100	0.50406	0.68771	0.88755	**H95**	0.12723	0.17807	0.20368	**H106**	0.83745	0.35439	0.55494
H101	0.31189	0.81584	0.89233	**H96**	0.82206	0.94914	0.20395	**H107**	0.64563	0.48307	0.55447
H102	0.18412	0.49601	0.89209	**H103**	0.17094	1.02134	0.22116	**H108**	0.5169	0.16243	0.55468
H109	0.58591	0.68557	0.80996	**H104**	-0.02114	0.14976	0.22131	**H115**	0.91917	0.35213	0.4767
H110	0.31307	0.89882	0.8127	**H105**	0.85043	0.8291	0.22117	**H116**	0.64788	0.5671	0.4766
H111	0.10109	0.41418	0.81276	**H112**	0.25275	1.01912	0.14338	**H117**	0.43288	0.08061	0.47692
H118	0.59785	0.64575	0.8915	**H113**	-0.0189	0.2338	0.1435	**H124**	0.93121	0.31238	0.55822
H119	0.35343	0.95137	0.89182	**H114**	0.76642	0.74729	0.14335	**H125**	0.68763	0.61884	0.55824
H120	0.04857	0.40203	0.89191	**H121**	0.26466	0.97925	0.22478	**H126**	0.38111	0.06871	0.55833
H127	0.58913	0.69231	0.95294	**H122**	0.02096	0.28557	0.22493	**H133**	0.92261	0.35902	0.61965
H128	0.30754	0.89649	0.95597	**H123**	0.71463	0.73536	0.22476	**H134**	0.64099	0.56356	0.61955
H129	0.10345	0.41102	0.95604	**H130**	0.25604	1.02584	0.28636	**H135**	0.43633	0.07735	0.61991
H136	0.3961	0.2895	0.73926	**H131**	-0.02564	0.23035	0.28648	**H142**	0.72964	-0.04379	0.40604
H137	0.71112	0.10797	0.74065	**H132**	0.76985	0.74399	0.28634	**H143**	1.04382	0.77346	0.40606
H138	0.89237	0.60353	0.74075	**H139**	0.06298	0.62284	0.07453	**H144**	0.22657	0.27034	0.40576
H145	0.39269	0.34318	0.7058	**H140**	0.37711	0.44012	0.07237	**H151**	0.72618	0.00985	0.37249
H146	0.65777	0.05101	0.70499	**H141**	0.55993	0.93707	0.0746	**H152**	0.99018	0.71637	0.37252
H147	0.94927	0.60702	0.70498	**H148**	0.05951	0.67641	0.04024	**H153**	0.28367	0.27379	0.37232
H154	0.38772	0.32397	0.84279	**H149**	0.32346	0.38301	0.03897	**H160**	0.72117	-0.00936	0.5095
H155	0.67623	0.06431	0.84257	**H150**	0.61698	0.94056	0.04038	**H161**	1.00938	0.73057	0.50953
H156	0.93603	0.6122	0.84259	**H157**	0.05458	0.65754	0.17748	**H162**	0.26944	0.27881	0.5093
H163	0.44778	0.70581	0.81068	**H158**	0.34274	0.39726	0.17593	**H169**	0.78126	0.3724	0.47761
H164	0.2934	0.74149	0.81267	**H159**	0.60297	0.94539	0.17763	**H170**	0.62767	0.4089	0.47696
H165	0.25831	0.5519	0.81113	**H166**	0.11471	1.03934	0.14339	**H171**	0.59111	0.21862	0.47692
H172	0.36877	0.60703	0.88673	**H167**	0.96082	1.07551	0.14356	**H178**	0.70218	0.27386	0.55462
H173	0.39169	0.7606	0.89022	**H168**	0.92465	0.88537	0.14335	**H179**	0.72619	0.42836	0.5542
H174	0.23941	0.631	0.89022	**H175**	0.03569	0.94084	0.22067	**H180**	0.57165	0.29768	0.55407
H181	0.5453	0.2832	0.76323	**H176**	0.05936	0.095	0.22061	**H187**	0.87868	-0.04984	0.43013
H182	0.71705	0.263	0.76665	**H177**	0.90515	0.96435	0.22082	**H188**	0.04986	-0.07144	0.4301
H183	0.73716	0.45485	0.76513	**H184**	0.21198	0.61682	0.09865	**H189**	0.07144	0.12131	0.43006
H190	0.60844	0.38427	0.67856	**H185**	0.38322	0.59524	0.09652	**H196**	0.94196	0.05126	0.34505
H191	0.61647	0.22521	0.67932	**H186**	0.40492	0.78802	0.09881	**H197**	0.94876	0.89072	0.34499
H192	0.77469	0.39152	0.67995	**H193**	0.27533	0.71787	0.0134	**H198**	0.10926	0.05803	0.345
C11	0.53213	-0.01409	0.87026	**H194**	0.28204	0.55743	0.01203	**C223**	-0.0493	-0.0069	0.48616
C12	1.01415	0.54631	0.87016	**H195**	0.4426	0.7248	0.01257	**C224**	1.0069	-0.04238	0.48614
C20	0.48257	1.01507	0.86876	**C193**	1.04688	1.00196	0.06592	**C232**	-0.04241	-0.04903	0.50345
C21	-0.01511	0.4675	0.86862	**C194**	-0.00183	1.04504	0.06604	**C234**	0.99336	0.04241	0.50349
C29	0.45015	-0.03674	0.82291	**C202**	1.0451	1.04677	0.04446	**C242**	1.01349	0.92349	0.43846
C30	1.03671	0.48689	0.82286	**C204**	0.00167	0.95501	0.04446	**N17**	-0.02554	-0.11588	0.38231
C38	0.51352	1.0082	0.95013	**C212**	-0.00437	0.07756	0.13017				
C39	-0.00822	0.50536	0.95026	**N5**	1.03514	1.10712	0.20028				

Table S2. Fractional atomic coordinates for the unit cell of ND-COF-1.

ND-COF-1 in eclipsed AA model (Space group *P*1)											
a = 34.39 Å, b = 34.19 Å, c = 10.89 Å, α = 90.33°, β = 89.02°, γ = 60.14°											
Atoms	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**
N1	0.65752	0.66105	0.05009	**H100**	0.21953	0.61947	0.37629	**C61**	0.26944	0.22564	0.70738
H2	0.66486	0.66059	-0.04364	**H102**	0.22613	0.61911	0.21118	**C63**	0.23505	0.21503	0.72666
C2	0.9094	0.55369	0.17845	**H104**	0.18753	0.60379	0.27885	**C65**	0.24492	0.17063	0.74573
C4	0.86688	0.57055	0.26177	**C126**	0.52769	0.50558	0.27615	**C67**	0.28933	0.13758	0.75959
C6	0.85955	0.52602	0.12587	**H106**	0.52862	0.48644	0.35901	**H55**	0.20053	0.24049	0.71262
C8	0.90454	0.52301	0.0854	**H108**	0.52251	0.48941	0.19424	**H57**	0.21892	0.16171	0.74029
H4	0.9152	0.58013	0.13757	**H110**	0.56052	0.50413	0.26496	**C69**	0.48038	0.94471	0.68966
H6	0.9077	0.53057	-0.01164	**C128**	0.24532	0.37485	0.28407	**C71**	0.43685	0.97713	0.72298
C10	0.86002	0.52981	0.26504	**C130**	0.21758	0.42019	0.22987	**C73**	0.40186	0.96748	0.72046
H8	0.82834	0.53628	0.31175	**C132**	0.17065	0.43367	0.19685	**C75**	0.40931	0.92539	0.67889
H10	0.88753	0.49963	0.30822	**C134**	0.15216	0.40349	0.22742	**C77**	0.45427	0.89066	0.65553
C12	0.82715	0.60442	0.18414	**C136**	0.18475	0.35485	0.24558	**C79**	0.48937	0.90091	0.66225
H12	0.83022	0.63267	0.14425	**C138**	0.2332	0.33973	0.25808	**H59**	0.50607	0.95384	0.67664
C14	0.82234	0.57403	0.09004	**O2**	0.17172	0.32755	0.25202	**H61**	0.52315	0.87615	0.63433
H14	0.8224	0.58375	-0.00652	**O4**	0.27842	0.36594	0.34373	**C81**	0.36954	0.91999	0.6508
H16	0.8693	0.58472	0.35092	**O6**	0.14752	0.46926	0.14481	**H63**	0.34901	0.92595	0.73584
H18	0.85484	0.49818	0.09075	**C140**	0.10758	0.41911	0.24036	**H65**	0.34865	0.94484	0.58126
C16	0.78068	0.61752	0.23036	**H112**	0.09602	0.39636	0.2715	**H67**	0.37929	0.88601	0.61392
C18	0.74498	0.6599	0.26289	**C142**	0.26581	0.29738	0.22905	**C83**	0.35374	0.19694	0.67312
C20	0.70297	0.67333	0.21109	**H114**	0.30037	0.28909	0.23857	**H69**	0.38582	0.16441	0.67124
C22	0.69856	0.64701	0.1158	**C144**	0.23478	0.44694	0.20018	**H71**	0.34839	0.21072	0.57915
C24	0.73643	0.60584	0.07947	**H116**	0.21505	0.47638	0.14466	**H73**	0.35787	0.21951	0.73812
C26	0.77617	0.59042	0.14236	**N3**	0.07514	0.46566	0.21935	**C85**	0.36758	0.51462	0.73712
H20	0.67474	0.70521	0.24097	**H118**	0.07289	0.4834	0.3002	**C87**	0.40275	0.51798	0.8176
H22	0.7356	0.58756	-0.00091	**N5**	0.28031	0.43475	0.22647	**C89**	0.3452	0.58828	0.82234
C28	0.99272	0.50789	0.24614	**H120**	0.29847	0.42117	0.14434	**C91**	0.32782	0.56281	0.74254
C30	0.95115	0.51275	0.21939	**N7**	0.25646	0.2686	0.15348	**H75**	0.37944	0.49964	0.64393
C32	0.94705	0.48465	0.13373	**H122**	0.27285	0.2637	0.06838	**H77**	0.31403	0.5779	0.6524
C34	0.98454	0.45173	0.0685	**C146**	0.54847	0.76371	0.15751	**C93**	0.37377	0.55292	0.91472
C36	0.02713	0.44408	0.10196	**C148**	0.50312	0.7756	0.20556	**H79**	0.39269	0.56337	0.97484
C38	0.0317	0.47119	0.19335	**C150**	0.49801	0.73884	0.26069	**H81**	0.35451	0.54223	0.97428
H24	0.99458	0.5333	0.30126	**C152**	0.52617	0.6922	0.21059	**C95**	0.42049	0.54381	0.73937
H26	0.0567	0.41829	0.05376	**C154**	0.57021	0.68021	0.15132	**H83**	0.43468	0.52913	0.64712
C40	0.97922	0.42598	-0.03525	**C156**	0.58239	0.7159	0.12751	**C97**	0.38064	0.592	0.74044
H28	0.96261	0.40736	-0.00066	**O8**	0.59632	0.64091	0.12256	**H85**	0.36925	0.60732	0.64911
H30	0.95831	0.44954	-0.10675	**O10**	0.55889	0.79294	0.14968	**H87**	0.4292	0.48539	0.85363
H32	1.01212	0.40141	-0.07781	**O12**	0.47009	0.7471	0.34253	**H89**	0.31859	0.62069	0.86279
C42	0.75175	0.6898	0.35058	**C158**	0.51114	0.6624	0.20717	**C99**	0.44602	0.56247	0.80472
H34	0.7636	0.67241	0.43927	**H124**	0.53025	0.63177	0.15238	**C101**	0.49006	0.55324	0.78953
H36	0.77722	0.69751	0.31207	**C160**	0.62278	0.70634	0.07914	**C103**	0.49768	0.59009	0.78631
H38	0.72012	0.72203	0.36828	**H126**	0.62959	0.73353	0.0594	**C105**	0.46125	0.63503	0.77396
C44	0.40881	0.02285	0.16874	**C162**	0.46639	0.8169	0.19301	**C107**	0.41699	0.64236	0.77798
C46	0.39105	0.06474	0.25476	**H128**	0.43507	0.82331	0.23657	**C109**	0.41014	0.60633	0.8029
C48	0.33533	0.04941	0.25983	**N9**	0.4674	0.67362	0.25547	**H91**	0.53194	0.58314	0.78641
C50	0.37014	0.01295	0.1695	**H130**	0.44495	0.69359	0.18845	**H93**	0.38874	0.67502	0.75752

H40	0.42112	0.02625	0.07678	**N11**	0.46316	0.84855	0.10099	**C111**	0.33054	0.46462	0.76747
H42	0.35728	0.01143	0.07795	**H132**	0.49052	0.83571	0.03955	**C113**	0.33762	0.50008	0.79905
C52	0.36467	0.05535	0.3516	**C28**	-0.00728	0.50789	0.24614	**C115**	0.30186	0.54408	0.80729
H44	0.34563	0.08369	0.41722	**C34**	-0.01546	0.45173	0.0685	**C117**	0.25782	0.55383	0.79302
H46	0.38557	0.02459	0.40449	**C36**	1.02713	0.44408	0.10196	**C119**	0.24987	0.51742	0.78032
C54	0.35375	0.10395	0.18131	**C38**	1.0317	0.47119	0.19335	**C121**	0.28622	0.47249	0.761
H48	0.36369	0.10857	0.08739	**C44**	0.40881	1.02285	0.16874	**H95**	0.35874	0.43215	0.74105
C56	0.31518	0.09407	0.18827	**C50**	0.37014	1.01295	0.1695	**H97**	0.21545	0.52498	0.77813
H50	0.3003	0.09397	0.09854	**C72**	0.43685	-0.02287	0.22298	**C123**	0.22051	0.60179	0.78957
H52	0.41722	0.07146	0.29047	**C74**	0.40186	-0.03252	0.22046	**H99**	0.21953	0.61947	0.87629
H54	0.31031	0.04139	0.3001	**H1**	0.66486	0.66059	0.45636	**H101**	0.22613	0.61911	0.71118
C58	0.324	0.14761	0.24876	**C1**	0.9094	0.55369	0.67845	**H103**	0.18753	0.60379	0.77885
C60	0.31519	0.19073	0.21443	**C3**	0.86688	0.57055	0.76177	**C125**	0.52769	0.50558	0.77615
C62	0.26944	0.22564	0.20738	**C5**	0.85955	0.52602	0.62587	**H105**	0.52862	0.48644	0.85901
C64	0.23505	0.21503	0.22666	**C7**	0.90454	0.52301	0.5854	**H107**	0.52251	0.48941	0.69424
C66	0.24492	0.17063	0.24573	**H3**	0.9152	0.58013	0.63757	**H109**	0.56052	0.50413	0.76496
C68	0.28933	0.13758	0.25959	**H5**	0.9077	0.53057	0.48836	**C127**	0.24532	0.37485	0.78407
H56	0.20053	0.24049	0.21262	**C9**	0.86002	0.52981	0.76504	**C129**	0.21758	0.42019	0.72987
H58	0.21892	0.16171	0.24029	**H7**	0.82834	0.53628	0.81175	**C131**	0.17065	0.43367	0.69685
C70	0.48038	0.94471	0.18966	**H9**	0.88753	0.49963	0.80822	**C133**	0.15216	0.40349	0.72742
C72	0.43685	0.97713	0.22298	**C11**	0.82715	0.60442	0.68414	**C135**	0.18475	0.35485	0.74558
C74	0.40186	0.96748	0.22046	**H11**	0.83022	0.63267	0.64425	**C137**	0.2332	0.33973	0.75808
C76	0.40931	0.92539	0.17889	**C13**	0.82234	0.57403	0.59004	**O1**	0.17172	0.32755	0.75202
C78	0.45427	0.89066	0.15553	**H13**	0.8224	0.58375	0.49348	**O3**	0.27842	0.36594	0.84373
C80	0.48937	0.90091	0.16225	**H15**	0.8693	0.58472	0.85092	**O5**	0.14752	0.46926	0.64481
H60	0.50607	0.95384	0.17664	**H17**	0.85484	0.49818	0.59075	**C139**	0.10758	0.41911	0.74036
H62	0.52315	0.87615	0.13433	**C15**	0.78068	0.61752	0.73036	**H111**	0.09602	0.39636	0.7715
C82	0.36954	0.91999	0.1508	**C17**	0.74498	0.6599	0.76289	**C141**	0.26581	0.29738	0.72905
H64	0.34901	0.92595	0.23584	**C19**	0.70297	0.67333	0.71109	**H113**	0.30037	0.28909	0.73857
H66	0.34865	0.94484	0.08126	**C21**	0.69856	0.64701	0.6158	**C143**	0.23478	0.44694	0.70018
H68	0.37929	0.88601	0.11392	**C23**	0.73643	0.60584	0.57947	**H115**	0.21505	0.47638	0.64466
C84	0.35374	0.19694	0.17312	**C25**	0.77617	0.59042	0.64236	**N2**	0.07514	0.46566	0.71935
H70	0.38582	0.16441	0.17124	**H19**	0.67474	0.70521	0.74097	**H117**	0.07289	0.4834	0.8002
H72	0.34839	0.21072	0.07915	**H21**	0.7356	0.58756	0.49909	**N4**	0.28031	0.43475	0.72647
H74	0.35787	0.21951	0.23812	**C27**	0.99272	0.50789	0.74614	**H119**	0.29847	0.42117	0.64434
C86	0.36758	0.51462	0.23712	**C29**	0.95115	0.51275	0.71939	**N6**	0.25646	0.2686	0.65348
C88	0.40275	0.51798	0.3176	**C31**	0.94705	0.48465	0.63373	**H121**	0.27285	0.2637	0.56838
C90	0.3452	0.58828	0.32234	**C33**	0.98454	0.45173	0.5685	**C145**	0.54847	0.76371	0.65751
C92	0.32782	0.56281	0.24254	**C35**	0.02713	0.44408	0.60196	**C147**	0.50312	0.7756	0.70556
H76	0.37944	0.49964	0.14393	**C37**	0.0317	0.47119	0.69335	**C149**	0.49801	0.73884	0.76069
H78	0.31403	0.5779	0.1524	**H23**	0.99458	0.5333	0.80126	**C151**	0.52617	0.6922	0.71059
C94	0.37377	0.55292	0.41472	**H25**	0.0567	0.41829	0.55376	**C153**	0.57021	0.68021	0.65132
H80	0.39269	0.56337	0.47484	**C39**	0.97922	0.42598	0.46475	**C155**	0.58239	0.7159	0.62751
H82	0.35451	0.54223	0.47428	**H27**	0.96261	0.40736	0.49934	**O7**	0.59632	0.64091	0.62256
C96	0.42049	0.54381	0.23937	**H29**	0.95831	0.44954	0.39325	**O9**	0.55889	0.79294	0.64968
H84	0.43468	0.52913	0.14712	**H31**	1.01212	0.40141	0.42219	**O11**	0.47009	0.7471	0.84253
C98	0.38064	0.592	0.24044	**C41**	0.75175	0.6898	0.85058	**C157**	0.51114	0.6624	0.70717
H86	0.36925	0.60732	0.14911	**H33**	0.7636	0.67241	0.93927	**H123**	0.53025	0.63177	0.65238
H88	0.4292	0.48539	0.35363	**H35**	0.77722	0.69751	0.81207	**C159**	0.62278	0.70634	0.57914
H90	0.31859	0.62069	0.36279	**H37**	0.72012	0.72203	0.86828	**H125**	0.62959	0.73353	0.5594

