Synthesis of Novel 2D In-Plane Anisotropic Covalent Organic Frameworks through a Solvent Modulated Orthogonal Strategy

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General methods and materials

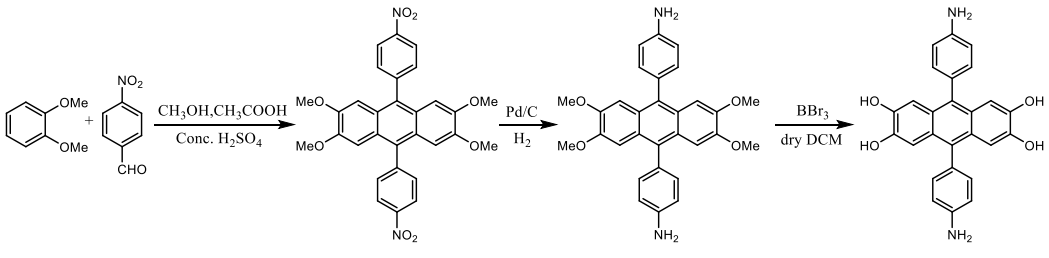
General methods

^{1}H NMR and ^{13}C NMR spectra were recorded at room temperature on a Bruker AV500 NMR spectrometer. Solid-state ^{13}C NMR spectra were recorded on a Bruker 400MHz Avance III SS-NMR spectrometer with a CPMAS probe. Chemical shifts are given in ppm relative to tetramethylsilane. High resolution mass spectra were recorded on an FT-MS instrument using the ESI technique. SEM measurements were carried out on Hitachi S-4800. Fourier transform infrared spectra were recorded as KBr-pellet on a Nicolet 380 FT-IR spectrometer. Powder X-ray diffraction(PXRD) data were collected at 35 kV, 15 mA on an Ultima IV XRD diffractometer using Cu-Kα radiation (λ = 1.5418 Å) at room temperature. Elemental analyses were carried out on an Elementar Vario EL III Elemental Analyzer. Thermogravimetric analysis (TGA) was carried out under nitrogen flow (100mL/min) on a SDT-Q600 thermoanalyzer with a heating rate of 10 ℃/min. N_2 adsorption–desorption analyses were carried out at 77 K using a Micromeritics ASAP 2460 Surface Area and Porosity Analyzer.

Materials

Deuterated solvents were purchased from Cambridge Isotope Laboratories. The other materials and solvents were commercially available and used without further purification.

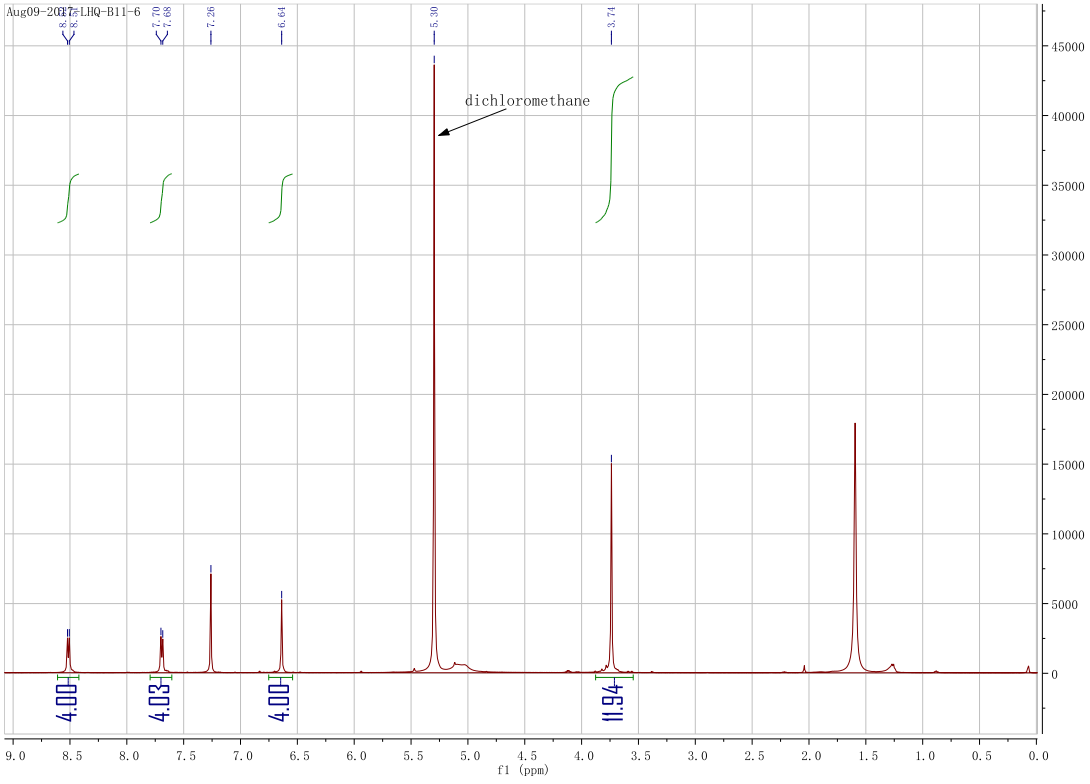
Scheme S1. Chemical synthesis of the **BAAT**.