C100	0.44602	0.56247	0.30472	**C43**	0.40881	0.02285	0.66874	**C161**	0.46639	0.8169	0.69301
C102	0.49006	0.55324	0.28953	**C45**	0.39105	0.06474	0.75476	**H127**	0.43507	0.82331	0.73657
C104	0.49768	0.59009	0.28631	**C47**	0.33533	0.04941	0.75983	**N8**	0.4674	0.67362	0.75547
C106	0.46125	0.63503	0.27396	**C49**	0.37014	0.01295	0.6695	**H129**	0.44495	0.69359	0.68845
C108	0.41699	0.64236	0.27798	**H39**	0.42112	0.02625	0.57678	**N10**	0.46316	0.84855	0.60099
C110	0.41014	0.60633	0.3029	**H41**	0.35728	0.01143	0.57795	**H131**	0.49052	0.83571	0.53955
H92	0.53194	0.58314	0.28641	**C51**	0.36467	0.05535	0.8516	**N12**	0.65752	0.66105	0.55009
H94	0.38874	0.67502	0.25752	**H43**	0.34563	0.08369	0.91722	**C27**	-0.00728	0.50789	0.74614
C112	0.33054	0.46462	0.26747	**H45**	0.38557	0.02459	0.90449	**C33**	-0.01546	0.45173	0.5685
C114	0.33762	0.50008	0.29905	**C53**	0.35375	0.10395	0.68131	**C35**	1.02713	0.44408	0.60196
C116	0.30186	0.54408	0.30729	**H47**	0.36369	0.10857	0.58739	**C37**	1.0317	0.47119	0.69335
C118	0.25782	0.55383	0.29302	**C55**	0.31518	0.09407	0.68827	**C43**	0.40881	1.02285	0.66874
C120	0.24987	0.51742	0.28032	**H49**	0.3003	0.09397	0.59854	**C49**	0.37014	1.01295	0.6695
C122	0.28622	0.47249	0.261	**H51**	0.41722	0.07146	0.79047	**C71**	0.43685	-0.02287	0.72298
H96	0.35874	0.43215	0.24105	**H53**	0.31031	0.04139	0.8001	**C73**	0.40186	-0.03252	0.72046
H98	0.21545	0.52498	0.27813	**C57**	0.324	0.14761	0.74876				
C124	0.22051	0.60179	0.28957	**C59**	0.31519	0.19073	0.71443				

Table S3. Fractional atomic coordinates for the unit cell of ND-COF-1.

ND-COF-1 in staggered AB model (Space group *P*1)											
a = 34.12 Å, b = 33.64 Å, c = 9.16 Å, α = 91.11°, β = 89°, γ = 60.98°											
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
N1	0.0066	0.98948	-0.00466	**H98**	0.56323	0.86778	0.24922	**C61**	0.29703	0.2225	0.74616
H2	0.01392	0.98647	-0.11701	**C124**	0.57355	0.94141	0.30944	**C63**	0.26442	0.2102	0.78796
C2	0.25744	0.88638	0.18631	**H100**	0.57716	0.95508	0.41657	**C65**	0.27615	0.16486	0.81138
C4	0.21323	0.89774	0.27061	**H102**	0.57753	0.96151	0.22152	**C67**	0.32125	0.1325	0.80857
C6	0.21072	0.86017	0.07149	**H104**	0.53937	0.94527	0.30566	**H55**	0.22922	0.23516	0.78581
C8	0.25568	0.86087	0.04911	**C126**	0.88347	0.83317	0.29041	**H57**	0.2506	0.15471	0.81978
H4	0.26327	0.91558	0.16516	**H106**	0.88185	0.81043	0.37362	**C69**	0.51022	0.94238	0.64984
H6	0.25992	0.87496	-0.05522	**H108**	0.87846	0.82193	0.18088	**C71**	0.46809	0.97387	0.70584
C10	0.20778	0.85628	0.23619	**H110**	0.91727	0.83033	0.29099	**C73**	0.43374	0.96277	0.72047
H8	0.17537	0.85963	0.2767	**C128**	0.59618	0.71473	0.23234	**C75**	0.43999	0.92035	0.67143
H10	0.23484	0.82409	0.27863	**C130**	0.56374	0.76206	0.19357	**C77**	0.48402	0.88644	0.62684
C12	0.17548	0.93556	0.18252	**C132**	0.51507	0.77605	0.19625	**C79**	0.51879	0.89798	0.61769
H12	0.17927	0.9659	0.15979	**C134**	0.49949	0.74271	0.23267	**H59**	0.53503	0.95262	0.62487
C14	0.17348	0.90969	0.04619	**C136**	0.53366	0.69364	0.23653	**H61**	0.55161	0.87359	0.57386
H14	0.17576	0.92447	-0.05915	**C138**	0.58239	0.6792	0.22397	**C81**	0.39962	0.91368	0.65751
H16	0.21266	0.9062	0.38866	**O2**	0.52164	0.66515	0.25313	**H63**	0.38428	0.91623	0.76753
H18	0.20798	0.83371	0.00522	**O4**	0.6348	0.70434	0.26029	**H65**	0.37448	0.94031	0.58875
C16	0.12824	0.94617	0.21869	**O6**	0.48787	0.81516	0.16803	**H67**	0.40793	0.88038	0.60587
C18	0.09116	0.98673	0.26728	**C140**	0.45565	0.75587	0.26121	**C83**	0.37934	0.19698	0.67284
C20	0.04986	0.99957	0.20087	**H112**	0.44594	0.7309	0.29425	**H69**	0.41174	0.16492	0.66011
C22	0.04781	0.97623	0.07171	**C142**	0.61364	0.63591	0.18872	**H71**	0.37022	0.21175	0.56339
C24	0.08763	0.93861	0.01525	**H114**	0.64858	0.62747	0.18403	**H73**	0.38514	0.21989	0.74685
C26	0.12647	0.9225	0.09509	**C144**	0.5775	0.7911	0.14486	**C85**	0.40086	0.50949	0.7804
H20	0.02019	1.02909	0.24508	**H116**	0.55327	0.82272	0.09764	**C87**	0.43376	0.51195	0.89132
H22	0.0885	0.92293	-0.08989	**N3**	0.42147	0.80267	0.25376	**C89**	0.37855	0.58355	0.88852
C28	0.33905	0.83889	0.27497	**H118**	0.4169	0.81677	0.35963	**C91**	0.36293	0.55864	0.77995
C30	0.29886	0.84366	0.22425	**N5**	0.62397	0.77975	0.141	**H75**	0.41541	0.49432	0.67043

C32	0.29771	0.82037	0.09804	**H120**	0.63404	0.77667	0.03095	**H77**	0.35403	0.57312	0.66954
C34	0.33701	0.7923	0.01679	**N7**	0.60131	0.60594	0.1141	**C93**	0.40232	0.54801	1.00287
C36	0.3783	0.78406	0.07437	**H122**	0.61492	0.59998	0.00769	**H79**	0.41972	0.55805	1.08523
C38	0.37972	0.80667	0.20513	**C146**	0.90046	0.09692	0.11946	**H81**	0.38006	0.53825	1.06433
H24	0.33858	0.86183	0.36035	**C148**	0.85823	0.10892	0.2036	**C95**	0.45598	0.53656	0.81112
H26	0.4092	0.76203	0.01392	**C150**	0.8567	0.07172	0.28343	**H83**	0.47259	0.52148	0.70319
C40	0.3347	0.77302	-0.1297	**C152**	0.87973	0.02504	0.2149	**C97**	0.41772	0.58553	0.80662
H28	0.31838	0.75161	-0.11719	**C154**	0.91717	0.01427	0.10695	**H85**	0.41071	0.60007	0.69592
H30	0.31478	0.80101	-0.20394	**C156**	0.93221	0.04843	0.07945	**H87**	0.45774	0.47889	0.93729
H32	0.36863	0.75175	-0.18035	**O8**	0.93526	-0.02238	0.04012	**H89**	0.35151	0.61686	0.93195
C42	0.09584	1.01596	0.38369	**O10**	0.91039	0.12633	0.09145	**C99**	0.48047	0.55459	0.90254
H34	0.10773	0.99655	0.48499	**O12**	0.83613	0.07975	0.40048	**C101**	0.52516	0.54467	0.89651
H36	0.12055	1.02641	0.3465	**C158**	0.86657	0.9936	0.24023	**C103**	0.53398	0.58145	0.9021
H38	0.06341	1.04711	0.40889	**H124**	0.88366	0.96153	0.17818	**C105**	0.49892	0.6269	0.8883
C44	0.75527	0.3592	0.13147	**C160**	0.97356	0.03636	0.0229	**C107**	0.45438	0.63508	0.87777
C46	0.73935	0.4028	0.22824	**H126**	0.983	0.06229	0.00103	**C109**	0.44575	0.59914	0.89604
C48	0.68451	0.38587	0.26221	**C162**	0.82072	0.15009	0.20044	**H91**	0.56835	0.57438	0.90556
C50	0.7171	0.34819	0.15059	**H128**	0.79223	0.15619	0.27077	**H93**	0.42726	0.66825	0.85279
H40	0.76451	0.3613	0.01583	**N9**	0.83349	0.99963	0.35197	**C111**	0.359	0.46194	0.79159
H42	0.70227	0.34523	0.04638	**H130**	0.80433	1.02999	0.33203	**C113**	0.36692	0.49698	0.83818
C52	0.71604	0.39424	0.35736	**N11**	0.81177	0.18143	0.08424	**C115**	0.33267	0.54194	0.84049
H44	0.69875	0.42385	0.43515	**H132**	0.83619	0.1693	0.00011	**C117**	0.28919	0.55329	0.80358
H46	0.73853	0.3645	0.4221	**N1**	1.0066	-0.01052	-0.00466	**C119**	0.27945	0.51764	0.77842
C54	0.69975	0.44045	0.1452	**C152**	0.87973	1.02504	0.2149	**C121**	0.31461	0.47146	0.76653
H48	0.70643	0.44346	0.02765	**C158**	0.86657	-0.0064	0.24023	**H95**	0.38695	0.4284	0.76733
C56	0.66173	0.42979	0.17362	**C160**	-0.02644	1.03636	0.0229	**H97**	0.24505	0.52682	0.75849
H50	0.64445	0.42795	0.07383	**H1**	0.69323	0.644	0.44179	**C123**	0.25474	0.60204	0.78554
H52	0.76618	0.41097	0.2569	**C1**	0.93496	0.55018	0.72286	**H99**	0.25061	0.62171	0.88875
H54	0.66091	0.37765	0.32209	**C3**	0.89236	0.56135	0.81763	**H101**	0.26583	0.61662	0.69657
C58	0.67194	0.48519	0.22535	**C5**	0.8875	0.52185	0.62778	**H103**	0.22174	0.60545	0.75753
C60	0.66205	0.52841	0.17871	**C7**	0.93122	0.52349	0.59213	**C125**	0.56222	0.49644	0.88247
C62	0.61619	0.56326	0.18384	**H3**	0.93955	0.57964	0.69377	**H105**	0.56015	0.47709	0.97628
C64	0.58257	0.55234	0.2259	**H5**	0.93331	0.53691	0.48384	**H107**	0.55904	0.48044	0.7795
C66	0.59305	0.5075	0.25276	**C9**	0.88747	0.51914	0.79366	**H109**	0.59564	0.49457	0.88101
C68	0.63785	0.47465	0.25647	**H7**	0.85606	0.52211	0.84258	**C127**	0.27178	0.37594	0.80987
H56	0.54762	0.5777	0.21993	**H9**	0.91574	0.48761	0.83515	**C129**	0.24422	0.42045	0.7409
H58	0.56692	0.49813	0.25989	**C11**	0.8524	0.59799	0.73303	**C131**	0.19654	0.43415	0.7114
C70	0.82837	0.28202	0.15507	**H11**	0.85478	0.6287	0.70381	**C133**	0.17782	0.40386	0.75321
C72	0.78511	0.31445	0.19833	**C13**	0.84949	0.57072	0.60239	**C135**	0.2101	0.3551	0.77652
C74	0.75065	0.30345	0.21055	**H13**	0.84991	0.58492	0.49398	**C137**	0.25873	0.34015	0.78946
C76	0.75815	0.25986	0.17066	**H15**	0.89364	0.57077	0.93359	**O1**	0.19661	0.32759	0.78771
C78	0.80302	0.22528	0.13975	**H17**	0.88425	0.49464	0.5679	**O3**	0.30558	0.36807	0.87545
C80	0.83779	0.23687	0.13463	**C15**	0.80586	0.60759	0.77798	**O5**	0.1729	0.47015	0.65303
H60	0.85345	0.29189	0.12922	**C17**	0.76854	0.64845	0.8239	**C139**	0.13321	0.41957	0.77224
H62	0.87141	0.21177	0.10019	**C19**	0.72729	0.66066	0.75788	**H111**	0.12136	0.39674	0.81082
C82	0.71852	0.25237	0.15037	**C21**	0.72536	0.63583	0.63259	**C141**	0.29083	0.29669	0.76227
H64	0.69813	0.26146	0.25362	**C23**	0.7648	0.59718	0.58095	**H113**	0.32558	0.28825	0.77251
H66	0.69742	0.27418	0.06274	**C25**	0.8037	0.58242	0.65877	**C143**	0.26214	0.44603	0.69252
H68	0.72852	0.21663	0.11951	**H19**	0.6976	0.69082	0.79878	**H115**	0.2424	0.47436	0.62328
C84	0.69923	0.5348	0.11225	**H21**	0.76564	0.58015	0.47853	**N2**	0.10114	0.4665	0.75092

H70	0.73102	0.50205	0.10152	**C27**	0.01892	0.50401	0.79247	**H117**	0.09846	0.48417	0.84914
H72	0.69062	0.54868	0.00147	**C29**	0.97774	0.50804	0.75613	**N4**	0.30814	0.43402	0.71574
H74	0.70596	0.5576	0.18366	**C31**	0.97422	0.48374	0.63647	**H119**	0.32501	0.42266	0.61435
C86	0.71891	0.85159	0.21498	**C33**	0.01163	0.45509	0.54871	**N6**	0.28077	0.26601	0.68087
C88	0.75586	0.84965	0.31689	**C35**	0.05397	0.44746	0.59295	**H121**	0.29441	0.26158	0.57494
C90	0.70093	0.92108	0.34826	**C37**	0.05805	0.4713	0.716	**C145**	0.57716	0.75882	0.63938
C92	0.68088	0.90026	0.24047	**H23**	0.02022	0.52751	0.87207	**C147**	0.53207	0.77263	0.70517
H76	0.72915	0.84135	0.0983	**H25**	0.08364	0.42481	0.528	**C149**	0.52713	0.73787	0.78863
H78	0.667	0.91916	0.13901	**C39**	0.00613	0.43444	0.40942	**C151**	0.55347	0.68917	0.73849
C94	0.72881	0.88129	0.44495	**H27**	-0.01024	0.41364	0.43386	**C153**	0.5931	0.6765	0.63885
H80	0.7492	0.88825	0.52425	**H29**	-0.01514	0.46169	0.33473	**C155**	0.60953	0.7097	0.61457
H82	0.70895	0.86913	0.50899	**H31**	0.03899	0.41224	0.3532	**O7**	0.61198	0.63907	0.57684
C96	0.77535	0.87715	0.23966	**C41**	0.77287	0.67862	0.93766	**O9**	0.58847	0.78739	0.61383
H84	0.78846	0.8661	0.12553	**H33**	0.78505	0.65983	1.03995	**O11**	0.5008	0.74963	0.8931
C98	0.73706	0.92625	0.25699	**H35**	0.79717	0.68935	0.8984	**C157**	0.5421	0.65703	0.77418
H86	0.72607	0.94462	0.15311	**H37**	0.7402	0.70956	0.96215	**H123**	0.56212	0.62317	0.72522
H88	0.78129	0.81491	0.34684	**C43**	0.43696	0.02027	0.65131	**C159**	0.65247	0.69616	0.5731
H90	0.67576	0.95259	0.40725	**C45**	0.42277	0.0618	0.75706	**H125**	0.66316	0.72122	0.55223
C100	0.8026	0.89196	0.33013	**C47**	0.36879	0.04381	0.79435	**C161**	0.49538	0.81343	0.68513
C102	0.84751	0.88102	0.32349	**C49**	0.39919	0.00882	0.67288	**H127**	0.46443	0.82095	0.74343
C104	0.85735	0.91673	0.3476	**H39**	0.44389	0.02504	0.53563	**N8**	0.50818	0.66455	0.88444
C106	0.8228	0.96292	0.34536	**H41**	0.38236	0.00827	0.57044	**H129**	0.47868	0.69337	0.85616
C108	0.77769	0.97254	0.33422	**C51**	0.40207	0.05025	0.88661	**N10**	0.49175	0.84317	0.5686
C110	0.76839	0.93666	0.34154	**H43**	0.38618	0.07815	0.97099	**H131**	0.51893	0.82887	0.49403
H92	0.89197	0.90895	0.3551	**H45**	0.42595	0.01912	0.94303	**N12**	0.68479	0.6488	0.5535
H94	0.75081	1.00669	0.31851	**C53**	0.3814	0.10127	0.68607	**C27**	1.01892	0.50401	0.79247
C112	0.67794	0.80328	0.21872	**H47**	0.38587	0.107	0.56908	**C29**	-0.02226	0.50804	0.75613
C114	0.68788	0.83584	0.27647	**C55**	0.34422	0.08952	0.71608	**C31**	-0.02578	0.48374	0.63647
C116	0.65388	0.8802	0.30528	**H49**	0.32532	0.08959	0.61814	**C33**	1.01163	0.45509	0.54871
C118	0.60894	0.89262	0.29027	**H51**	0.45007	0.06946	0.78367	**C43**	0.43696	1.02027	0.65131
C120	0.59827	0.85825	0.25363	**H53**	0.34645	0.03414	0.85528	**C49**	0.39919	1.00882	0.67288
C122	0.63272	0.81363	0.21006	**C57**	0.35451	0.14423	0.77659	**C71**	0.46809	-0.02613	0.70584
H96	0.70458	0.77162	0.17234	**C59**	0.34322	0.18849	0.73685	**C73**	0.43374	-0.03723	0.72047