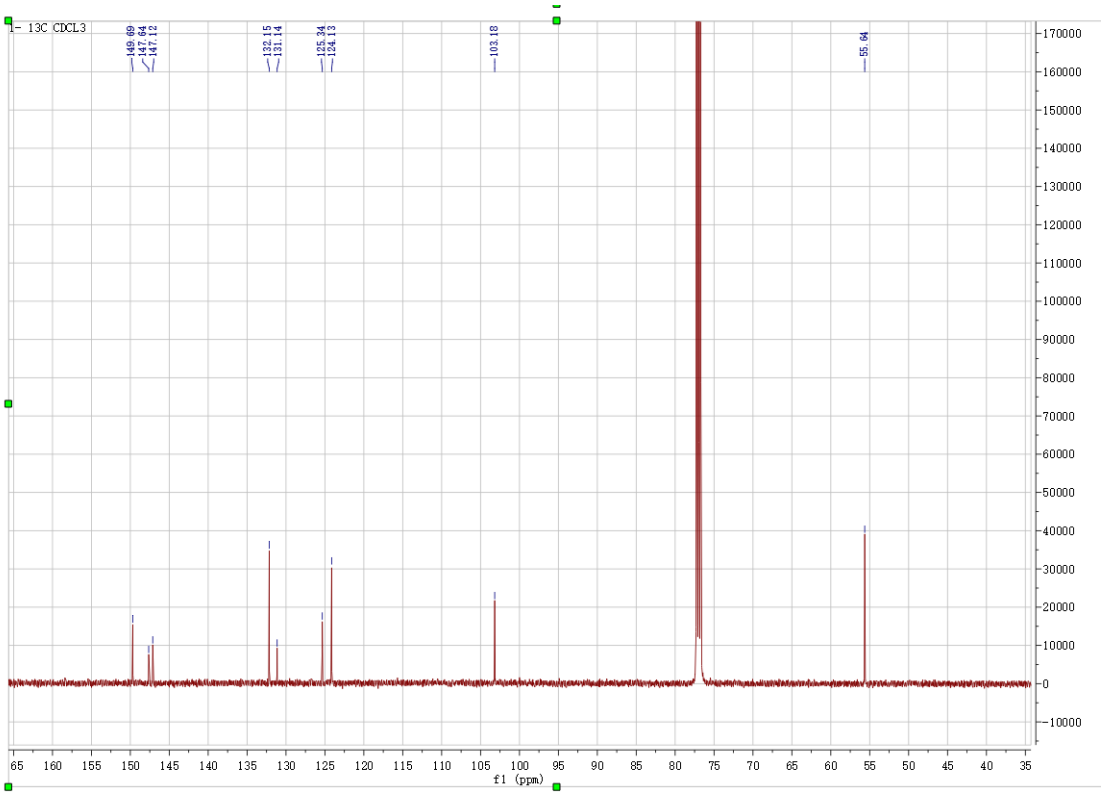


1 2 BAAT

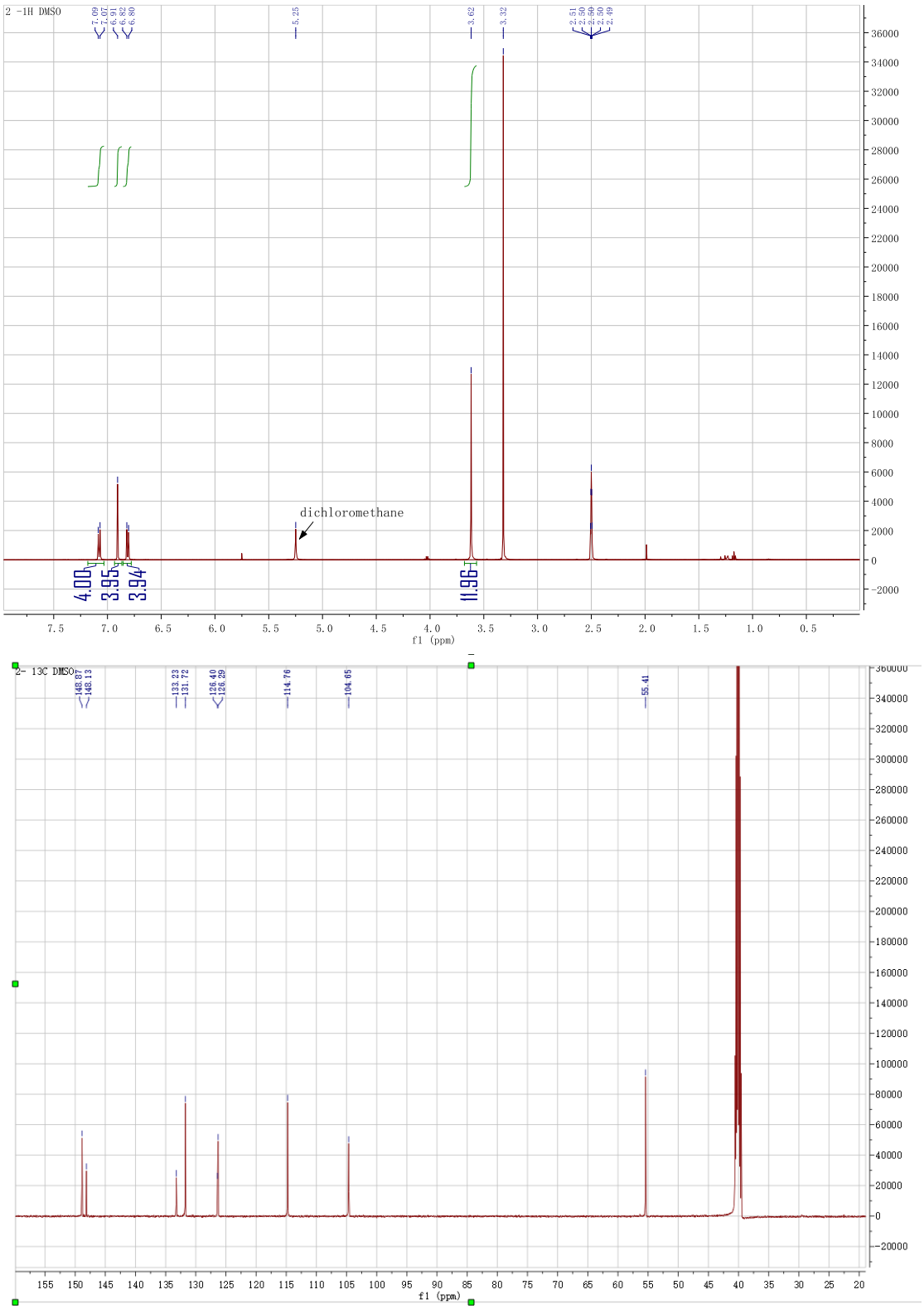
Compound 1: To a cooled solution (0 °C) of 4-Nitrobenzaldehyde (18.97 g,125.5 mmol) in acetic acid (31 mL) was slowly added solution of veratrole (8 mL, 62.7 mmol)

in methanol (6 mL). The resulting mixture was then stirred for 1h and concentrated H_2SO_4 (98 %, 40 mL) was added dropwise over 2 h. The reaction mixture was then stirred at 0 °C for 24 hours and then poured into water. The resultant precipitate was filtered and washed with water. Then recrystallised from ethyl acetate to give yellow crystals (4.6 g, 27.1% yield).^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.54 (d, *J*=8.7 Hz, 4H, -*Ar*H), 7.72 (d, *J*=8.7 Hz, 4H, -*Ar*H), 6.66 (s, 4H, -*Ar*H), 3.76 (s, 12H, -OMe). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 149.7, 147.6, 147.1, 132.2, 131.1, 125.3, 124.1, 103.2, 55.6. MS (MALDI-TOF) m/z: $[M+H]^+$ Calcd for $C_{30}H_{25}N_2O_8^+$ 541.15; Found 541.76. HR-MS (MALDI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{30}H_{24}N_2O_8Na^+$ 563.1425; Found 563.1416.