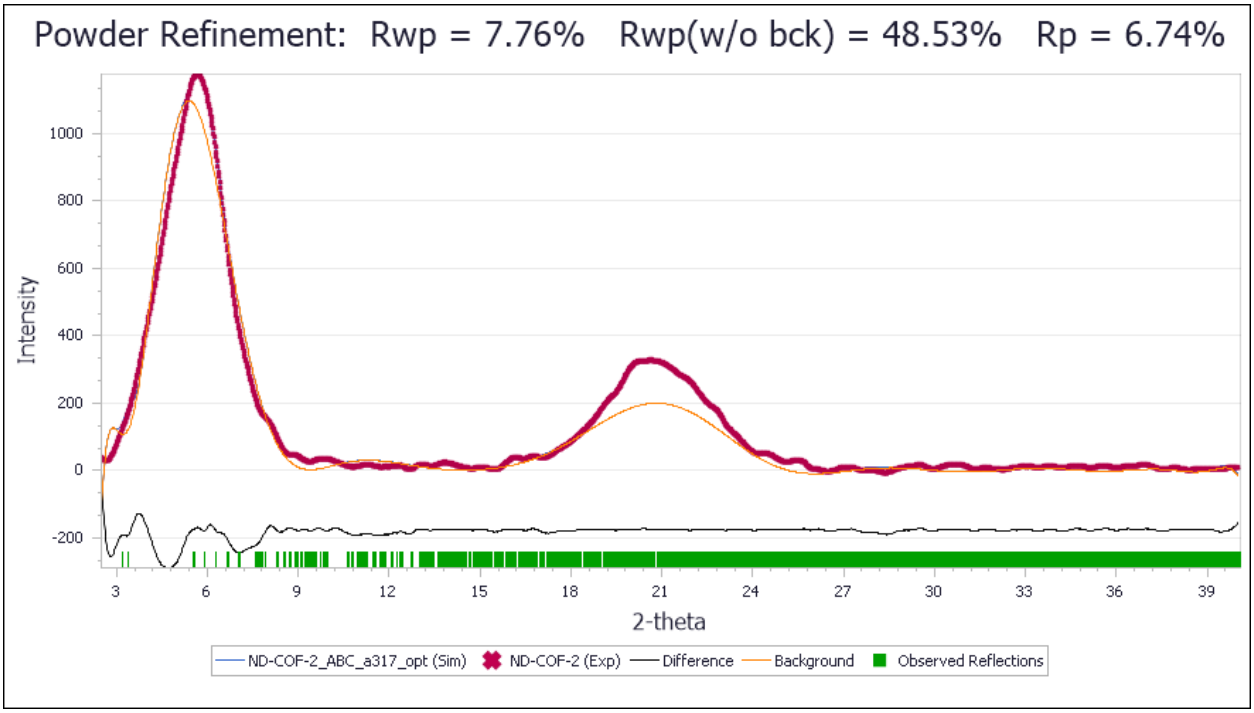

Figure S12. Pawley refinement for ND-COF-2. Pawley refinement suggests that the simulated (blue) and experimental (red) PXRD patterns are in good agreement. The black line denotes the refinement difference, and green lines denote observed reflections.

Table S4. Fractional atomic coordinates for the unit cell of ND-COF-2.

ND-COF-2 in ABC stacking model (Space group = *P*1)											
a = 30.53 Å, b = 32.44 Å, c = 12.74 Å, α = 90.59°, β = 91.95°, γ = 117.74°											
Atoms	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**	**Atoms**	**X**	**Y**	**Z**
C1	0.45156	0.50706	0.8302	**C47**	0.56235	1.02661	0.79039	**C7**	0.78474	0.17388	0.49793
C2	0.49387	0.94326	0.81505	**C48**	-0.02717	0.53548	0.7857	**C8**	0.8279	0.61065	0.49137
C3	0.0551	0.54855	0.81475	**C4**	0.1179	0.84052	0.16407	**C9**	0.38708	0.21458	0.48989
C10	0.44884	0.46306	0.88062	**C5**	0.16118	0.2771	0.1583	**C16**	0.78206	0.12987	0.54815
C11	0.53903	0.98454	0.87181	**C6**	0.7207	0.88147	0.15694	**C17**	0.87146	0.65145	0.5442
C12	0.01372	0.55275	0.86963	**C13**	0.11505	0.79652	0.2148	**C18**	0.34623	0.21774	0.5409
C19	0.52411	0.51221	0.87879	**C14**	0.20481	0.31778	0.21126	**C25**	0.85732	0.17906	0.5463
C20	0.48775	0.01125	0.87251	**C15**	0.67982	0.88463	0.20781	**C26**	0.82187	0.67701	0.54452
C21	0.98557	0.47448	0.86734	**C22**	0.19032	0.84573	0.21405	**C27**	0.31928	0.14232	0.5384
C28	0.50535	0.54246	0.83063	**C23**	0.15524	0.34336	0.21264	**C34**	0.83851	0.2093	0.49826
C29	0.45801	0.96152	0.81762	**C24**	0.65292	0.80921	0.20552	**C35**	0.79213	0.62855	0.49376
C30	0.03589	0.49424	0.81478	**C31**	0.17168	0.87594	0.16514	**C36**	0.36825	0.16072	0.48987
C37	0.48788	0.48335	0.96125	**C32**	0.12543	0.29501	0.16148	**C43**	0.82111	0.15015	0.62875
C38	0.51742	0.00264	0.95392	**C33**	0.7019	0.82761	0.15708	**C44**	0.85059	0.66898	0.62616
C39	0.99401	0.51221	0.94997	**C40**	0.15382	0.81683	0.29603	**C45**	0.32714	0.17855	0.62118
C46	0.46526	0.4392	0.80135	**C41**	0.18404	0.33515	0.29377	**C52**	0.79849	0.10608	0.46872
C47	0.56235	0.02661	0.79039	**C42**	0.66073	0.84548	0.28819	**C53**	0.89536	0.69267	0.46724
C48	0.97283	0.53548	0.7857	**C49**	0.13176	0.77272	0.136	**C54**	0.30608	0.20179	0.46168

C55	0.51918	0.4754	0.7983	**C50**	0.22864	0.35914	0.13463	**C61**	0.8524	0.14229	0.46574
C56	0.52564	0.04409	0.78861	**C51**	0.63969	0.86863	0.12852	**C62**	0.85878	0.70984	0.46532
C57	0.95388	0.48097	0.78259	**C58**	0.18567	0.80896	0.13385	**C63**	0.28752	0.14773	0.45826
C64	0.47822	0.40235	0.83355	**C59**	0.19208	0.37632	0.13347	**C70**	0.81141	0.06919	0.50074
C65	0.59907	0.07621	0.83129	**C60**	0.62117	0.81457	0.12525	**C71**	0.93163	0.74233	0.5017
C66	0.92336	0.52385	0.8241	**C67**	0.14462	0.73585	0.16864	**C72**	0.25668	0.18983	0.49385
C73	0.45991	0.35396	0.80275	**C68**	0.26498	0.40873	0.1693	**C79**	0.79313	0.02084	0.46955
C74	0.64748	0.10723	0.80252	**C69**	0.59027	0.85665	0.16056	**C80**	0.97987	0.77274	0.47028
C75	0.89404	0.54303	0.79454	**C76**	0.12655	0.68757	0.13712	**C81**	0.22792	0.20945	0.4622
C82	0.4939	0.33825	0.78639	**C77**	0.31314	0.43916	0.13732	**C88**	0.82713	0.0052	0.45273
C83	0.66251	0.15678	0.78695	**C78**	0.56147	0.8762	0.12869	**C89**	0.99487	0.82203	0.45108
C84	0.84434	0.50996	0.77671	**C85**	0.16067	0.67203	0.12084	**C90**	0.17841	0.17659	0.44162
C91	0.54438	0.37274	0.78138	**C86**	0.32808	0.48845	0.11818	**C97**	0.87761	0.03971	0.44778
C92	0.62775	0.17239	0.78117	**C87**	0.51196	0.84329	0.10827	**C98**	0.95996	0.83742	0.44497
C93	0.82692	0.45924	0.77059	**C94**	0.21115	0.70661	0.11689	**C99**	0.1612	0.12594	0.43504
C100	0.5604	0.42295	0.79273	**C95**	0.29315	0.50383	0.11275	**C106**	0.89363	0.08989	0.4599
C101	0.57757	0.13813	0.79279	**C96**	0.4948	0.79263	0.10193	**C107**	0.91	0.80314	0.45985
C102	0.85965	0.4413	0.78367	**C103**	0.22705	0.75674	0.12946	**C108**	0.19405	0.10829	0.45019
C109	0.52655	0.43519	0.82911	**C104**	0.24325	0.46956	0.1284	**C115**	0.85974	0.10205	0.49641
C110	0.56516	0.09184	0.8277	**C105**	0.5277	0.77505	0.11708	**C116**	0.89839	0.75743	0.49775
C111	0.90619	0.47403	0.8197	**C112**	0.19296	0.76876	0.16518	**C117**	0.24013	0.14127	0.48873
C118	0.41323	0.55893	0.87455	**C113**	0.23173	0.42384	0.16605	**C124**	0.74637	0.22567	0.54263
C119	0.44296	0.85264	0.86116	**C114**	0.57377	0.80809	0.15558	**C125**	0.77598	0.51988	0.52893
C120	0.14486	0.58683	0.86715	**C121**	0.07944	0.89238	0.20737	**C126**	0.47723	0.25278	0.53324
C127	0.44663	0.54336	0.89316	**C122**	0.10927	0.18626	0.19487	**C133**	0.77982	0.21015	0.56107
C128	0.45869	0.90141	0.88187	**C123**	0.81084	0.91972	0.2003	**C134**	0.7913	0.56849	0.55155
C129	0.09573	0.5538	0.88391	**C130**	0.11282	0.87685	0.22662	**C135**	0.4283	0.21942	0.55242
C136	0.49571	0.57529	0.89553	**C131**	0.12463	0.23481	0.2182	**C142**	0.8289	0.24211	0.56327
C137	0.4258	0.91873	0.88641	**C132**	0.76192	0.88636	0.21957	**C143**	0.75914	0.58535	0.55646
C138	0.07782	0.50345	0.88529	**C139**	0.16188	0.9088	0.22945	**C144**	0.41092	0.17026	0.55416
C145	0.51479	0.62522	0.88107	**C140**	0.09249	0.25168	0.22386	**C151**	0.84792	0.29202	0.54866
C146	0.37597	0.88743	0.87331	**C141**	0.74456	0.83721	0.22146	**C152**	0.70937	0.55462	0.53985
C147	0.10894	0.48472	0.87179	**C148**	0.18098	0.95871	0.21463	**C153**	0.44166	0.15118	0.5379
C154	0.48203	0.6425	0.87007	**C149**	0.04269	0.221	0.20737	**C160**	0.81513	0.30925	0.5374
C155	0.35925	0.83771	0.85884	**C150**	0.77532	0.81813	0.20537	**C161**	0.69242	0.505	0.52315
C156	0.15887	0.51755	0.85971	**C157**	0.14823	0.97597	0.20296	**C162**	0.49152	0.18382	0.5239
C163	0.43129	0.60959	0.86391	**C158**	0.02571	0.1714	0.19016	**C169**	0.76438	0.27631	0.5315
C164	0.39228	0.82011	0.85078	**C159**	0.82517	0.85078	0.1913	**C170**	0.72543	0.48733	0.51629
C165	0.17709	0.56841	0.85534	**C166**	0.09749	0.94304	0.19647	**C171**	0.50964	0.23466	0.51992
C172	0.5686	0.6591	0.87102	**C167**	0.0587	0.15374	0.18249	**C178**	0.90173	0.32598	0.53883
C173	0.34128	0.90652	0.86915	**C168**	0.84326	0.90161	0.18701	**C179**	0.67511	0.57424	0.53512
C174	0.08954	0.43094	0.86501	**C175**	0.2348	0.99256	0.20463	**C180**	0.42193	0.09733	0.53102
C181	0.40648	0.32093	0.78446	**C176**	0.00846	0.24066	0.20315	**C187**	0.7397	-0.01219	0.45126
C182	0.68139	0.08784	0.78486	**C177**	0.7556	0.76428	0.19855	**C188**	1.01357	0.75297	0.45413
C183	0.91537	0.59676	0.77928	**C184**	0.0732	0.65451	0.11783	**C189**	0.24958	0.26329	0.44818
C190	0.37854	0.66351	0.69228	**C185**	0.34681	0.4194	0.1204	**C196**	0.71182	0.33023	0.35978
C191	0.33463	0.71057	0.68612	**C186**	0.5831	0.93001	0.1142	**C197**	0.66816	0.37752	0.35174
C192	0.28726	0.61945	0.69354	**C193**	0.04493	0.9969	0.02441	**C198**	0.62051	0.28633	0.3592
C199	0.37956	0.70891	0.66367	**C194**	0.00124	0.04418	0.01711	**C205**	0.71309	0.37566	0.33037
C200	0.28839	0.66545	0.66658	**C195**	0.95363	0.95302	0.02483	**C206**	0.62186	0.33244	0.33215

C201	0.33212	0.61794	0.67302	**C202**	0.04614	1.04233	-0.00476	**C207**	0.66542	0.28471	0.34006
O1	0.41808	0.74625	0.64561	**C203**	-0.04509	-0.0009	-0.00217	**O7**	0.75174	0.41293	0.3127
O2	0.25072	0.66629	0.65059	**C204**	0.99847	0.95139	0.00498	**O8**	0.58428	0.33342	0.3159
O3	0.33117	0.57918	0.66093	**O4**	0.08476	1.0796	-0.02259	**O9**	0.66443	0.24589	0.32856
C208	0.41142	0.66552	0.7623	**O5**	-0.08271	0.00007	-0.01793	**C214**	0.74449	0.33217	0.43
C209	0.33471	0.74326	0.75354	**O6**	0.99744	0.91256	-0.0068	**C215**	0.66824	0.41051	0.41819
C210	0.2549	0.58754	0.76253	**C211**	0.07767	0.99883	0.09443	**C216**	0.5876	0.25416	0.42695
N1	0.39865	0.6267	0.83669	**C212**	0.00143	0.07713	0.08388	**N7**	0.7317	0.29336	0.50407
N2	0.37525	0.77043	0.82294	**C213**	0.92096	0.92097	0.09315	**N8**	0.7087	0.43781	0.48769
N3	0.22707	0.60107	0.82937	**N4**	0.06486	0.9601	0.16874	**N9**	0.55943	0.26755	0.493
C217	0.6183	0.32633	0.86943	**N5**	0.04194	0.10428	0.15332	**C223**	0.9518	-0.00738	0.53142
C218	0.67676	0.29426	0.8604	**N6**	0.893	0.93446	0.15966	**C224**	0.00954	-0.04023	0.51921
C219	0.70871	0.38519	0.86203	**C220**	0.2855	0.65938	0.19989	**C225**	0.04235	0.05086	0.52234
C226	0.62761	0.28595	0.88547	**C221**	0.34301	0.62629	0.18629	**C232**	0.96069	-0.0481	0.5458
C227	0.71789	0.34402	0.8736	**C222**	0.37605	0.71742	0.18994	**C233**	0.05103	0.00931	0.53215
C228	0.65963	0.3758	0.88775	**C229**	0.29427	0.61855	0.21355	**C234**	-0.00647	0.04189	0.54929
O10	0.59577	0.24675	0.9196	**C230**	0.38462	0.67578	0.19903	**O16**	0.92894	-0.08705	0.58113
O11	0.75838	0.35108	0.89659	**C231**	0.32736	0.70857	0.21772	**O17**	0.09124	0.01583	0.55587
O12	0.65312	0.40795	0.9234	**O13**	0.26257	0.57966	0.24925	**O18**	-0.01241	0.07418	0.58634
C235	0.57836	0.31866	0.81682	**O14**	0.42483	0.68217	0.22223	**C241**	0.9116	-0.01458	0.48077
C236	0.68311	0.26113	0.80784	**O15**	0.32163	0.74088	0.25539	**C242**	0.01535	-0.07367	0.46664
C237	0.73955	0.42595	0.81004	**C238**	0.24524	0.65236	0.14978	**C243**	0.07363	0.09199	0.47212
N10	0.5785	0.35719	0.75767	**C239**	0.34862	0.59276	0.13358	**N16**	0.91172	0.02427	0.42303
N11	0.64301	0.22174	0.75449	**C240**	0.4073	0.75858	0.13977	**N17**	0.97475	0.8864	0.41589
N12	0.77701	0.42724	0.74497	**N13**	0.24542	0.69134	0.09246	**N18**	0.11154	0.09377	0.40785
H1	0.43267	0.4993	0.75456	**N14**	0.30783	0.55276	0.08348	**H7**	0.7658	0.16616	0.42236
H2	0.5002	0.93286	0.73471	**N15**	0.44511	0.76039	0.0751	**H8**	0.83613	0.6007	0.41482
H3	0.06686	0.5662	0.73551	**H4**	0.09921	0.83277	0.08819	**H9**	0.39819	0.23347	0.41423
H10	0.41295	0.43827	0.91177	**H5**	0.16934	0.26733	0.08147	**H16**	0.74618	0.10504	0.57927
H11	0.56454	0.9733	0.9038	**H6**	0.73182	0.90032	0.08124	**H17**	0.89636	0.64027	0.57424
H12	0.0252	0.58932	0.90304	**H13**	0.07907	0.7717	0.24543	**H18**	0.35769	0.25365	0.57246
H19	0.56103	0.5339	0.90803	**H14**	0.22971	0.30651	0.24085	**H25**	0.89425	0.20075	0.57549
H20	0.46537	0.0262	0.90511	**H15**	0.69125	0.92055	0.23927	**H26**	0.79987	0.69167	0.57496
H21	0.9697	0.4368	0.89847	**H22**	0.22714	0.86744	0.24382	**H27**	0.30374	0.10533	0.56735
H28	0.52272	0.55883	0.75559	**H23**	0.1333	0.35798	0.2436	**H34**	0.85584	0.22568	0.4232
H29	0.4418	0.96167	0.73932	**H24**	0.63737	0.77224	0.23456	**H35**	0.77596	0.6303	0.41903
H30	0.03623	0.47858	0.7359	**H31**	0.18925	0.89227	0.09025	**H36**	0.36696	0.14334	0.41466
H37	0.48361	0.50336	1.02633	**H32**	0.10918	0.29693	0.087	**H43**	0.81686	0.17012	0.69391
H38	0.49714	-0.02263	1.0172	**H33**	0.70064	0.8102	0.08193	**H44**	0.83045	0.64385	0.6899
H39	1.01838	0.51609	1.01438	**H40**	0.14933	0.83681	0.36084	**H45**	0.35138	0.18243	0.68602
H46	0.49402	0.45758	1.00566	**H41**	0.16396	0.3099	0.35737	**H52**	0.82728	0.12436	0.67304
H47	0.54303	0.03419	0.99935	**H42**	0.68496	0.8494	0.35308	**H53**	0.87602	0.70049	0.67215
H48	0.96219	0.5065	0.99395	**H49**	0.15985	0.79106	0.34078	**H54**	0.29536	0.17269	0.66577
H55	0.44503	0.43011	0.72735	**H50**	0.20953	0.36658	0.33991	**H61**	0.77827	0.09706	0.39471
H56	0.57119	0.01758	0.71108	**H51**	0.62893	0.83962	0.33269	**H62**	0.905	0.68254	0.39261
H57	0.98317	0.5539	0.70704	**H58**	0.11182	0.76371	0.06164	**H63**	0.31747	0.22206	0.38775
H64	0.53541	0.49112	0.72203	**H59**	0.23817	0.34913	0.05971	**H70**	0.86864	0.15803	0.3895
H65	0.51149	0.04522	0.70839	**H60**	0.6511	0.88886	0.05455	**H71**	0.84322	0.71074	0.38909
H66	0.95312	0.46612	0.70211	**H67**	0.20218	0.82469	0.0578	**H72**	0.28686	0.13155	0.38188
H73	0.48131	0.3004	0.76832	**H68**	0.17643	0.37735	0.05745	**H79**	0.81455	-0.03262	0.43418

H74	0.70032	0.18236	0.7694	**H69**	0.62054	0.79836	0.04893	**H80**	1.03252	0.84733	0.43144
H75	0.81984	0.52354	0.75893	**H76**	0.14822	0.63428	0.10192	**H81**	0.15411	0.19025	0.42245
C244	0.61041	0.46235	0.76011	**H77**	0.36566	0.51373	0.09805	**C250**	0.94375	0.1294	0.42824
C245	0.53804	0.1487	0.76092	**H78**	0.48762	0.85689	0.08906	**C251**	0.8699	0.81299	0.4287
C246	0.84788	0.38999	0.75962	**C247**	0.27733	0.79639	0.09921	**C252**	0.18284	0.05715	0.42604
C253	0.36105	0.52158	0.85114	**C248**	0.20305	0.47941	0.09815	**C259**	0.69413	0.18826	0.52005
C254	0.48012	0.83793	0.83454	**C249**	0.51656	0.72393	0.09296	**C260**	0.81345	0.5054	0.50357
C255	0.16059	0.63954	0.8479	**C256**	0.02731	0.855	0.18361	**C261**	0.49247	0.30536	0.51365
H82	0.49632	0.68117	0.86014	**C257**	0.1467	0.17187	0.16835	**H88**	0.82941	0.34789	0.52712
H83	0.32067	0.81339	0.8481	**C258**	0.82605	0.97228	0.1805	**H89**	0.65395	0.481	0.51007
H84	0.18291	0.50304	0.84801	**H85**	0.16254	1.01463	0.19277	**H90**	0.51536	0.16919	0.51057
H91	0.57701	0.67682	0.79184	**H86**	-0.01278	0.14742	0.17727	**H97**	0.91019	0.34369	0.45963
H92	0.32311	0.89838	0.79048	**H87**	0.84904	0.83617	0.17806	**H98**	0.65794	0.56727	0.45546
H93	0.09833	0.42166	0.7862	**H94**	0.24326	1.01011	0.12527	**H99**	0.42981	0.08785	0.4515
H100	0.58898	0.63924	0.88022	**H95**	-0.00873	0.23384	0.12354	**H106**	0.92216	0.30618	0.54824
H101	0.36056	0.94653	0.88216	**H96**	0.76349	0.75479	0.11903	**H107**	0.69454	0.61409	0.55049
H102	0.04942	0.41031	0.8762	**H103**	0.25516	0.9727	0.21429	**H108**	0.38192	0.07687	0.54417
H109	0.5811	0.68755	0.93341	**H104**	0.02792	0.28048	0.21886	**H115**	0.91411	0.35444	0.60119
H110	0.31319	0.88878	0.93189	**H105**	0.71559	0.74381	0.21169	**H116**	0.64623	0.55594	0.59604
H111	0.10655	0.41977	0.92785	**H112**	0.24729	1.02113	0.26672	**H117**	0.43946	0.08612	0.59255
H118	0.39829	0.28366	0.7625	**H113**	-0.0204	0.22227	0.26407	**H124**	0.73153	-0.04945	0.42919
H119	0.71864	0.11758	0.76487	**H114**	0.77314	0.75309	0.26009	**H125**	1.05069	0.78233	0.43206
H120	0.88675	0.60587	0.75929	**H121**	0.06517	0.61734	0.09541	**H126**	0.22128	0.27262	0.4266
H127	0.39408	0.33552	0.71887	**H122**	0.38386	0.44876	0.09785	**H133**	0.72728	0.00242	0.38577
H128	0.66781	0.06136	0.71823	**H123**	0.5548	0.93927	0.09195	**H134**	0.9995	0.72549	0.38949
H129	0.94235	0.60944	0.71366	**H130**	0.06098	0.66927	0.05225	**H135**	0.27732	0.27632	0.38409
H136	0.38602	0.31871	0.85771	**H131**	0.33254	0.3919	0.05581	**H142**	0.71924	-0.01446	0.52455
H137	0.68336	0.06926	0.8578	**H132**	0.61096	0.94298	0.05037	**H143**	1.01604	0.73552	0.52842
H138	0.93391	0.61624	0.85325	**H139**	0.05245	0.65199	0.1908	**H144**	0.26726	0.28229	0.52316
H145	0.44464	0.6999	0.77575	**H140**	0.34951	0.40198	0.19451	**H151**	0.77764	0.36643	0.44356
H146	0.30088	0.74261	0.77	**H141**	0.60062	0.94913	0.18919	**H152**	0.63446	0.41008	0.43386
H147	0.25612	0.5549	0.78185	**H148**	0.11088	1.03306	0.10776	**H153**	0.58856	0.22138	0.4461
H154	0.36236	0.60645	0.86079	**H149**	-0.03232	0.0767	0.09991	**H160**	0.6954	0.27308	0.52813
H155	0.39595	0.7547	0.84577	**H150**	0.92199	0.88823	0.11226	**H161**	0.72932	0.42209	0.5112
H156	0.24265	0.63766	0.85088	**H157**	0.02856	0.93987	0.19286	**H162**	0.57486	0.3041	0.51471
H163	0.54856	0.28187	0.80469	**H158**	0.06258	0.08851	0.17638	**H169**	0.88144	-0.05122	0.46908
H164	0.7195	0.26784	0.79125	**H159**	0.90847	0.97104	0.1811	**H170**	0.05158	-0.06721	0.44903
H165	0.73189	0.45554	0.80302	**H166**	0.21498	0.61578	0.13811	**H171**	0.06646	0.12196	0.467
H172	0.61081	0.38142	0.71885	**H167**	0.38477	0.59914	0.1155	**H178**	0.9439	0.04859	0.38393
H173	0.61833	0.22949	0.71673	**H168**	0.40022	0.78863	0.13524	**H179**	0.9495	0.89362	0.37908
H174	0.76737	0.39818	0.69305	**H175**	0.27764	0.71576	0.05361	**H180**	0.10245	0.06485	0.35587
H181	0.35325	0.52326	0.76603	**H176**	0.28248	0.55993	0.04706	**H190**	0.20876	0.05826	0.36564
H182	0.33589	0.52794	0.90048	**H177**	0.43598	0.73145	0.02318	**H191**	0.14588	0.03317	0.39468
H183	0.35374	0.48417	0.86878	**H184**	0.20546	0.51018	0.14413	**H192**	0.18718	0.04023	0.49929
H196	0.63885	0.46049	0.80696	**H185**	0.16654	0.44738	0.11335	**H193**	0.52236	0.32931	0.56817
H197	0.61521	0.49919	0.77193	**H186**	0.20579	0.48796	0.01247	**H194**	0.46181	0.31223	0.52744
H198	0.6158	0.45803	0.67492	**H187**	0.18425	0.20234	0.18305	**H195**	0.50481	0.31513	0.43033
H208	0.51777	0.86847	0.84774	**H188**	0.14363	0.16162	0.08339	**H199**	0.8722	0.8438	0.47435
H209	0.47653	0.82704	0.74993	**H189**	0.14145	0.14081	0.21798	**H200**	0.83335	0.78098	0.44364
H210	0.47511	0.80722	0.88515	**H202**	0.54256	0.72507	0.03273	**H201**	0.87287	0.8215	0.34296

H211	0.53971	0.17863	0.80895	**H203**	0.47965	0.69996	0.06136	**H214**	0.85096	0.53591	0.51839
H212	0.50125	0.11646	0.77209	**H204**	0.52082	0.707	0.16628	**H215**	0.81056	0.49493	0.41879
H213	0.54234	0.15891	0.67601	**H205**	0.85602	0.99629	0.23477	**H216**	0.80806	0.47446	0.55383
H217	0.87326	0.39076	0.69818	**H206**	0.7954	0.97916	0.1945	**H220**	0.68603	0.18975	0.43505
H218	0.81059	0.36608	0.72983	**H207**	0.83825	0.98196	0.09708	**H221**	0.66913	0.19474	0.56971
H219	0.8527	0.37319	0.83253	**H226**	0.01962	0.85668	0.09843	**H222**	0.68688	0.1509	0.53797
H223	0.19023	0.6632	0.90326	**H227**	0.00206	0.86132	0.2327	**H229**	0.97197	0.12742	0.47568
H224	0.13002	0.64665	0.86074	**H228**	0.02001	0.8176	0.20134	**H230**	0.94847	0.16619	0.44032
H225	0.17345	0.64949	0.76495	**H232**	0.30525	0.7944	0.14776	**H231**	0.94952	0.12535	0.34313
C11	0.53903	-0.01546	0.87181	**H233**	0.28188	0.83312	0.11106	**C223**	-0.0482	-0.00738	0.53142
C12	1.01372	0.55275	0.86963	**H234**	0.28371	0.79253	0.01437	**C224**	1.00954	-0.04023	0.51921
C20	0.48775	1.01125	0.87251	**C193**	1.04493	0.9969	0.02441	**C232**	-0.03931	-0.0481	0.5458
C21	-0.01443	0.47448	0.86734	**C194**	0.00124	1.04418	0.01711	**C234**	0.99353	0.04189	0.54929
C29	0.45801	-0.03848	0.81762	**C195**	-0.04637	-0.04698	0.02483	**C242**	1.01535	0.92633	0.46664
C30	1.03589	0.49424	0.81478	**C202**	0.04614	0.04233	-0.00476	**N17**	-0.02525	-0.1136	0.41589
C38	0.51742	1.00264	0.95392	**C203**	0.95491	0.9991	-0.00217				
C39	-0.00599	0.51221	0.94997	**C204**	-0.00153	0.95139	0.00498				

Table S5. Fractional atomic coordinates for the unit cell of ND-COF-2.

ND-COF-2 in eclipsed AA model (Space group P1)											
a = 34.48 Å, b = 33.14 Å, c = 10.89 Å, α = 89.83°, β = 88.81°, γ = 60.25°											
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
N1	0.6572	0.6642	0.04811	**C137**	0.18545	0.35457	0.24198	**C69**	0.47959	0.94455	0.69261
H2	0.66411	0.66657	-0.04474	**C139**	0.2336	0.34019	0.25562	**C71**	0.43601	0.97705	0.72474
C2	0.90906	0.55397	0.1728	**O2**	0.1731	0.32666	0.24694	**C73**	0.40102	0.96747	0.72196
C4	0.86682	0.57052	0.25616	**O4**	0.27855	0.36703	0.33877	**C75**	0.40835	0.92542	0.68082
C6	0.85967	0.52568	0.12187	**O6**	0.14552	0.47125	0.15167	**C77**	0.45314	0.89066	0.65779
C8	0.90444	0.52307	0.08063	**C141**	0.10788	0.4177	0.23625	**C79**	0.48823	0.90079	0.66508
H4	0.91476	0.58054	0.131	**H111**	0.09689	0.39398	0.26337	**H60**	0.52183	0.87581	0.63787
H6	0.90753	0.53071	-0.01668	**C143**	0.26653	0.29781	0.22906	**C82**	0.36864	0.92007	0.65305
C10	0.8603	0.52948	0.2609	**H113**	0.30084	0.28972	0.24101	**H62**	0.34772	0.9268	0.73769
H8	0.82893	0.53561	0.30806	**C145**	0.23299	0.44891	0.19754	**H64**	0.3483	0.94448	0.58154
H10	0.88789	0.4994	0.30456	**H115**	0.21243	0.47872	0.1436	**H66**	0.37831	0.88582	0.61892
C12	0.8273	0.60411	0.17771	**N3**	0.07506	0.46461	0.22201	**C84**	0.3547	0.1968	0.67511
H12	0.83033	0.6323	0.13604	**H117**	0.0741	0.47991	0.30569	**H68**	0.38667	0.16429	0.6764
C14	0.82211	0.57361	0.08563	**N5**	0.2789	0.43647	0.21631	**H70**	0.35026	0.21	0.5802
H14	0.82188	0.58329	-0.01153	**H119**	0.29451	0.42618	0.12977	**H72**	0.35814	0.21986	0.73947
H16	0.86906	0.58485	0.34497	**N7**	0.2581	0.26876	0.15239	**C86**	0.36767	0.51478	0.74021
H18	0.85521	0.49761	0.08776	**H121**	0.27533	0.26381	0.06861	**C88**	0.40256	0.51786	0.82179
C16	0.78129	0.61725	0.22539	**C147**	0.54799	0.76446	0.16204	**C90**	0.3454	0.58823	0.8258
C18	0.74639	0.65966	0.25811	**C149**	0.50271	0.77529	0.2075	**C92**	0.32825	0.56301	0.74477
C20	0.70441	0.67403	0.20641	**C151**	0.49806	0.73775	0.2606	**H74**	0.37983	0.50007	0.64711
C22	0.69868	0.64799	0.11331	**C153**	0.52772	0.69116	0.21266	**H76**	0.31492	0.57836	0.65429
C24	0.73575	0.60532	0.0791	**C155**	0.57195	0.68025	0.15731	**C94**	0.37349	0.55259	0.91857
C26	0.77601	0.59007	0.13998	**C157**	0.58275	0.71697	0.13276	**H78**	0.39225	0.56283	0.97951
H20	0.67707	0.70643	0.23552	**O8**	0.59931	0.64101	0.13234	**H80**	0.35396	0.54179	0.97714
H22	0.75718	0.57152	-0.09587	**O10**	0.55758	0.79436	0.15539	**C96**	0.4205	0.54387	0.74403

C28	0.99191	0.50848	0.24599	**O12**	0.46932	0.7453	0.3393	**H82**	0.43459	0.52952	0.65165
C30	0.95071	0.51322	0.2152	**C159**	0.51367	0.6606	0.20631	**C98**	0.38103	0.59208	0.74509
C32	0.94697	0.48506	0.12996	**H123**	0.53413	0.62991	0.15347	**H84**	0.36997	0.60757	0.65337
C34	0.98458	0.45212	0.06663	**C161**	0.6226	0.70871	0.08368	**H86**	0.42875	0.48514	0.8582
C36	0.02684	0.44428	0.10267	**H125**	0.62851	0.73665	0.06486	**H88**	0.31883	0.62059	0.86587
C38	0.0313	0.47104	0.1953	**C163**	0.46571	0.81641	0.19492	**C100**	0.44612	0.56218	0.80954
H24	1.01024	0.55933	0.27639	**H127**	0.43456	0.82204	0.23752	**C102**	0.48991	0.55282	0.79156
H26	0.05642	0.41843	0.05525	**N9**	0.46851	0.67234	0.24044	**C104**	0.49781	0.58944	0.78313
C40	0.97973	0.42631	-0.03727	**H129**	0.45027	0.68702	0.16138	**C106**	0.46171	0.63466	0.77141
H28	0.96274	0.40788	-0.00318	**N11**	0.46202	0.84861	0.10311	**C108**	0.41707	0.64265	0.78329
H30	0.95942	0.44981	-0.11003	**H131**	0.4892	0.83609	0.04128	**C110**	0.41052	0.60617	0.80854
H32	1.01273	0.40155	-0.07805	**C164**	0.37085	0.41883	0.24333	**H90**	0.53217	0.58183	0.77909
C42	0.75397	0.68851	0.34691	**H132**	0.3941	0.40948	0.32107	**H92**	0.38428	0.71608	0.77324
H34	0.76554	0.67039	0.43519	**H133**	0.36218	0.39179	0.23322	**C112**	0.33057	0.46437	0.76857
H36	0.77989	0.69576	0.30916	**C166**	0.37665	0.68826	0.26456	**C114**	0.33741	0.50008	0.80085
H38	0.72285	0.72098	0.36545	**H136**	0.36298	0.68946	0.1723	**C116**	0.302	0.54419	0.80786
C44	0.40816	0.02282	0.16944	**H137**	0.35058	0.69425	0.33539	**C118**	0.2582	0.5543	0.79107
C46	0.39076	0.06458	0.25498	**H143**	0.69985	0.58938	-0.05803	**C120**	0.24995	0.51823	0.77525
C48	0.3349	0.04959	0.26038	**C169**	0.20895	0.1589	0.24327	**C122**	0.28586	0.47304	0.75696
C50	0.36948	0.01307	0.17051	**H145**	0.17556	0.18923	0.23231	**H94**	0.38835	0.42014	0.658
H40	0.42047	0.02625	0.07721	**H146**	0.21515	0.13535	0.16562	**H96**	0.2155	0.52645	0.77004
H42	0.35657	0.01167	0.07908	**C171**	0.99299	0.54369	0.32621	**C124**	0.22143	0.60246	0.78763
C52	0.36426	0.05527	0.35211	**H149**	0.95872	0.57074	0.35231	**H98**	0.22033	0.61962	0.87517
H44	0.34543	0.08359	0.41747	**H150**	1.01061	0.52816	0.41243	**H100**	0.22767	0.62003	0.71033
H46	0.38495	0.02438	0.40533	**H151**	0.52902	0.95042	0.08409	**H102**	0.1884	0.60494	0.77515
C54	0.35381	0.10401	0.1811	**C174**	0.51593	0.95635	0.18029	**C126**	0.52704	0.50497	0.7788
H48	0.36381	0.10878	0.08707	**H155**	0.50343	0.99227	0.20486	**H104**	0.52784	0.48589	0.86233
C56	0.31519	0.09431	0.18799	**H156**	0.5435	0.93486	0.24253	**H106**	0.52145	0.48897	0.69756
H50	0.30046	0.09434	0.09804	**C28**	-0.00809	0.50848	0.24599	**H108**	0.55998	0.50311	0.76675
H52	0.41705	0.071	0.29055	**C34**	-0.01542	0.45212	0.06663	**C128**	0.24516	0.37579	0.78118
H54	0.30971	0.04181	0.30092	**C36**	1.02684	0.44428	0.10267	**C130**	0.21656	0.42149	0.72897
C58	0.32426	0.14756	0.24841	**C38**	1.0313	0.47104	0.1953	**C132**	0.1696	0.43471	0.69887
C60	0.31594	0.19068	0.21458	**C44**	0.40816	1.02282	0.16944	**C134**	0.15221	0.40318	0.72553
C62	0.27051	0.22582	0.207	**C50**	0.36948	1.01307	0.17051	**C136**	0.18545	0.35457	0.74198
C64	0.23586	0.2156	0.22626	**C72**	0.43601	-0.02295	0.22474	**C138**	0.2336	0.34019	0.75562
C66	0.24512	0.17111	0.24537	**C74**	0.40102	-0.03253	0.22196	**O1**	0.1731	0.32666	0.74694
C68	0.28944	0.13779	0.25904	**H1**	0.66411	0.66657	0.45526	**O3**	0.27855	0.36703	0.83877
H56	0.20165	0.24171	0.21271	**C1**	0.90906	0.55397	0.6728	**O5**	0.14552	0.47125	0.65167
H58	0.20867	0.14228	0.3308	**C3**	0.86682	0.57052	0.75616	**C140**	0.10788	0.4177	0.73625
C70	0.47959	0.94455	0.19261	**C5**	0.85967	0.52568	0.62187	**H110**	0.09689	0.39398	0.76337
C72	0.43601	0.97705	0.22474	**C7**	0.90444	0.52307	0.58063	**C142**	0.26653	0.29781	0.72906
C74	0.40102	0.96747	0.22196	**H3**	0.91476	0.58054	0.631	**H112**	0.30084	0.28972	0.74101
C76	0.40835	0.92542	0.18082	**H5**	0.90753	0.53071	0.48332	**C144**	0.23299	0.44891	0.69754
C78	0.45314	0.89066	0.15779	**C9**	0.8603	0.52948	0.7609	**H114**	0.21243	0.47872	0.6436
C80	0.48823	0.90079	0.16508	**H7**	0.82893	0.53561	0.80806	**N2**	0.07506	0.46461	0.72201
H59	0.74335	0.54207	0.01896	**H9**	0.88789	0.4994	0.80456	**H116**	0.0741	0.47991	0.80569
C81	0.73362	0.57576	-0.01973	**C11**	0.8273	0.60411	0.67771	**N4**	0.2789	0.43647	0.71631
H61	0.52183	0.87581	0.13787	**H11**	0.83033	0.6323	0.63604	**H118**	0.29451	0.42618	0.62977
C83	0.36864	0.92007	0.15305	**C13**	0.82211	0.57361	0.58563	**N6**	0.2581	0.26876	0.65239
H63	0.34772	0.9268	0.23769	**H13**	0.82188	0.58329	0.48847	**H120**	0.27533	0.26381	0.56861