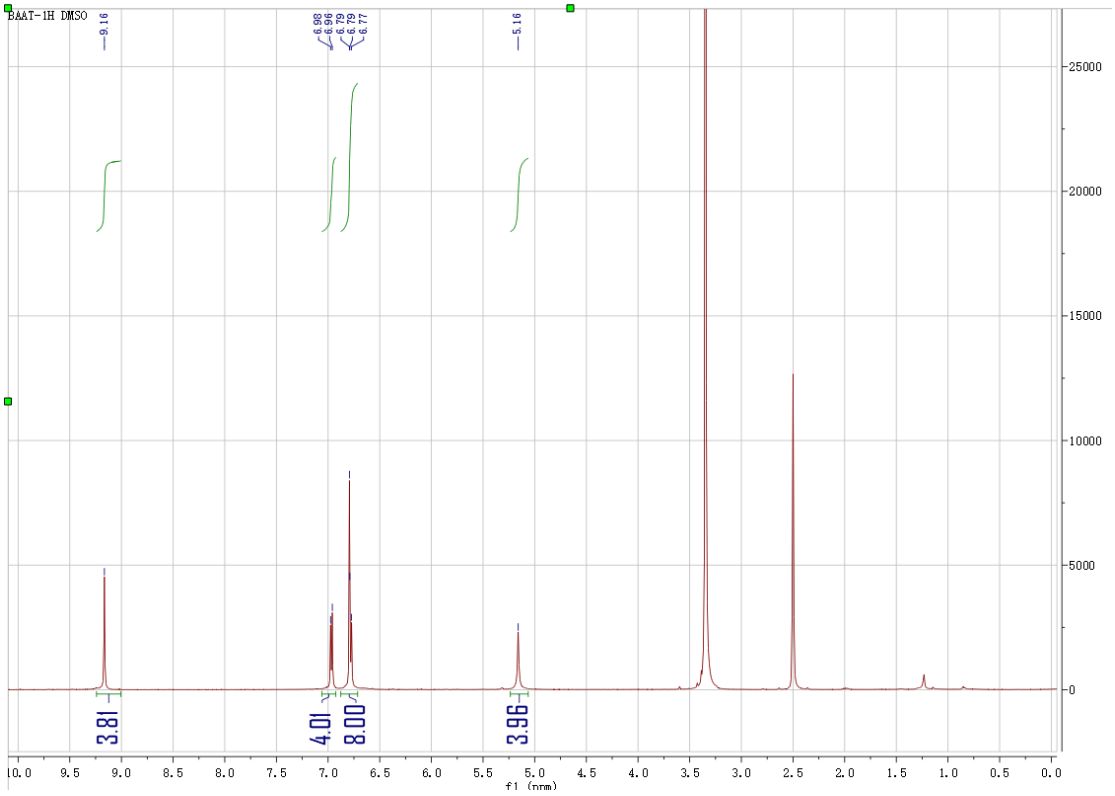


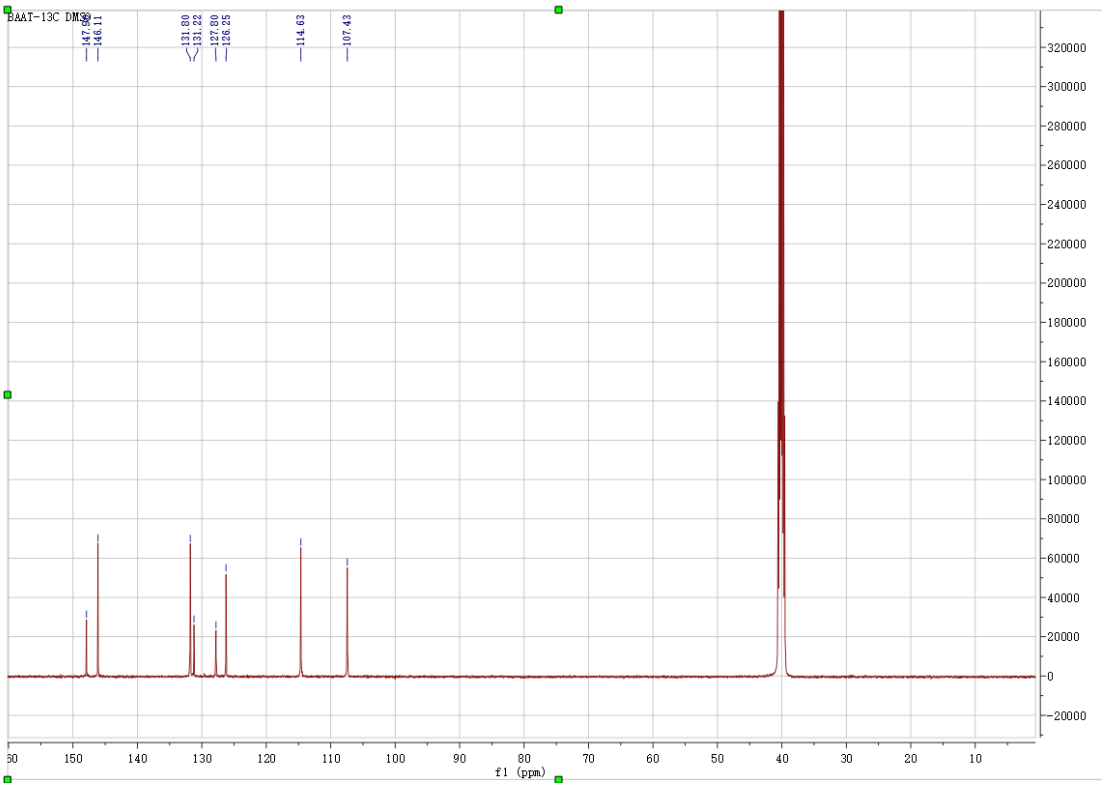
Compound 2: **1** (271 mg, 0.5 mmol) was dissolved in dry CH_2Cl_2 (20 mL) at room temperature. To the mixture was added 10% Pd/C (50 mg). The mixture was then degassed, backfilled with H_2 three times, and stirred under H_2 atmosphere at room temperature for 24 h. After the reaction was completed, the reaction mixture was filtered through Celite to afford a clear solution. The solution was then evaporated under reduced pressure to give **2** (221 mg, 92% yield). ^{1}H NMR (500 MHz, DMSO-d_6) δ = 7.08 (d, *J*=8.4 Hz, 4H, -*Ar*H), 6.91 (s, 4H, -*Ar*H), 6.82 (d, *J*=8.4 Hz, 4H, -*Ar*H), 5.26 (s, 4H, -NH_2), 3.62 (s, 12H, -OMe). ^{13}C NMR (126 MHz, DMSO-d_6) δ = 148.9, 148.1, 133.2, 131.7, 126.4, 126.3, 114.8, 104.7, 55.4. MS (MALDI-TOF) m/z: $[M+H]^+$ Calcd for $C_{30}H_{29}N_2O_4^+$ 481.21; Found 481.05. HR-MS (MALDI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{30}H_{28}N_2O_4Na^+$ 503.1942; Found 503.1933.



Compound BAAT: Borontribromide (1.14 mL, 12 mmol) was added dropwise to a stirred solution of **2** (961.2 mg, 2.0 mmol) in dry dichloromethane (60 mL) at -78 °C under a nitrogen atmosphere and then the reaction mixture was stirred at room temperature overnight. Methanol (10 mL) was added and the mixture stirred for 1 h.

Volatiles were removed in vacuo. The resultant was basified with sat.aq.$NaHCO_3$ until pH neutral. The precipitate was collected by filtration and washed with water to afford **BAAT** as a dark brown solid (798 mg, 95 %). ^{1}H NMR (500 MHz, DMSO-d_6) δ = 9.18 (s, 4H, -OH), 6.98 (d, *J*=8.1 Hz, 4H, -*Ar*H), 6.87 – 6.69 (m, 8H, -*Ar*H), 5.17 (s, 4H, -NH_2). ^{13}C NMR (126 MHz, DMSO-d_6) δ = 147.9, 146.1, 131.8, 131.2, 127.8, 126.3, 114.6, 107.4. MS (MALDI-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2O_4^+$ 425.15; Found 425.24. HR-MS (MALDI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{20}N_2O_4Na^+$ 447.1316; Found 447.1307.





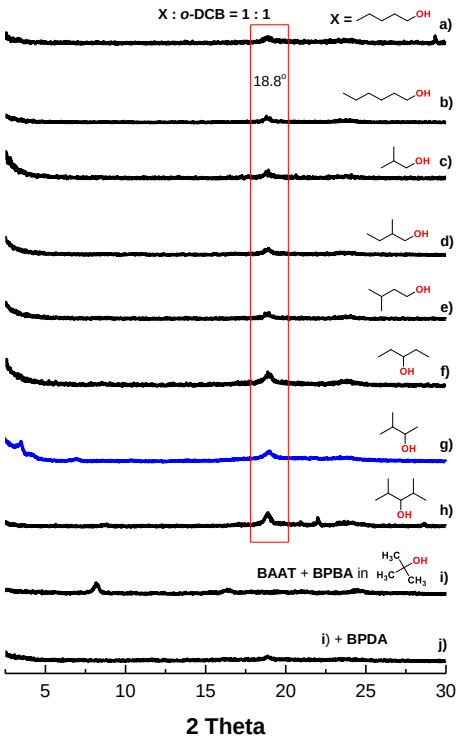


Figure S1. PXRD patterns of the products after reaction (**BAAT** + **BPBA** + **BPDA**) for 3 days at 120 ^{0}C under solvothermal conditions in different solvent pairs.

Scheme S2: Standard conditions for synthesis of **aniso-COFs**:

In a typical protocol, a 10 mL Pyrex tube was charged with **BAAT** (21.2 mg, 0.05 mmol), **PBA** (8.3 mg, 0.05 mmol) and **TPA** (6.7 mg, 0.05 mmol) in a 1/1 v/v solution (1 mL) of *t*-BuOH/*o*-DCB. The

tube was sonicated for 5 min and degassed by three freeze-pump-thaw cycles and sealed under vacuum. The tube was stand in an oven at 120 ℃ for 3 d to afford a black precipitate. The precipitate was collected by centrifuge, washed with solvents, and dried under vacuum in a Schlenk line under room temperature to afford **aniso-COF 1** (22.5 mg, 73%) as black powders.

The following **aniso-COFs** were prepared by similar methodology:

aniso-COF 2. Yield: 24.9 mg, 72 %.

aniso-COF 3. Yield: 26.3 mg, 76 %.

aniso-COF 4. Yield: 31.7 mg, 83 %.

aniso-COF 5. Yield: 28.0 mg, 78 %.

aniso-COF 6. Yield: 31.2 mg, 79 %.

aniso-COF 4. 79% in 2-BuOH/*o*-DCB, 77% in 2-Methyl-2-butanol/ *o*-DCB, 82% in 3-Methyl-3 -pentanol/ *o*-DCB.

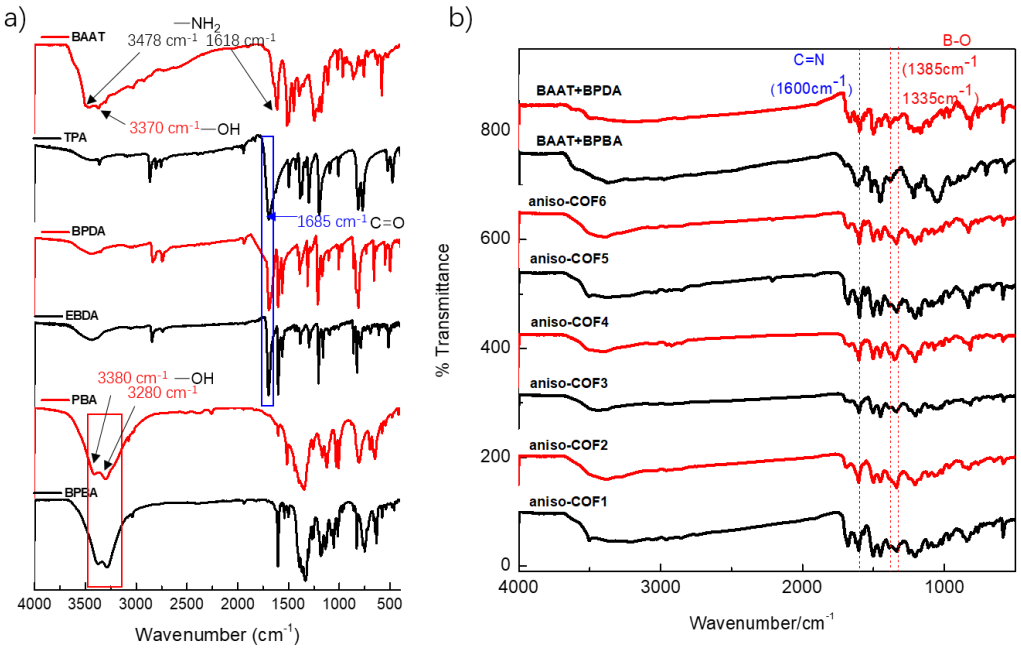


Figure S2: FT-IR spectra of **BAAT**, aldehyde, boronic acid and **aniso-COFs**.