H65	0.3483	0.94448	0.08154	**H15**	0.86906	0.58485	0.84497	**C146**	0.54799	0.76446	0.66204
H67	0.37831	0.88582	0.11892	**H17**	0.85521	0.49761	0.58776	**C148**	0.50271	0.77529	0.7075
C85	0.3547	0.1968	0.17511	**C15**	0.78129	0.61725	0.72539	**C150**	0.49806	0.73775	0.7606
H69	0.38667	0.16429	0.1764	**C17**	0.74639	0.65966	0.75811	**C152**	0.52772	0.69116	0.71266
H71	0.35026	0.21	0.0802	**C19**	0.70441	0.67403	0.70641	**C154**	0.57195	0.68025	0.65731
H73	0.35814	0.21986	0.23947	**C21**	0.69868	0.64799	0.61331	**C156**	0.58275	0.71697	0.63276
C87	0.36767	0.51478	0.24021	**C23**	0.73575	0.60532	0.5791	**O7**	0.59931	0.64101	0.63234
C89	0.40256	0.51786	0.32179	**C25**	0.77601	0.59007	0.63998	**O9**	0.55758	0.79436	0.65539
C91	0.3454	0.58823	0.3258	**H19**	0.67707	0.70643	0.73552	**O11**	0.46932	0.7453	0.8393
C93	0.32825	0.56301	0.24477	**H21**	0.75718	0.57152	0.40413	**C158**	0.51367	0.6606	0.70631
H75	0.37983	0.50007	0.14711	**C27**	0.99191	0.50848	0.74599	**H122**	0.53413	0.62991	0.65347
H77	0.31492	0.57836	0.15429	**C29**	0.95071	0.51322	0.7152	**C160**	0.6226	0.70871	0.58368
C95	0.37349	0.55259	0.41857	**C31**	0.94697	0.48506	0.62996	**H124**	0.62851	0.73665	0.56486
H79	0.39225	0.56283	0.47951	**C33**	0.98458	0.45212	0.56663	**C162**	0.46571	0.81641	0.69492
H81	0.35396	0.54179	0.47714	**C35**	0.02684	0.44428	0.60267	**H126**	0.43456	0.82204	0.73752
C97	0.4205	0.54387	0.24403	**C37**	0.0313	0.47104	0.6953	**N8**	0.46851	0.67234	0.74044
H83	0.43459	0.52952	0.15165	**H23**	1.01024	0.55933	0.77639	**H128**	0.45027	0.68702	0.66138
C99	0.38103	0.59208	0.24509	**H25**	0.05642	0.41843	0.55525	**N10**	0.46202	0.84861	0.60311
H85	0.36997	0.60757	0.15337	**C39**	0.97973	0.42631	0.46273	**H130**	0.4892	0.83609	0.54128
H87	0.42875	0.48514	0.3582	**H27**	0.96274	0.40788	0.49682	**N12**	0.6572	0.6642	0.54811
H89	0.31883	0.62059	0.36587	**H29**	0.95942	0.44981	0.38997	**C165**	0.37085	0.41883	0.74333
C101	0.44612	0.56218	0.30954	**H31**	1.01273	0.40155	0.42195	**H134**	0.3941	0.40948	0.82107
C103	0.48991	0.55282	0.29156	**C41**	0.75397	0.68851	0.84691	**H135**	0.36218	0.39179	0.73322
C105	0.49781	0.58944	0.28313	**H33**	0.76554	0.67039	0.93519	**C167**	0.37665	0.68826	0.76456
C107	0.46171	0.63466	0.27141	**H35**	0.77989	0.69576	0.80916	**H138**	0.36298	0.68946	0.6723
C109	0.41707	0.64265	0.28329	**H37**	0.72285	0.72098	0.86545	**H139**	0.35058	0.69425	0.83539
C111	0.41052	0.60617	0.30854	**C43**	0.40816	0.02282	0.66944	**H140**	0.69985	0.58938	0.44197
H91	0.53217	0.58183	0.27909	**C45**	0.39076	0.06458	0.75498	**C168**	0.73362	0.57576	0.48027
H93	0.38428	0.71608	0.27324	**C47**	0.3349	0.04959	0.76038	**H141**	1.01061	0.52816	0.91243
C113	0.33057	0.46437	0.26857	**C49**	0.36948	0.01307	0.67051	**H142**	0.74335	0.54207	0.51896
C115	0.33741	0.50008	0.30085	**H39**	0.42047	0.02625	0.57721	**H144**	0.95872	0.57074	0.85231
C117	0.302	0.54419	0.30786	**H41**	0.35657	0.01167	0.57908	**C170**	0.20895	0.1589	0.74327
C119	0.2582	0.5543	0.29107	**C51**	0.36426	0.05527	0.85211	**H147**	0.17556	0.18923	0.73231
C121	0.24995	0.51823	0.27525	**H43**	0.34543	0.08359	0.91747	**H148**	0.21515	0.13535	0.66562
C123	0.28586	0.47304	0.25696	**H45**	0.38495	0.02438	0.90533	**C172**	0.99299	0.54369	0.82621
H95	0.38835	0.42014	0.158	**C53**	0.35381	0.10401	0.6811	**H152**	0.52902	0.95042	0.58409
H97	0.2155	0.52645	0.27004	**H47**	0.36381	0.10878	0.58707	**C173**	0.51593	0.95635	0.68029
C125	0.22143	0.60246	0.28763	**C55**	0.31519	0.09431	0.68799	**H153**	0.50343	0.99227	0.70486
H99	0.22033	0.61962	0.37517	**H49**	0.30046	0.09434	0.59804	**H154**	0.5435	0.93486	0.74253
H101	0.22767	0.62003	0.21033	**H51**	0.41705	0.071	0.79055	**C27**	-0.00809	0.50848	0.74599
H103	0.1884	0.60494	0.27515	**H53**	0.30971	0.04181	0.80092	**C33**	-0.01542	0.45212	0.56663
C127	0.52704	0.50497	0.2788	**C57**	0.32426	0.14756	0.74841	**C35**	1.02684	0.44428	0.60267
H105	0.52784	0.48589	0.36233	**C59**	0.31594	0.19068	0.71458	**C37**	1.0313	0.47104	0.6953
H107	0.52145	0.48897	0.19756	**C61**	0.27051	0.22582	0.707	**C43**	0.40816	1.02282	0.66944
H109	0.55998	0.50311	0.26675	**C63**	0.23586	0.2156	0.72626	**C49**	0.36948	1.01307	0.67051
C129	0.24516	0.37579	0.28118	**C65**	0.24512	0.17111	0.74537	**C71**	0.43601	-0.02295	0.72474
C131	0.21656	0.42149	0.22897	**C67**	0.28944	0.13779	0.75904	**C73**	0.40102	-0.03253	0.72196
C133	0.1696	0.43471	0.19887	**H55**	0.20165	0.24171	0.71271				
C135	0.15221	0.40318	0.22553	**H57**	0.20867	0.14228	0.8308				

Table S6. Fractional atomic coordinates for the unit cell of ND-COF-2.

ND-COF-2 in staggered AB model (Space group P1)											
a = 34.27 Å, b = 32.91 Å, c = 9.70 Å, α = 88.54°, β = 84.80°, γ = 61.95°											
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
N1	0.33907	0.32784	0.07643	**C135**	0.82071	0.05916	0.26946	**H57**	0.20196	0.14744	0.85642
H2	0.34853	0.33528	-0.02261	**C137**	0.85295	0.00977	0.28575	**C69**	0.47473	0.95038	0.65594
C2	0.58195	0.20606	0.24758	**C139**	-0.10047	0.99667	0.31199	**C71**	0.43118	0.983	0.69692
C4	0.53788	0.21646	0.33429	**O2**	0.84094	-0.01971	0.28055	**C73**	0.39749	0.97041	0.72102
C6	0.53437	0.18277	0.14324	**O4**	0.93954	0.02661	0.41997	**C75**	0.40587	0.92511	0.69658
C8	0.57958	0.18307	0.11652	**O6**	0.81663	0.12979	0.19457	**C77**	0.4505	0.89086	0.66363
H4	0.58859	0.23586	0.229	**C141**	0.77666	0.07282	0.27773	**C79**	0.48458	0.90388	0.6471
H6	0.5845	0.19915	0.01867	**H111**	0.76487	0.0477	0.30118	**H60**	0.51817	0.87835	0.61424
C10	0.5309	0.1757	0.29864	**C143**	-0.06676	0.95377	0.28701	**C82**	0.36712	0.91543	0.69572
H8	0.49825	0.17901	0.34089	**H113**	-0.03363	0.94707	0.3063	**H62**	0.34764	0.92503	0.79827
H10	0.55694	0.14201	0.33243	**C145**	0.90208	0.10801	0.25301	**H64**	0.34535	0.9361	0.61515
C12	0.50157	0.25687	0.25913	**H115**	0.8843	0.1379	0.19043	**H66**	0.37748	0.87869	0.67411
H12	0.50677	0.28756	0.24015	**N3**	0.74494	0.12063	0.26762	**C84**	0.34079	0.20519	0.55249
C14	0.49912	0.23374	0.12844	**H117**	0.74283	0.13609	0.36247	**H68**	0.3732	0.17338	0.55033
H14	0.50262	0.25052	0.03034	**N5**	0.94732	0.09481	0.27619	**H70**	0.3345	0.2159	0.44393
H16	0.5375	0.22264	0.4465	**H119**	0.96545	0.08386	0.17961	**H72**	0.34426	0.23159	0.61103
H18	0.53063	0.15774	0.07827	**N7**	-0.07167	0.92166	0.20203	**C86**	0.34651	0.5271	0.70897
C16	0.45417	0.26822	0.29868	**H121**	-0.05198	0.91635	0.1087	**C88**	0.37029	0.53275	0.83061
C18	0.41925	0.31027	0.34687	**C147**	0.22766	0.41816	0.23595	**C90**	0.326	0.60516	0.77497
C20	0.38006	0.32888	0.27902	**C149**	0.18225	0.42301	0.26396	**C92**	0.31604	0.57679	0.67141
C22	0.37769	0.3081	0.15473	**C151**	0.17821	0.38073	0.29706	**H74**	0.36846	0.50491	0.6202
C24	0.41497	0.2669	0.10312	**C153**	0.2157	0.33504	0.25253	**H76**	0.31931	0.58457	0.55989
C26	0.45197	0.24689	0.17913	**C155**	0.2608	0.33072	0.22663	**C94**	0.33437	0.57627	0.90481
H20	0.35256	0.36073	0.32001	**C157**	0.26601	0.3726	0.19794	**H78**	0.34614	0.58883	0.98907
H22	0.44714	0.21229	-0.05284	**O8**	0.29339	0.29279	0.22812	**H80**	0.30504	0.57299	0.95043
C28	0.66241	0.15673	0.31534	**O10**	0.2338	0.45144	0.24943	**C96**	0.40351	0.54881	0.76297
C30	0.6223	0.16193	0.2747	**O12**	0.14395	0.38354	0.3563	**H82**	0.42717	0.52679	0.67671
C32	0.62037	0.1409	0.15397	**C159**	0.20922	0.29944	0.21753	**C98**	0.373	0.5985	0.7236
C34	0.65871	0.11424	0.06828	**H123**	0.23768	0.26801	0.17664	**H84**	0.37798	0.60653	0.61329
C36	0.69981	0.10551	0.113	**C161**	0.30361	0.37036	0.13378	**H86**	0.38527	0.50209	0.8967
C38	0.70235	0.12607	0.23641	**H125**	0.30645	0.40168	0.11609	**H88**	0.30004	0.64161	0.78968
H24	0.67639	0.2083	0.39677	**C163**	0.14516	0.46313	0.24661	**C100**	0.42313	0.56834	0.85784
H26	0.73	0.08472	0.04806	**H127**	0.11319	0.46502	0.27926	**C102**	0.46663	0.55423	0.88699
C40	0.65554	0.09734	-0.07023	**N9**	0.16563	0.30558	0.20047	**C104**	0.47953	0.58868	0.90121
H28	0.63881	0.07549	-0.05605	**H129**	0.16474	0.30013	0.09531	**C106**	0.45224	0.63478	0.86164
H30	0.63596	0.12704	-0.13528	**N11**	0.14475	0.49757	0.15062	**C108**	0.41047	0.64636	0.81065
H32	0.68889	0.07659	-0.12542	**H131**	0.17437	0.48594	0.08669	**C110**	0.3957	0.61329	0.82147
C42	0.42438	0.33544	0.46482	**C164**	1.0374	0.07226	0.33368	**H90**	0.51196	0.57933	0.93456
H34	0.43158	0.31365	0.55798	**H132**	1.05617	0.06357	0.42695	**H92**	0.37071	0.72009	0.82312
H36	0.45216	0.34339	0.43703	**H133**	1.02637	0.04593	0.32168	**C112**	0.29652	0.4864	0.71101
H38	0.39372	0.36827	0.49024	**C166**	0.07372	0.33251	0.26325	**C114**	0.30537	0.52208	0.74558
C44	0.08295	0.67563	0.24164	**H136**	0.07884	0.33741	0.15066	**C116**	0.2776	0.56761	0.71224
C46	0.06179	0.71915	0.33648	**H137**	0.04008	0.33557	0.28505	**C118**	0.23968	0.57943	0.64433
C48	0.00884	0.69802	0.34414	**H143**	0.41396	0.2688	-0.11852	**C120**	0.22784	0.54476	0.62116
C50	0.04643	0.66169	0.24374	**C169**	-0.1177	0.80294	0.31054	**C122**	0.25572	0.49822	0.65501

H40	0.09626	0.6797	0.13609	**H145**	-0.15064	0.83191	0.29166	**H94**	0.3629	0.43135	0.66893
H42	0.03697	0.65872	0.13912	**H146**	-0.10751	0.77679	0.22625	**H96**	0.19843	0.55326	0.56876
C52	0.03424	0.7079	0.44758	**C171**	0.66144	0.18604	0.43352	**C124**	0.21317	0.62759	0.59568
H44	0.01293	0.73718	0.52013	**H149**	0.62691	0.20868	0.47779	**H98**	0.20291	0.65217	0.68446
H46	0.05419	0.67776	0.51097	**H150**	0.68	0.16375	0.51755	**H100**	0.23363	0.63582	0.516
C54	0.02615	0.75655	0.2507	**H151**	0.20219	0.61301	0.13536	**H102**	0.18278	0.63202	0.55067
H48	0.03777	0.761	0.14316	**C174**	0.18961	0.61589	0.24612	**C126**	0.49829	0.50415	0.9009
C56	-0.01063	0.7428	0.25964	**H155**	0.17563	0.65232	0.28137	**H104**	0.48503	0.48946	0.98547
H50	-0.02192	0.74013	0.15777	**H156**	0.21771	0.59416	0.3078	**H106**	0.50239	0.48549	0.80247
H52	0.08578	0.72895	0.3752	**C93**	1.00747	0.21639	0.3066	**H108**	0.5314	0.49894	0.92479
H54	-0.01599	0.68769	0.38985	**C113**	-0.00071	0.12034	0.35039	**C128**	0.23073	0.38436	0.68482
C58	-0.00628	0.80082	0.32376	**C115**	1.00839	0.15589	0.38353	**C130**	0.1952	0.43302	0.70279
C60	-0.01496	0.84515	0.28234	**C117**	-0.02406	0.20194	0.38263	**C132**	0.14878	0.44177	0.74073
C62	-0.05993	0.87825	0.26752	**C129**	-0.09045	1.03413	0.34746	**C134**	0.13694	0.4037	0.73085
C64	-0.09361	0.86493	0.28827	**C137**	-0.14705	1.00977	0.28575	**C136**	0.17169	0.35805	0.67271
C66	-0.08348	0.81899	0.31486	**C139**	0.89953	-0.00333	0.31199	**C138**	0.21939	0.34722	0.65396
C68	-0.03979	0.78767	0.33597	**H1**	0.66152	0.64712	0.43191	**O1**	0.1607	0.32944	0.64065
H56	-0.12722	0.8895	0.26882	**C1**	0.90013	0.55478	0.7134	**O3**	0.26936	0.37486	0.69559
H58	-0.12094	0.7873	0.41082	**C3**	0.85435	0.56742	0.79359	**O5**	0.12046	0.48037	0.77959
C70	0.15526	0.59972	0.26365	**C5**	0.85532	0.5264	0.61302	**C140**	0.09595	0.40914	0.77346
C72	0.11105	0.63005	0.30467	**C7**	0.90037	0.52715	0.58842	**H110**	0.0899	0.3795	0.77376
C74	0.0779	0.61656	0.30258	**H3**	0.90718	0.58394	0.68718	**C142**	0.25225	0.30561	0.60654
C76	0.08793	0.57273	0.25346	**H5**	0.90745	0.53955	0.48614	**H112**	0.2861	0.3002	0.59547
C78	0.13324	0.54041	0.21972	**C9**	0.84887	0.52486	0.77029	**C144**	0.20381	0.46895	0.68007
C80	0.16628	0.5545	0.2263	**H7**	0.81589	0.52858	0.81032	**H114**	0.17641	0.50373	0.69277
H59	0.38761	0.23761	-0.03045	**H9**	0.87423	0.49303	0.81569	**N2**	0.05963	0.45284	0.82098
C81	0.416	0.24516	-0.03257	**C11**	0.81911	0.60416	0.70467	**H116**	0.05279	0.44843	0.92593
H61	0.20023	0.53176	0.18853	**H11**	0.82358	0.6348	0.67657	**N4**	0.24586	0.46244	0.61467
C83	0.05021	0.56358	0.22508	**C13**	0.81979	0.5758	0.58095	**H118**	0.24346	0.46445	0.50784
H63	0.03077	0.56467	0.32417	**H13**	0.82449	0.58929	0.47786	**N6**	0.24323	0.27204	0.54448
H65	0.02796	0.59025	0.15621	**H15**	0.85136	0.57777	0.90367	**H120**	0.25893	0.26434	0.44433
H67	0.06154	0.52984	0.1731	**H17**	0.85359	0.49853	0.55605	**C146**	0.54674	0.75917	0.64722
C85	0.02368	0.85425	0.24205	**C15**	0.77165	0.61452	0.73891	**C148**	0.50397	0.77233	0.73273
H69	0.0558	0.82222	0.24369	**C17**	0.73393	0.65517	0.78097	**C150**	0.50071	0.73563	0.81693
H71	0.02187	0.86799	0.13592	**C19**	0.69441	0.66561	0.7207	**C152**	0.52387	0.68756	0.76039
H73	0.02439	0.87859	0.31727	**C21**	0.69456	0.63983	0.60381	**C154**	0.56515	0.67411	0.66612
C87	0.04307	0.16633	0.31091	**C23**	0.73547	0.60177	0.55241	**C156**	0.57936	0.70946	0.62173
C89	0.07736	0.1687	0.40039	**C25**	0.77235	0.58855	0.62745	**O7**	0.58706	0.63421	0.62447
C91	0.0261	0.24196	0.38993	**H19**	0.66414	0.69507	0.76123	**O9**	0.55646	0.78891	0.60564
C93	0.00747	0.21639	0.3066	**H21**	0.73416	0.59845	0.33184	**O11**	0.47889	0.74499	0.92931
H75	0.05639	0.14923	0.20726	**C27**	0.97931	0.5042	0.80625	**C158**	0.50721	0.65756	0.78437
H77	-0.00131	0.22921	0.20064	**C29**	0.93971	0.51167	0.75463	**H122**	0.52547	0.62332	0.73686
C95	0.04851	0.20799	0.50248	**C31**	0.93966	0.48691	0.6411	**C160**	0.62058	0.69779	0.56103
H79	0.06764	0.21845	0.56694	**C33**	0.97898	0.45454	0.57141	**H124**	0.62927	0.72459	0.52804
H81	0.0253	0.20089	0.57414	**C35**	0.01872	0.44199	0.63238	**C162**	0.46768	0.8144	0.73122
C97	0.10132	0.18981	0.30395	**C37**	0.01933	0.46538	0.75402	**H126**	0.43911	0.82115	0.80369
H83	0.11615	0.17194	0.20201	**H23**	1.00149	0.55102	0.87316	**N8**	0.46749	0.66867	0.87515
C99	0.06603	0.23973	0.29422	**H25**	0.04908	0.41553	0.5804	**H128**	0.44306	0.70099	0.84858
H85	0.05899	0.25167	0.18648	**C39**	0.97901	0.43345	0.43649	**N10**	0.45974	0.84574	0.61773
H87	0.09972	0.13566	0.44748	**H27**	0.99369	0.39562	0.4476	**H130**	0.48417	0.83345	0.53468

H89	0.00122	0.27709	0.42723	**H29**	0.94476	0.44656	0.40561	**N12**	0.65418	0.65059	0.5392
C101	0.12897	0.20732	0.36818	**H31**	0.99886	0.44153	0.35418	**C165**	0.33127	0.43741	0.72783
C103	0.17394	0.19339	0.33553	**C41**	0.73593	0.68647	0.88643	**H134**	0.3369	0.43096	0.83898
C105	0.18677	0.22703	0.29524	**H33**	0.74658	0.66758	0.98391	**H135**	0.32172	0.41221	0.68961
C107	0.15455	0.27356	0.27636	**H35**	0.76023	0.69833	0.84704	**C167**	0.38258	0.69169	0.74527
C109	0.10895	0.28626	0.30426	**H37**	0.70309	0.71716	0.90929	**H138**	0.40241	0.69749	0.65744
C111	0.09695	0.25327	0.35587	**C43**	0.40169	0.02612	0.62372	**H139**	0.35292	0.69245	0.70505
H91	0.22161	0.2157	0.26785	**C45**	0.38338	0.07304	0.70118	**H140**	0.71569	0.56206	0.43039
H93	0.07535	0.36009	0.32207	**C47**	0.33017	0.05319	0.7528	**C168**	0.74002	0.57554	0.42213
C113	0.99929	0.12034	0.35039	**C49**	0.3646	0.0132	0.65498	**H141**	0.99033	0.51856	1.01034
C115	0.00839	0.15589	0.38353	**H39**	0.4122	0.0258	0.51158	**H142**	0.7738	0.5458	0.40394
C117	0.97594	0.20194	0.38263	**H41**	0.3518	0.00661	0.5612	**H144**	0.94516	0.56598	0.93565
C119	0.93268	0.21398	0.35575	**C51**	0.35909	0.06635	0.83173	**C170**	0.20234	0.15683	0.74576
C121	0.9217	0.17847	0.3365	**H43**	0.34016	0.09811	0.89709	**H147**	0.16872	0.18435	0.72601
C123	0.95513	0.13136	0.32596	**H45**	0.38096	0.0387	0.89929	**H148**	0.21022	0.12621	0.68086
H95	1.06004	0.07023	0.24166	**C53**	0.34486	0.10752	0.61727	**C172**	0.97902	0.53683	0.91248
H97	0.88759	0.1885	0.32101	**H47**	0.3531	0.10791	0.50371	**H152**	0.52208	0.95476	0.5043
C125	0.89955	0.26367	0.34215	**C55**	0.30808	0.09464	0.65649	**C173**	0.50966	0.96459	0.6144
H99	0.8955	0.28272	0.4397	**H49**	0.2932	0.08872	0.56666	**H153**	0.49627	1.0024	0.62706
H101	0.91138	0.27903	0.25573	**H51**	0.40879	0.08382	0.71863	**H154**	0.53768	0.94706	0.6801
H103	0.86662	0.26767	0.321	**H53**	0.30657	0.04498	0.8181	**C27**	-0.02069	0.5042	0.80625
C127	0.20702	0.1432	0.33283	**C57**	0.31454	0.1543	0.68123	**C33**	-0.02102	0.45454	0.57141
H105	0.20477	0.12819	0.43499	**C59**	0.30392	0.19722	0.62206	**C35**	1.01872	0.44199	0.63238
H107	0.19984	0.12483	0.25248	**C61**	0.25807	0.23003	0.6206	**C37**	1.01933	0.46538	0.75402
H109	0.24149	0.13776	0.30959	**C63**	0.22531	0.21728	0.66917	**C43**	0.40169	1.02612	0.62372
C129	0.90955	0.03413	0.34746	**C65**	0.23679	0.17239	0.71349	**C49**	0.3646	1.0132	0.65498
C131	0.88384	0.08016	0.28653	**C67**	0.28151	0.14181	0.7222	**C71**	0.43118	-0.017	0.69692
C133	0.83866	0.09255	0.24691	**H55**	0.19074	0.24122	0.65976	**C73**	0.39749	-0.02959	0.72102

Section S4: FTIR spectroscopic characterizations of as-synthesized COFs

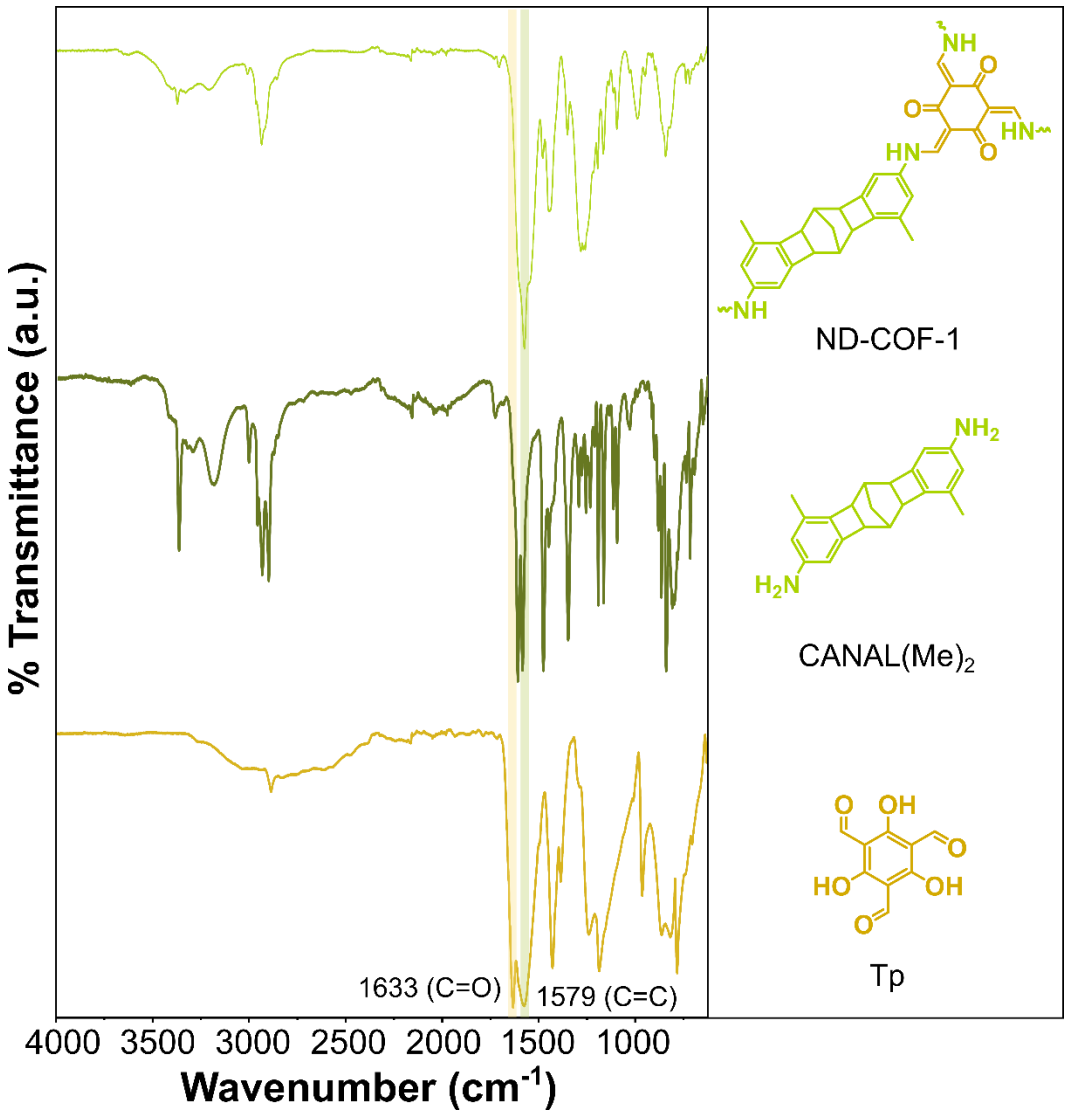

Figure S13. FTIR spectra of ND-COF-1 synthesized in green solvent media. FTIR spectra of as-synthesized **ND-COF-1** demonstrated an appearance of characteristic stretches corresponding to the β-ketoenamine-linked framework structures. Both C=O and C=C peaks have been highlighted for ready reference.

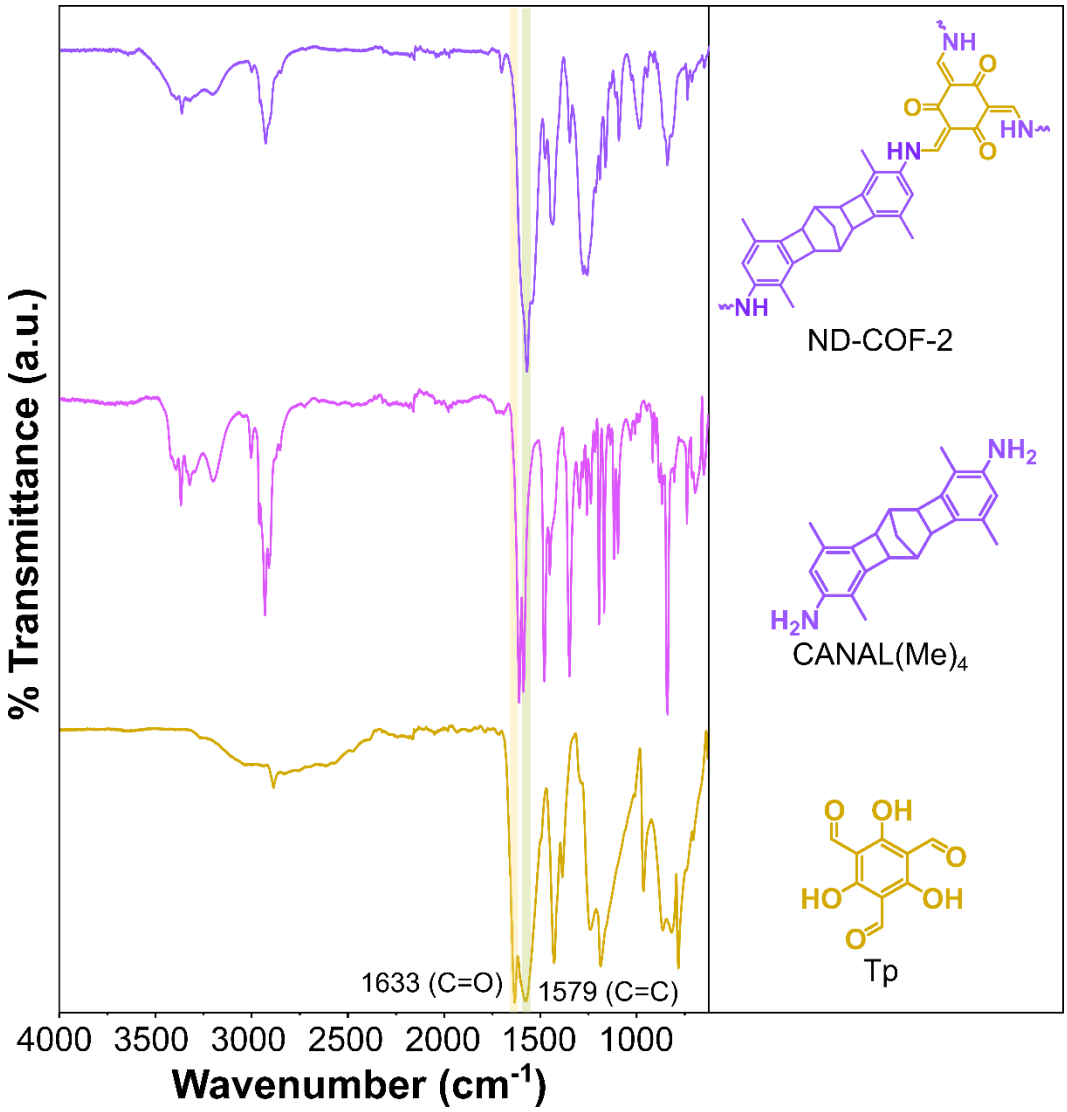

Figure S14. FTIR spectra of ND-COF-2 synthesized in green solvent media. FTIR spectra of as-synthesized **ND-COF-2** demonstrated an appearance of characteristic stretches corresponding to the β-ketoenamine-linked framework structures. Both C=O and C=C peaks have been highlighted for ready reference.