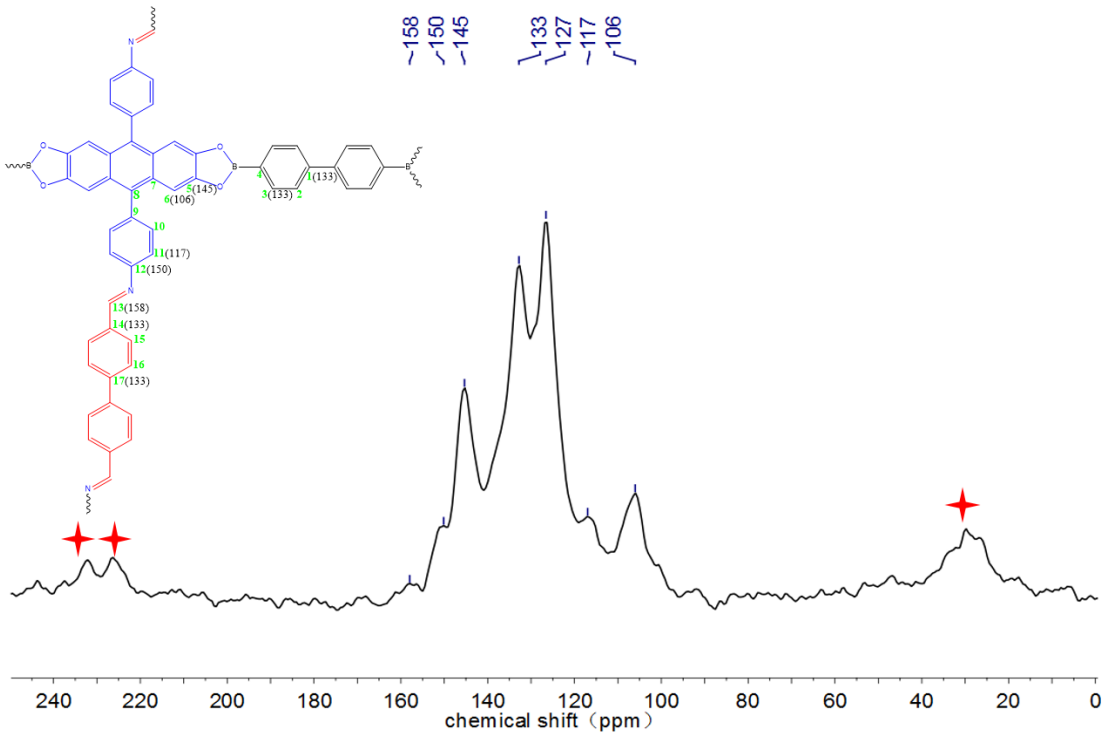


Figure S3: Solid-state ^{13}C CP/MAS NMR spectra and peak assignments for **aniso-COF 4**. ( ) denotes the rotation sidebands.

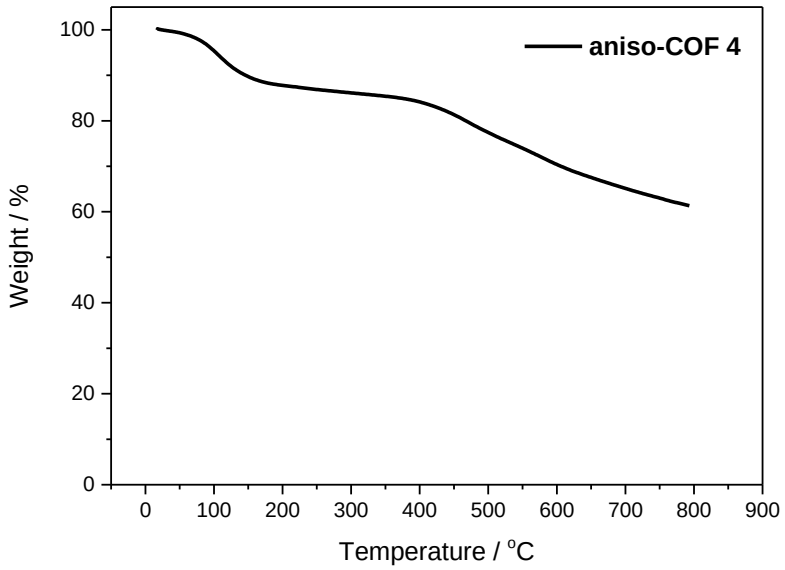


Figure S4: TGA of **aniso-COF 4**.

Table S1: Elemental analysis of **aniso-COFs**

Compound	Calculated:			Found:		
	C	H	N	C	H	N
aniso-COF 1	77.96	3.60	4.55	75.96	4.07	4.10
aniso-COF 2	79.80	3.79	4.05	75.83	4.63	4.68

aniso-COF 3	79.80	3.79	4.05	75.90	5.20	3.95
aniso-COF 4	81.28	3.94	3.65	80.10	4.63	4.29
aniso-COF 5	80.48	3.66	3.91	78.86	4.41	3.87
aniso-COF 6	81.85	3.82	3.54	77.12	4.93	3.62

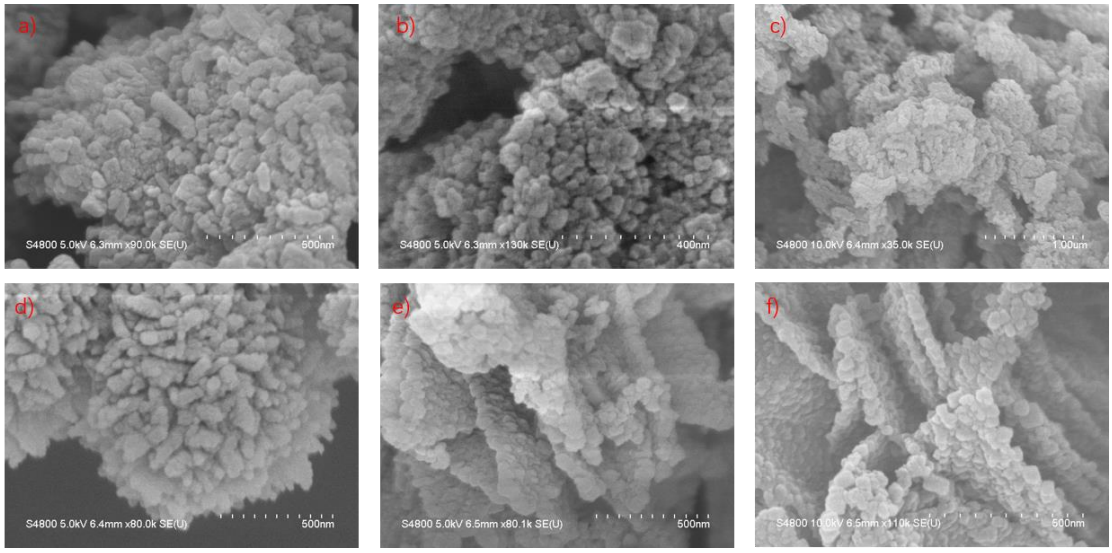


Figure S5: SEM images of a) **aniso-COF 1**, b) **aniso-COF 2**, c) **aniso-COF 3**, d) **aniso-COF 4**, e) **aniso-COF 5**, f) **aniso-COF 6**.

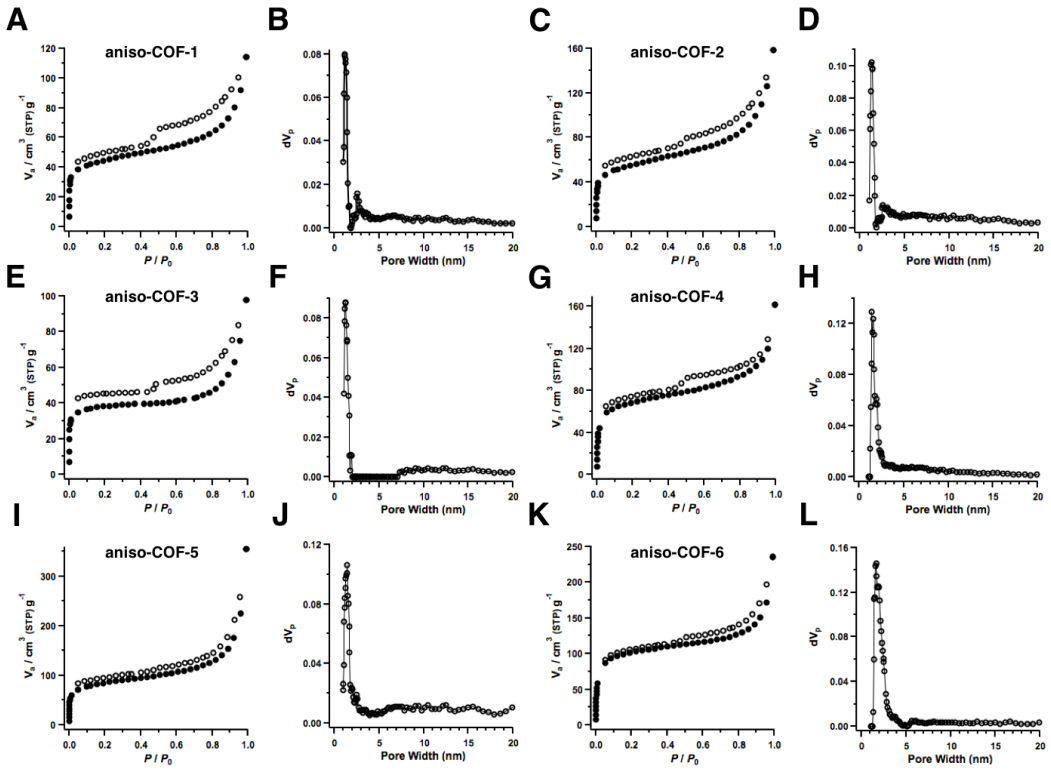


Figure S6: Gas adsorption. (**A**–**L**) Nitrogen sorption curves of (**A**) **aniso-COF 1**, (**C**) **aniso-COF 2** (**E**) **aniso-COF 3**, (**G**) **aniso-COF 4**, (**I**) **aniso-COF 5**, (**K**) **aniso-COF 6** (filled circles: adsorption, open circles: desorption) and pore size and pore size distribution profiles of (**B**) **aniso-COF 1**, (**D**) **aniso-COF 2** (**F**) **aniso-COF 3**, (**H**) **aniso-**

COF 4, (**J**) **aniso-COF 5**, (**L**) **aniso-COF 6**.

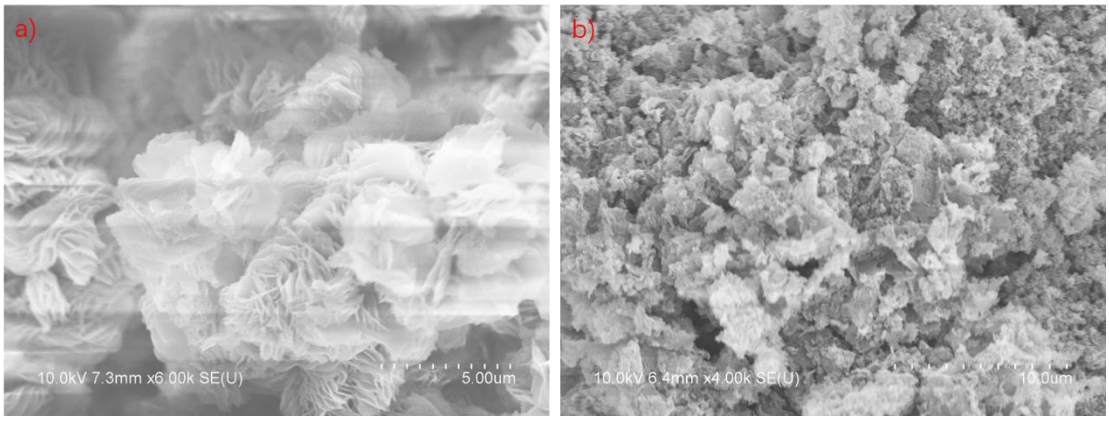
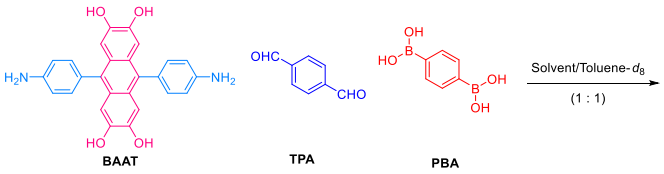
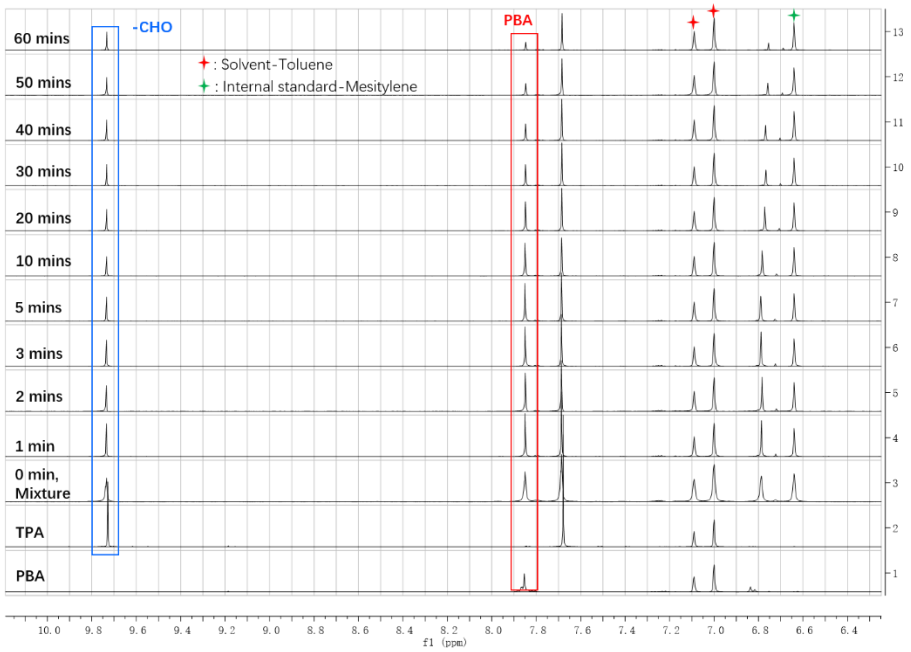


Figure S7: SEM images of stepwise reaction products a) **BAAT** + **BPDA**, b) **BAAT** + **BPBA**.

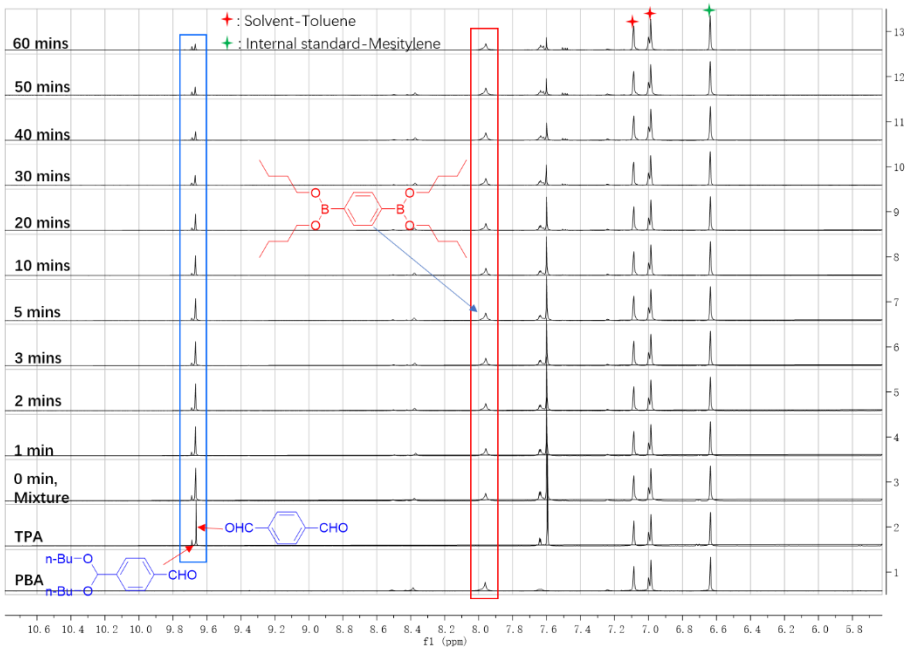
Scheme S3: Partial ^{1}H NMR spectra of orthogonal reactions (**BAAT** = **TPA** = **PBA** =7.5 mM) employing different solvent mixture. In a typical protocol, ten J-Young valve NMR tubes were added with a 1:1:1 mixture of **BAAT**-**TPA**-**PBA** and degassed, respectively. Then a 1:1 (v/v) mixture of hydrophilic solvent and toluene-d_8 was added. After sonicated for 5 min, one sample was monitored by ^{1}H NMR spectroscopy (as time = 0). Then the ten NMR tubes were dipped into a 120 ^{o}C oil bath for 1, 2, 3, 5, 10, 20, 30, 40, 50, 60 mins respectively, and monitored by ^{1}H NMR spectroscopy.