Section S5: XPS profiles of as-synthesized COFs

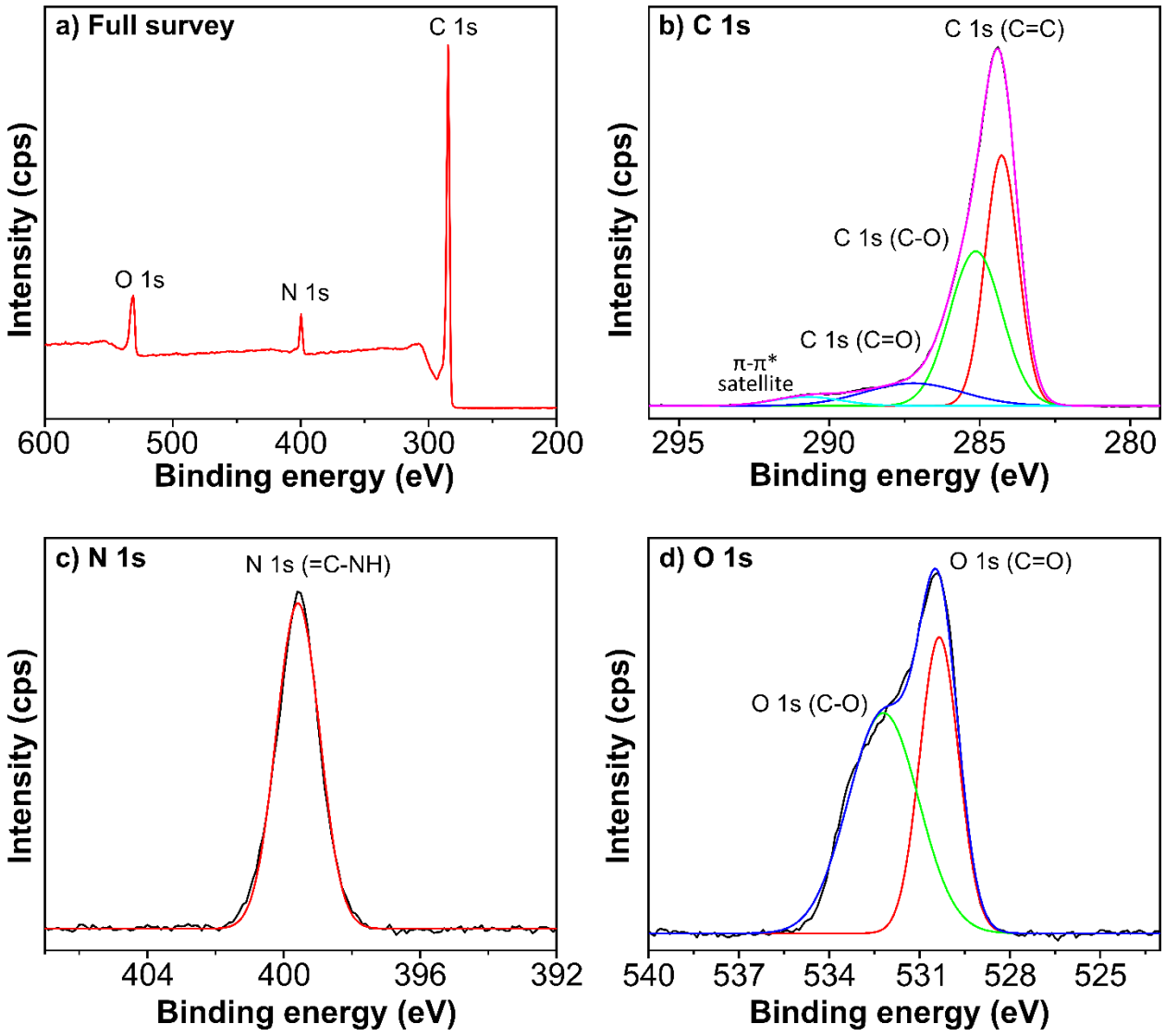

Figure S15. X-ray photoelectron spectroscopy (XPS) profile of ND-COF-1. a) Full survey XPS profile shows three peaks at 284.80 (for C 1s), 399.80 (for N 1s), and 530.80 eV (for O 1s), respectively. b) Deconvoluted XPS profile for C 1s shows 284.27 eV is assigned to C=C of aromatic ring system, and shoulders appearing at 285.13 and 287.21 are assigned to C-O and C=O bonds, respectively. In addition, a satellite peak was also observed at 290.74 eV arises from the π-π* transitions. c) For N 1s XPS profile only one peak is appeared at 399.57 eV and is assigned to =C-NH bond of the framework. d) Analysis of O 1s XPS profile shows one peak at 530.34 and a shoulder at 532.19 eV are assigned to C=O and C-O bonds of the framework.

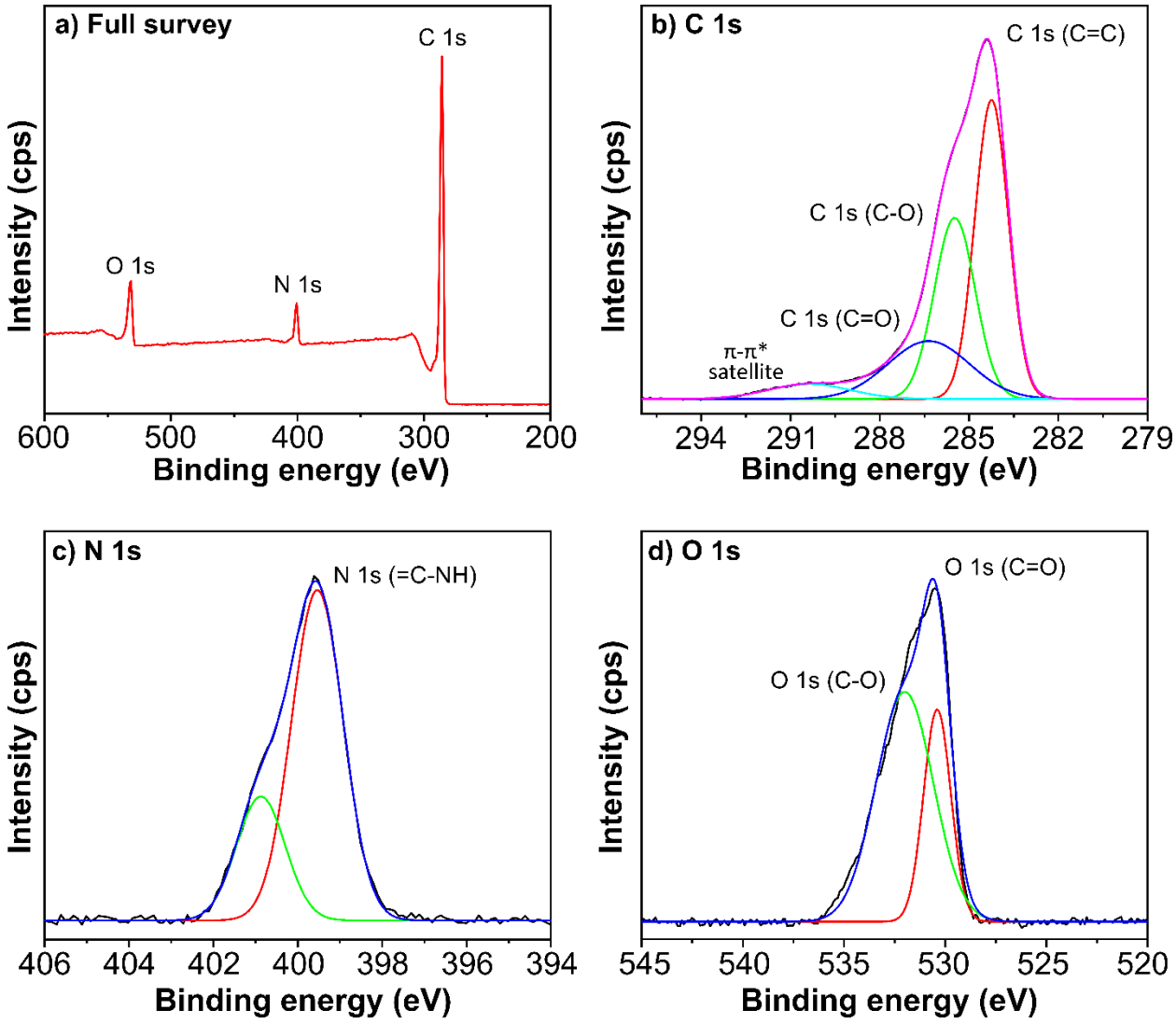

Figure S16. X-ray photoelectron spectroscopy (XPS) profile of a representative ND-COF-2. a) Full survey XPS profile shows three peaks at 284.71 (for C 1s), 399.71 (for N 1s), and 530.70 eV (for O 1s), respectively. b) Deconvoluted XPS profile for C 1s shows 284.24 eV is assigned to C=C of aromatic ring system, and shoulders appearing at 285.48 and 286.35 are assigned to C-O and C=O bonds, respectively. In addition, a satellite peak was also observed at 290.37 eV arises from the π-π* transitions. c) For N 1s XPS profile a peak appeared at 399.53 eV is assigned to =C–NH bond. The peak at 400.87 eV is attributed to the presence of another isomer of the monomer in the framework structure. d) Analysis of O 1s XPS profile shows one peak at 530.39 and a shoulder at 532.0 eV are assigned to C=O and C-O bonds of the framework.

Section S6: Thermal gravimetric analysis of as-synthesized COFs

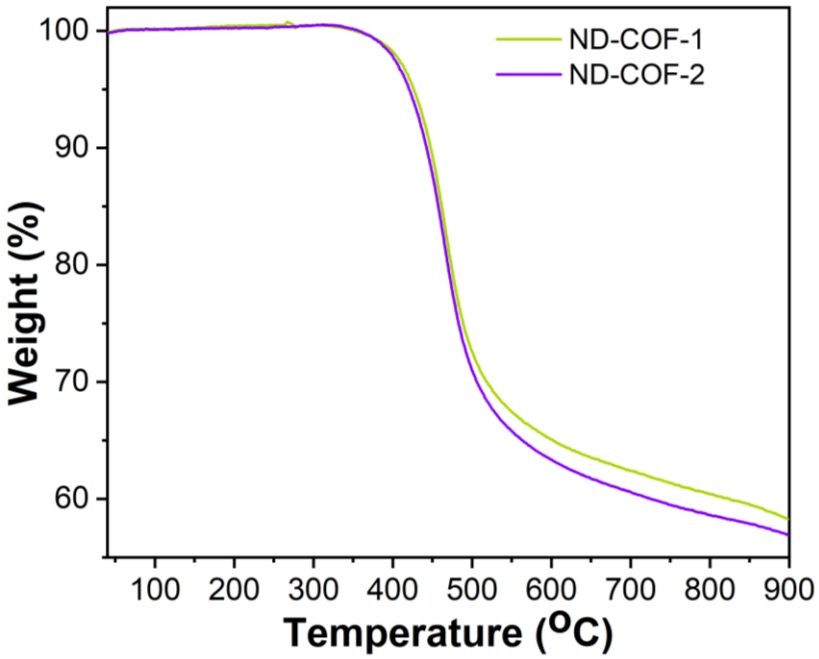

Figure S17. Thermal gravimetric analysis (TGA) profile of the as-synthesized COFs shows the thermal stability up to ~380 ˚C.

Section S7: Analysis of nitrogen gas uptake BET isotherms and pore size distribution of ND-COFs

BET theory is an extension of Langmuir theory, which is widely used to determine the adsorption of gas molecule forming a monolayer on the solid surface. Monolayer formation is related to the physical adsorption of gas molecules on a solid surface. BET equation describes the relationship between numbers of gas molecules adsorbed at a given relative pressure and thus, serves as the basis for the measurement of the specific surface area of a material.

The BET equation is

$$\frac{1}{v[(p_o/p)-1]} = \frac{c-1}{v_m c}\left(\frac{p}{p_o}\right) + \frac{1}{v_m c}$$

where p and p_o are the equilibrium and the saturation pressure of adsorbents at the temperature of adsorption, v is the adsorbed gas quantity (for example, in volume units), and v_m is the monolayer adsorbed gas quantity, c is the BET constant.

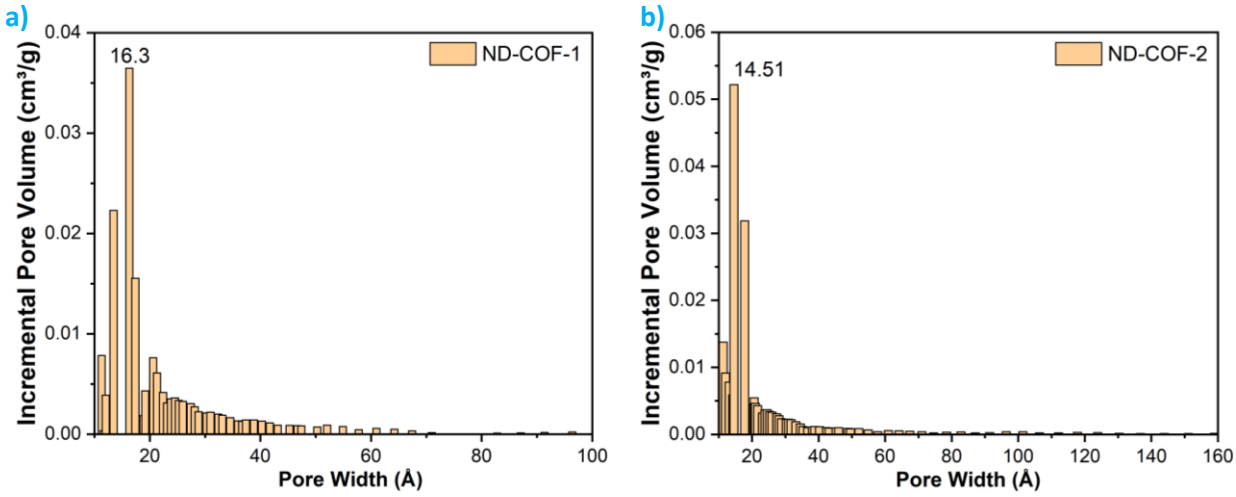

Figure S18. Pore size distribution of COFs. Pore size distribution curves of a series of COFs calculated using the non-local density functional theory (NLDFT) model show similar pore size distribution for **ND-COF-1** and **ND-COF-2**.

Table S7. Theoretical surface area measured for **ND-COF-1** and **ND-COF-2**.

	ND-COF-1		ND-COF-2	
	Theoretical	**Experimental**	**Theoretical**	**Experimental**
Unit cell_volume	10905.3	-	10972.2	-
Density	0.557057	-	0.59187	-
ASA_A^2	2478.85	-	2283.38	-
ASA_m^2/cm^3	2273.07	-	2081.06	-
ASA_m^2/g	4080.51	794	3516.08	879

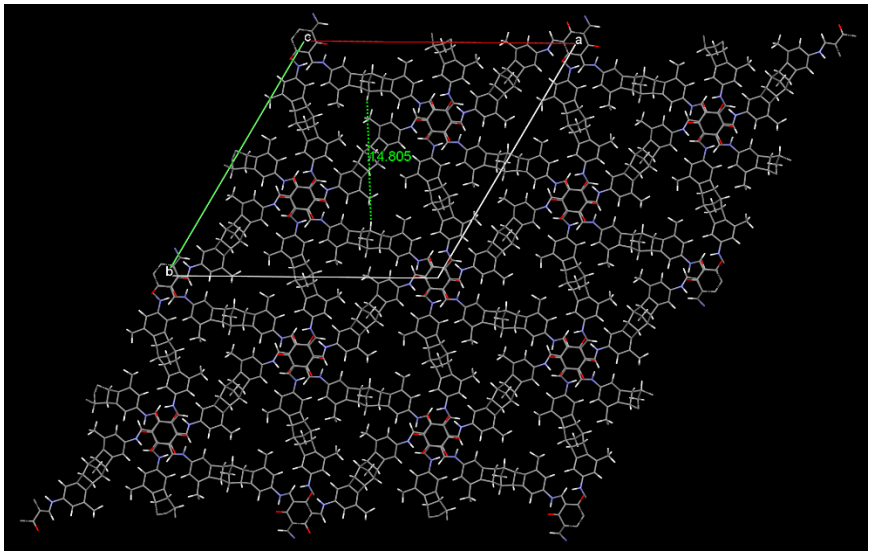

Figure S19. ND-COF-1 shows a pore size of 14.8 Å calculated from ABC crystal model.

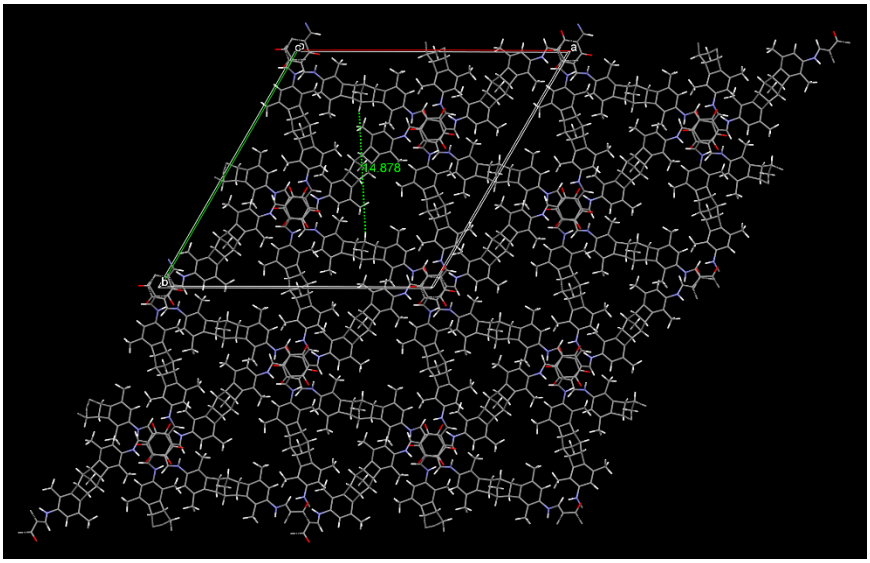

Figure S20. ND-COF-2 shows a pore size of 14.8 Å calculated from ABC crystal model.