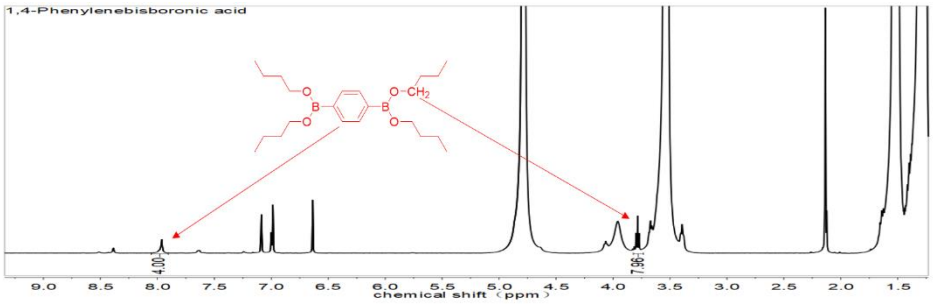


a): Solvent =1,4-dioxane/ Toluene-d_8

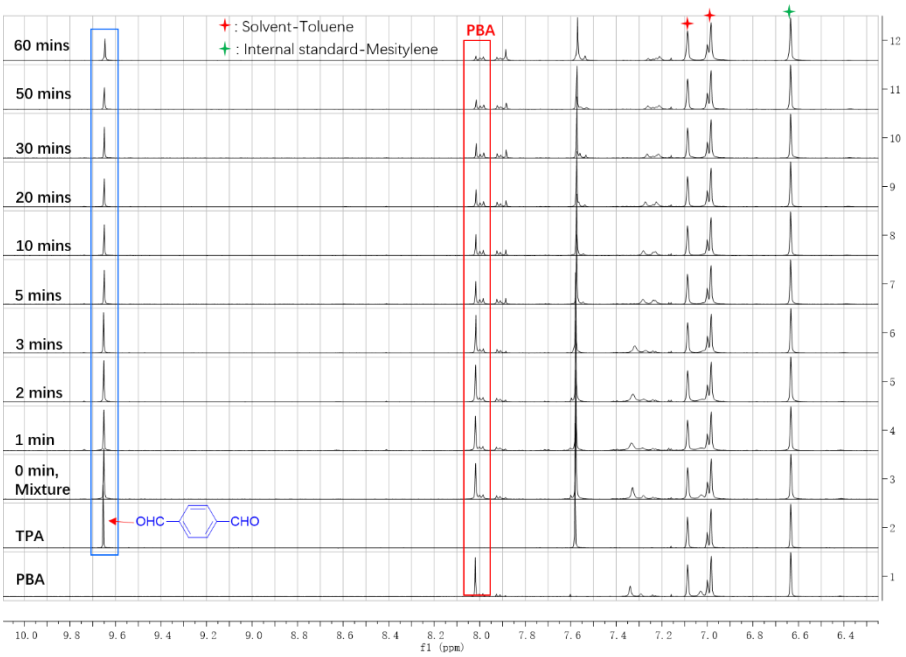


b): Solvent = *n*-BuOH/Toluene-d$_8$

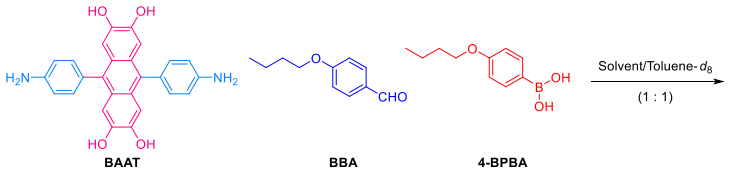




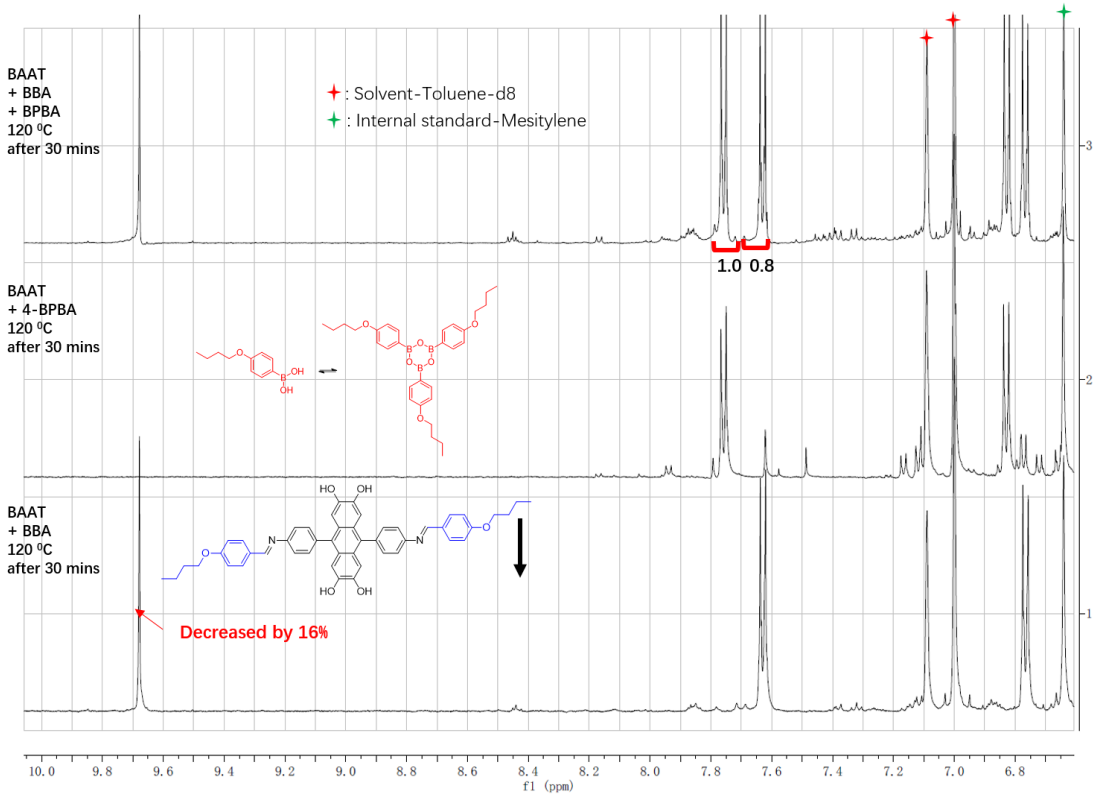
c): Solvent = *t*-BuOH/Toluene-d$_8$



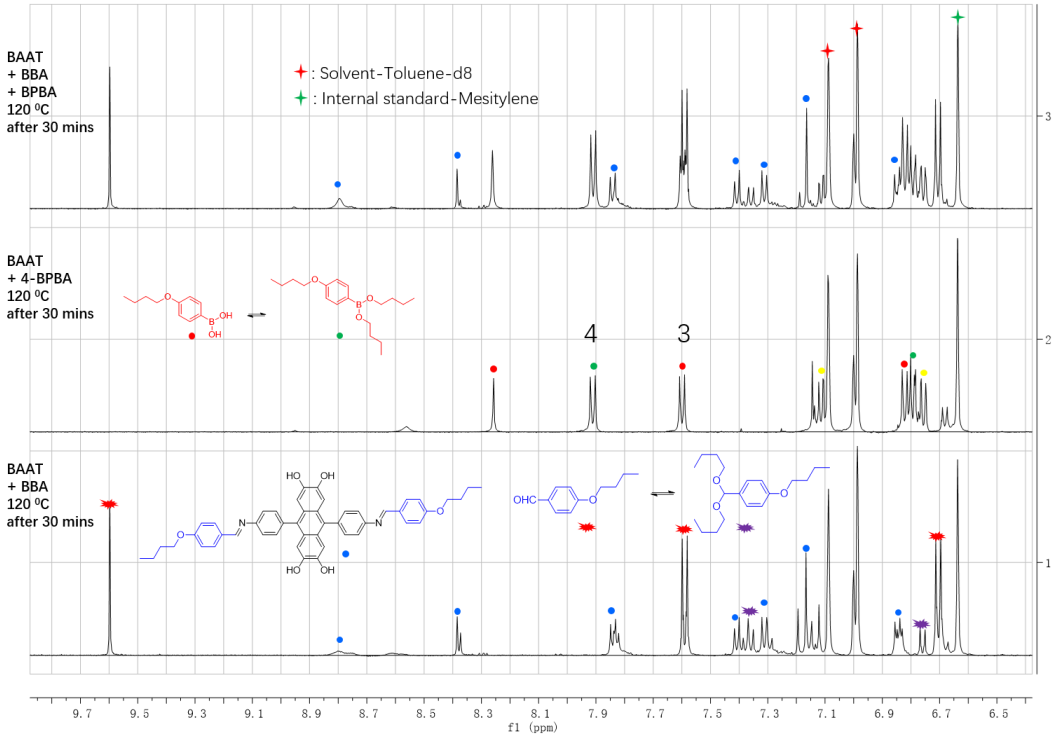
Scheme S4: Model reaction for the orthogonal reaction in different solvents (2**BAAT** = **BBA** = **4-BPBA** = 15 mM).



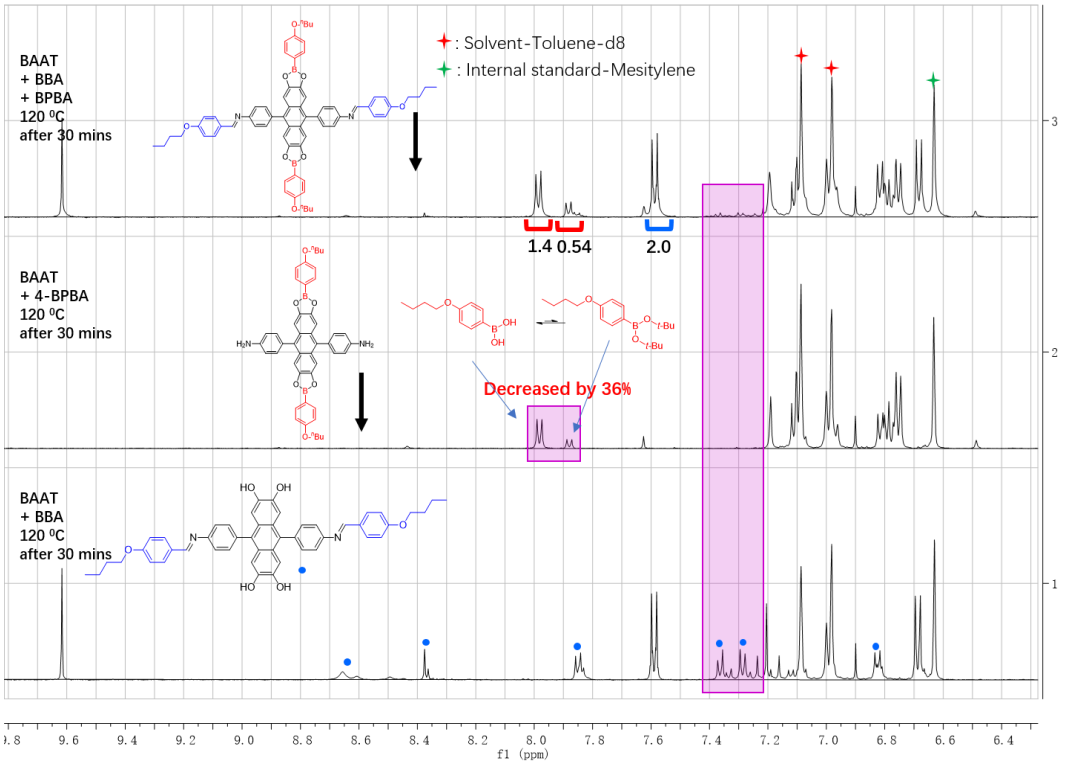
a): Solvent = 1,4-dioxane/Toluene-d_8



b): Solvent = *n*-BuOH/ Toluene-d$_8$



c): Solvent = *t*-BuOH/Toluene-d$_8$



Fractional atomic coordinates for the unit cell of **aniso-COFs** with AA stacking.

aniso-COF 1

Lattice parameters(A) Cell Angles

a = 22.000000 alpha = 75.000000

b = 18.000000 beta = 72.000000

c = 4.600000 gamma = 83.000000

Current cell volume = 1671.672263 A**3

Cell Contents

Total number of ions in cell = 70

Total number of species in cell = 5

Max number of any one species = 40

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	-0.180911	0.803550	-0.173020
H	2	-0.181579	0.666760	-0.171992
H	3	-0.005880	0.622678	0.082661
H	4	-0.005236	0.759428	0.081858
H	5	-0.202361	0.377310	-0.111403
H	6	0.012842	0.335703	0.046508
H	7	-0.198358	0.091503	-0.143939
H	8	0.016140	0.047871	0.020361
H	9	-0.214731	0.317735	-0.497092
H	10	-0.326906	0.323880	-0.496541
H	11	-0.368713	0.150727	0.376454
H	12	-0.257674	0.146722	0.375312
H	13	0.019454	0.104136	0.419368
H	14	0.127346	0.089396	0.473163
H	15	0.188537	0.266302	-0.376913
H	16	0.079348	0.278644	-0.431435
H	17	0.236846	0.122286	0.304691
H	18	0.328587	0.106297	0.378740
H	19	0.434794	0.101581	0.431804
H	20	0.483999	0.296513	-0.357470
H	21	0.375605	0.301942	-0.413639
H	22	0.542575	0.145137	0.271175
B	1	5.905946	-1.459809	-0.044114
B	2	5.907364	-2.114001	-0.046157
C	1	5.907011	-1.205715	-0.045826
C	2	5.857698	-1.235028	-0.115892
C	3	5.857289	-1.314224	-0.115172
C	4	5.906186	-1.368079	-0.044407

x	C	5	5.955500	-1.338756	0.025593	x
x	C	6	5.955893	-1.259578	0.025016	x
x	C	7	5.876971	-1.573049	-0.072443	x
x	C	8	5.935880	-1.584762	-0.024545	x
x	C	9	5.845516	-1.634886	-0.090707	x
x	C	10	5.875399	-1.711313	-0.069197	x
x	C	11	5.938852	-1.722560	-0.034677	x
x	C	12	5.967269	-1.658239	-0.001836	x
x	C	13	5.843010	-1.776235	-0.072225	x
x	C	14	5.875844	-1.850896	-0.061577	x
x	C	15	5.939000	-1.862418	-0.024345	x
x	C	16	5.971600	-1.797427	-0.021598	x
x	C	17	5.847139	-1.915053	-0.094190	x
x	C	18	5.877952	-1.988844	-0.068065	x
x	C	19	5.936482	-2.001016	-0.016283	x
x	C	20	5.968150	-1.939389	0.002052	x
x	C	21	6.039967	-1.807147	-0.004595	x
x	C	22	5.773225	-1.768607	-0.064023	x
x	C	23	5.751949	-1.718639	-0.306325	x
x	C	24	5.687658	-1.715026	-0.304594	x
x	C	25	5.642939	-1.763217	-0.066319	x
x	C	26	5.663750	-1.812471	0.181478	x
x	C	27	5.727821	-1.814651	0.182473	x
x	C	28	6.055636	-1.859966	0.246856	x
x	C	29	6.117830	-1.868661	0.274166	x
x	C	30	6.166741	-1.822787	0.054478	x
x	C	31	6.151956	-1.769519	-0.201072	x
x	C	32	6.089403	-1.762383	-0.231698	x
x	C	33	6.231390	-1.832782	0.106236	x
x	C	34	6.342449	-1.794766	-0.024147	x
x	C	35	6.360887	-1.851261	0.214053	x
x	C	36	6.422622	-1.854336	0.245482	x
x	C	37	6.468106	-1.801425	0.042642	x
x	C	38	6.450143	-1.744965	-0.195438	x
x	C	39	6.388091	-1.741840	-0.227584	x
x	C	40	6.533223	-1.807845	0.087531	x
x	N	1	6.279020	-1.789147	-0.067305	x
x	N	2	6.578165	-1.760692	-0.088437	x
x	O	1	5.853425	-1.496152	-0.088889	x
x	O	2	5.958616	-1.517423	-0.000796	x
x	O	3	5.959736	-2.078030	0.001406	x
x	O	4	5.855086	-2.056023	-0.092596	x