Section S8: Stability investigation of as-synthesized COFs

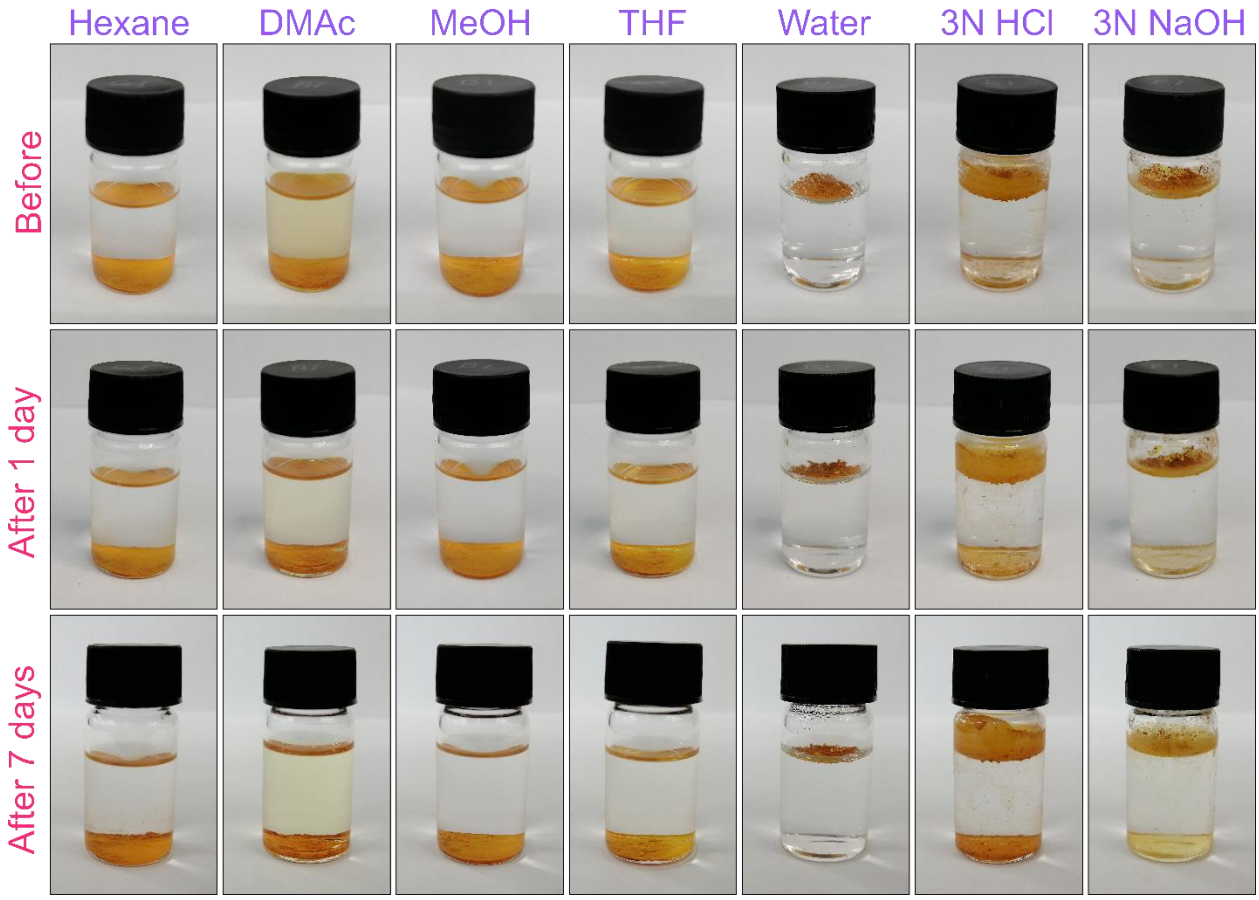

Figure S21. Chemical stability of ND-COF-1. The chemical stability of **ND-COF-1** was performed by immersing the COF in different solvents such as hexane, DMAc, MeOH, THF, Water, and acidic (3N HCl) and basic (3N NaOH) solution for 7 days. The images captured after 1 days suggest the high chemical stability of the COF in all these solvents. The chemical stability was observed maintained even after 7 days as shown above.

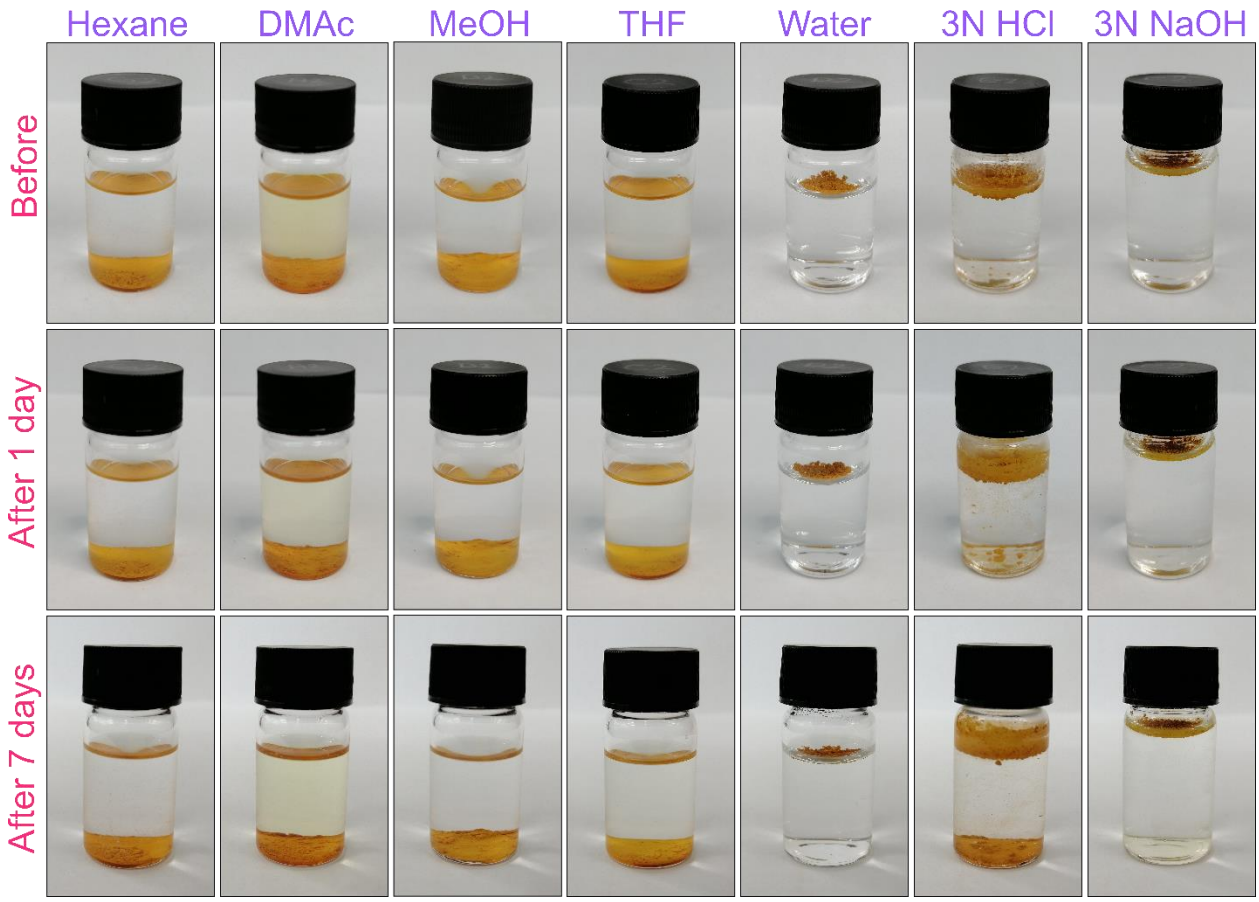

Figure S22. Chemical stability of ND-COF-2. The chemical stability of **ND-COF-2** was performed by immersing the COF in different solvents such as hexane, DMAc, MeOH, THF, Water, and acidic (3N HCl) and basic (3N NaOH) solution for 7 days. The images captured after 1 days suggest the high chemical stability of the COF in all these solvents. The chemical stability was observed maintained even after 7 days as shown above.

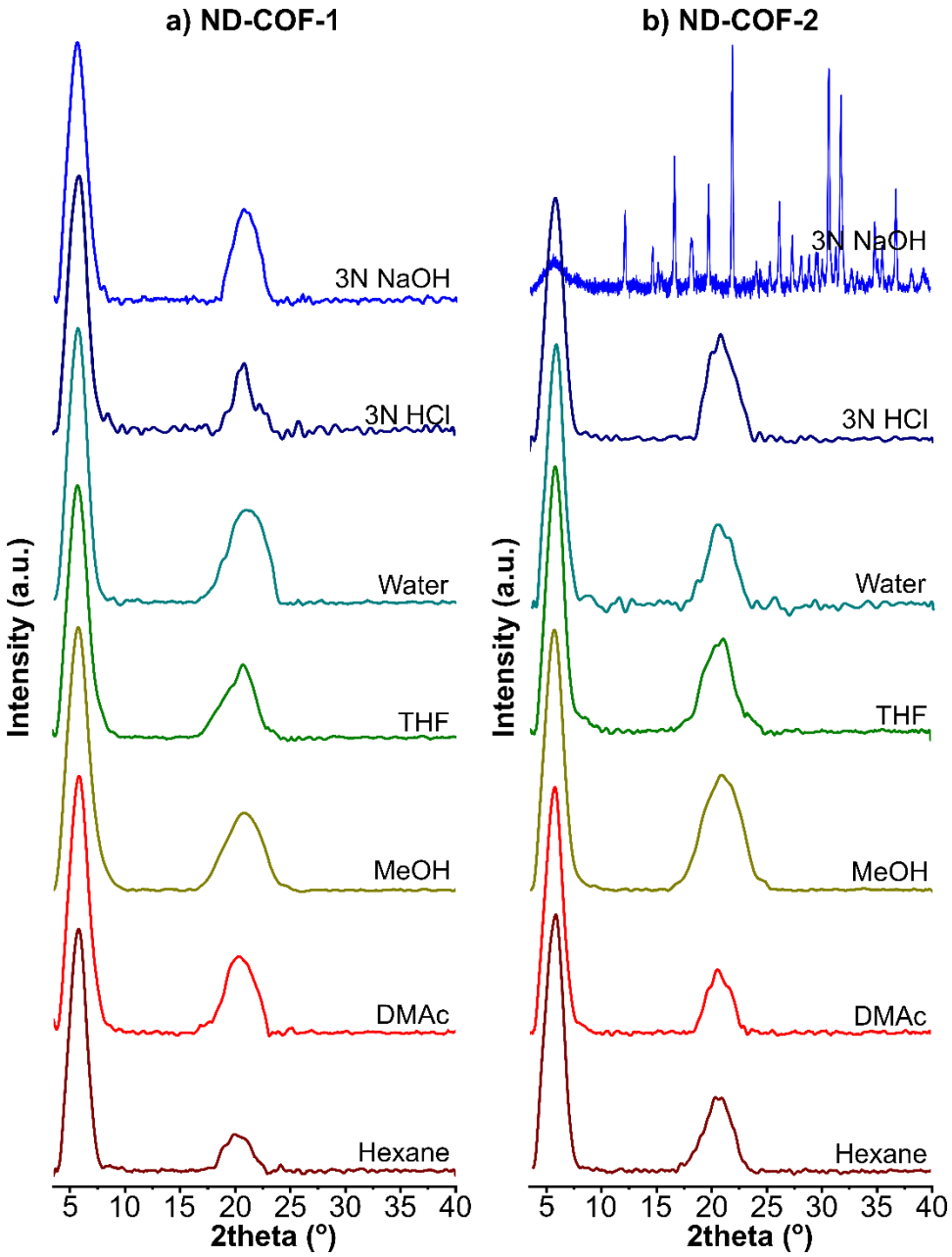

Figure S23. PXRD patterns of a) ND-COF-1 and b) ND-COF-2 treated with different solvents. Analysis of PXRD patterns of **ND-COF-1** and **ND-COF-2** suggest the high chemical stability in different organic solvents including acidic media. However, in the PXRD pattern measured for **ND-COF-2** treated in basic media displays additional number of sharp peaks along with characteristic COFs peak. This suggest that **ND-COF-2** is not stable and the framework disintegrate in the basic media.

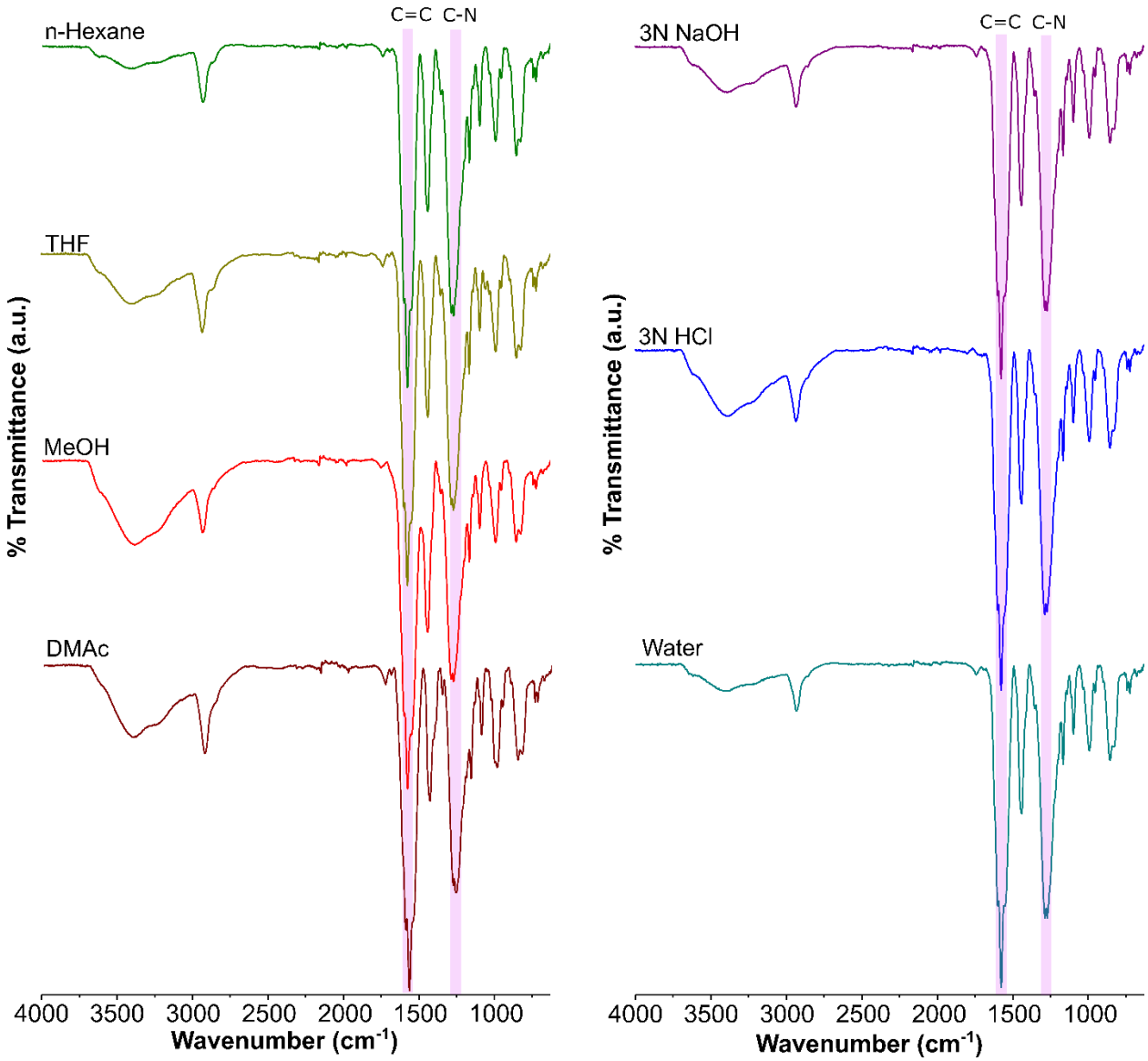

Figure S24. FTIR spectra of ND-COF-1 after treating with different solvents. Analysis of FTIR spectra of **ND-COF-1** after treatment with different solvents include acidic and basic media suggest high stability and intact nature of the framework.

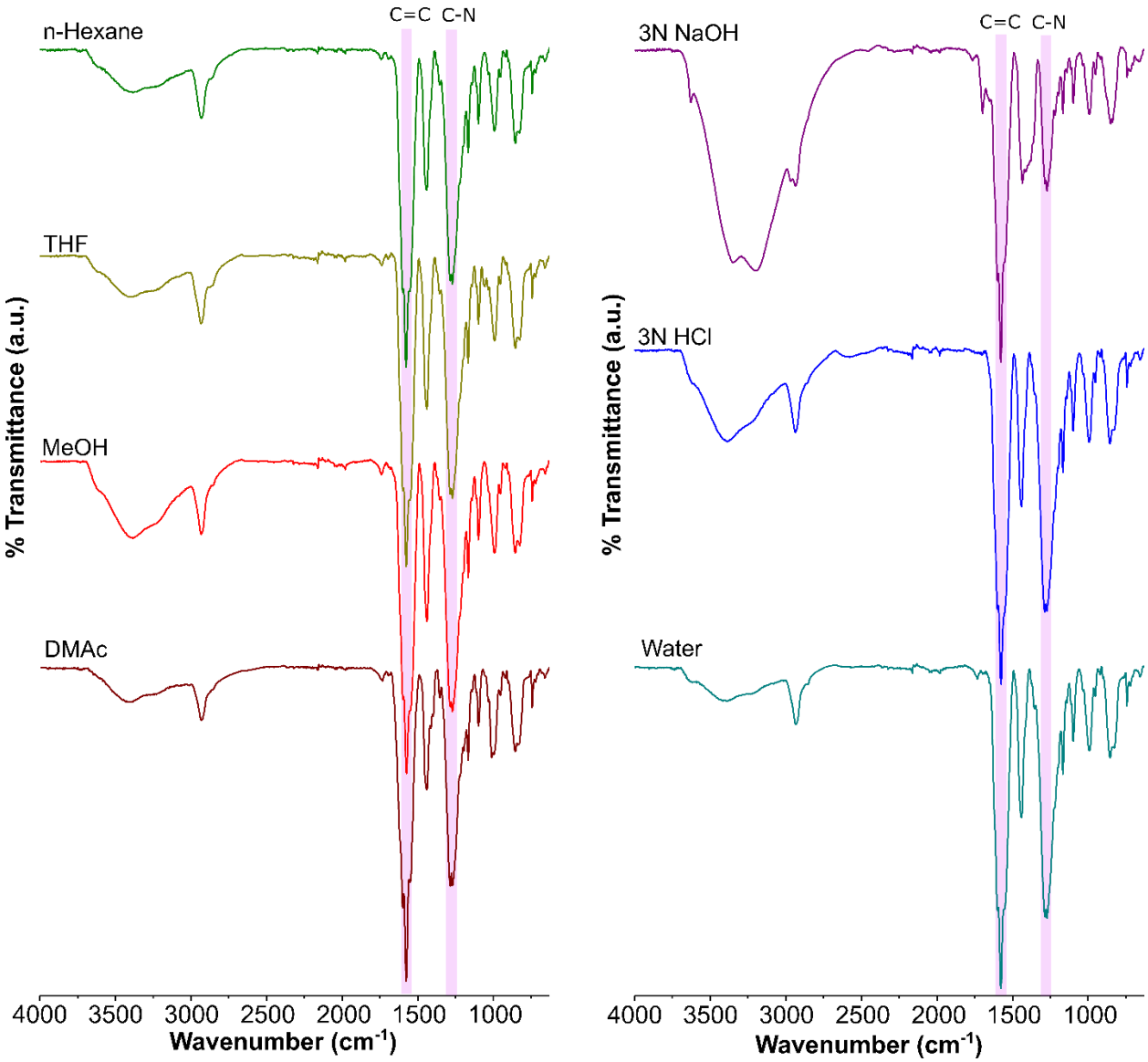

Figure S25. FTIR spectra of ND-COF-2 after treating with different solvents. Analysis of FTIR spectra of **ND-COF-2** after treatment with different solvents include acidic media suggest high stability and intact nature of the framework. However, as seen aforementioned in the PXRD pattern that the **ND-COF-2** is not stable in basic and the framework get disintegrate. In FTIR spectra there is a broadness in the NH stretch region when compared with the pristine COFs. This clearly suggest that the framework structure is disintegrated and the COF is not stable in basic media.

Section S9: References

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