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

aniso-COF 2

Lattice parameters(A) Cell Angles

a = 22.000000 alpha = 75.000000

b = 22.000000 beta = 72.000000

c = 4.250000 gamma = 83.000000

Current cell volume = 1887.697543 A**3

Cell Contents

Total number of ions in cell = 80

Total number of species in cell = 5

Max number of any one species = 46

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.385548	1.017754	-0.188919
H	2	0.386384	0.907131	-0.193571
H	3	0.551755	0.869263	0.185218
H	4	0.552809	0.980675	0.166402
H	5	0.360674	0.477004	-0.057136
H	6	0.579017	0.442807	0.066112
H	7	0.365202	0.246480	-0.130024
H	8	0.578711	0.207923	0.052582
H	9	0.343249	0.436394	-0.450520
H	10	0.231550	0.442071	-0.444979
H	11	0.194857	0.285595	0.431929
H	12	0.306062	0.282570	0.432792
H	13	0.590720	0.250533	0.442164
H	14	0.699631	0.236909	0.471099
H	15	0.753011	0.391404	-0.407472
H	16	0.642382	0.401400	-0.446460
H	17	0.807153	0.266378	0.289933
H	18	0.905174	0.239416	0.262070
H	19	1.009594	0.234303	0.346769
H	20	1.042618	0.422734	-0.274919
H	21	0.935531	0.429040	-0.354041
H	22	1.111821	0.277706	0.255780
H	23	0.367342	0.805954	0.075400
H	24	0.369015	0.695858	0.059485
H	25	0.571992	0.679019	-0.073075

x	H	26	0.571942	0.790217	-0.082597	x
x	B	1	7.471086	-1.393700	-0.011130	x
x	B	2	7.469393	-1.919310	-0.015059	x
x	C	1	7.469260	-0.991820	-0.012601	x
x	C	2	7.422138	-1.014353	-0.107547	x
x	C	3	7.422309	-1.078428	-0.105912	x
x	C	4	7.469106	-1.122376	-0.003751	x
x	C	5	7.515820	-1.099220	0.095013	x
x	C	6	7.516229	-1.034962	0.087271	x
x	C	7	7.441793	-1.484006	-0.040581	x
x	C	8	7.501956	-1.493203	-0.005523	x
x	C	9	7.409547	-1.533539	-0.054193	x
x	C	10	7.439253	-1.595377	-0.037052	x
x	C	11	7.503770	-1.604572	-0.011690	x
x	C	12	7.533197	-1.552538	0.017161	x
x	C	13	7.405612	-1.647671	-0.033420	x
x	C	14	7.438711	-1.707893	-0.027934	x
x	C	15	7.502332	-1.717665	0.008533	x
x	C	16	7.536514	-1.665181	0.000246	x
x	C	17	7.409952	-1.759209	-0.068663	x
x	C	18	7.440098	-1.819041	-0.037037	x
x	C	19	7.498113	-1.829563	0.024524	x
x	C	20	7.530420	-1.780413	0.041777	x
x	C	21	7.606278	-1.672938	0.002158	x
x	C	22	7.334979	-1.641481	-0.015870	x
x	C	23	7.311664	-1.596592	-0.257624	x
x	C	24	7.247326	-1.593083	-0.252083	x
x	C	25	7.204372	-1.636516	-0.014109	x
x	C	26	7.226562	-1.681182	0.235236	x
x	C	27	7.290667	-1.682860	0.236651	x
x	C	28	7.625040	-1.718513	0.256331	x
x	C	29	7.688165	-1.726534	0.269129	x
x	C	30	7.735275	-1.686625	0.036370	x
x	C	31	7.717780	-1.639958	-0.221254	x
x	C	32	7.654259	-1.634018	-0.241708	x
x	C	33	7.800579	-1.695504	0.082724	x
x	C	34	7.910394	-1.664117	-0.046832	x
x	C	35	7.933199	-1.719294	0.147490	x
x	C	36	7.993967	-1.722722	0.194232	x
x	C	37	8.034370	-1.671861	0.046081	x
x	C	38	8.012516	-1.617188	-0.153971	x
x	C	39	7.951311	-1.613579	-0.199892	x
x	C	40	8.098805	-1.678197	0.102090	x
x	C	41	7.469543	-1.191386	-0.003118	x

x	C	42	7.412854	-1.220248	0.035807	x
x	C	43	7.413539	-1.283997	0.030266	x
x	C	44	7.470576	-1.321456	-0.006924	x
x	C	45	7.527086	-1.293528	-0.041723	x
x	C	46	7.526755	-1.229444	-0.043490	x
x	N	1	7.847062	-1.657888	-0.094766	x
x	N	2	8.139938	-1.634030	-0.040658	x
x	O	1	7.417113	-1.422551	-0.043219	x
x	O	2	7.525542	-1.438743	0.014290	x
x	O	3	7.417306	-1.872880	-0.069086	x
x	O	4	7.521395	-1.891752	0.043124	x

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aniso-COF 3

Lattice parameters(A) Cell Angles

a = 26.500000 alpha = 75.000000

b = 18.000000 beta = 72.000000

c = 4.650000 gamma = 83.000000

Current cell volume = 2035.492239 A**3

Cell Contents

Total number of ions in cell = 80

Total number of species in cell = 5

Max number of any one species = 46

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x	Element	Atom Number	Fractional coordinates of atoms u	v	w	x
x	H	1	0.754559	0.599101	0.914459	x
x	H	2	0.754133	0.463320	0.900727	x
x	H	3	0.910124	0.423510	1.026875	x
x	H	4	0.910083	0.558897	1.047304	x
x	H	5	0.736326	0.168332	1.006872	x
x	H	6	0.929782	0.146588	0.861079	x
x	H	7	0.744488	-0.111637	0.898156	x
x	H	8	0.918103	-0.157298	1.121205	x
x	H	9	0.728048	0.115769	0.577057	x
x	H	10	0.634622	0.121981	0.581616	x
x	H	11	0.601097	-0.055886	1.429075	x

x	H	12	0.694189	-0.060715	1.424589	x
x	H	13	0.971144	-0.083909	0.669162	x
x	H	14	1.064507	-0.094636	0.646625	x
x	H	15	1.035216	0.062785	1.242436	x
x	H	16	0.939717	0.062770	1.311480	x
x	H	17	1.140776	-0.060772	0.768160	x
x	H	18	1.219167	-0.092023	0.849632	x
x	H	19	1.311176	-0.095679	0.854357	x
x	H	20	1.278467	0.107697	1.219481	x
x	H	21	1.185621	0.111506	1.215296	x
x	H	22	1.361083	-0.121386	1.248458	x
x	H	23	1.451763	-0.129832	1.285830	x
x	H	24	1.464523	0.114163	0.893715	x
x	H	25	1.372860	0.122974	0.861189	x
x	H	26	1.533200	-0.071860	1.252398	x
x	B	1	4.832183	-2.660421	-0.049196	x
x	B	2	4.832318	-3.317054	-0.007344	x
x	C	1	4.832349	-2.408236	-0.017493	x
x	C	2	4.788865	-2.438344	-0.059320	x
x	C	3	4.788591	-2.516993	-0.067148	x
x	C	4	4.832101	-2.569331	-0.037827	x
x	C	5	4.875726	-2.539112	0.002030	x
x	C	6	4.875702	-2.460717	0.014091	x
x	C	7	4.805918	-2.776281	-0.035411	x
x	C	8	4.859082	-2.783062	-0.069946	x
x	C	9	4.778371	-2.840445	-0.019003	x
x	C	10	4.805060	-2.915174	-0.024676	x
x	C	11	4.860571	-2.923414	-0.039585	x
x	C	12	4.887320	-2.854186	-0.086004	x
x	C	13	4.777713	-2.980647	-0.017419	x
x	C	14	4.806065	-3.054183	-0.020383	x
x	C	15	4.859035	-3.065173	0.010362	x
x	C	16	4.887700	-2.999185	-0.008925	x
x	C	17	4.782390	-3.118184	-0.054128	x
x	C	18	4.808253	-3.191709	-0.031423	x
x	C	19	4.856036	-3.204411	0.030386	x
x	C	20	4.881504	-3.143097	0.059216	x
x	C	21	4.946322	-3.008429	-0.011498	x
x	C	22	4.719199	-2.973539	-0.003361	x
x	C	23	4.700766	-2.921977	-0.237159	x
x	C	24	4.647176	-2.918321	-0.233322	x
x	C	25	4.610329	-2.967676	-0.000586	x
x	C	26	4.628242	-3.018563	0.238689	x
x	C	27	4.681752	-3.020974	0.237718	x

x	C	28	4.983548	-3.053556	-0.193366	x
x	C	29	5.037820	-3.058790	-0.211344	x
x	C	30	5.057954	-3.016448	-0.059547	x
x	C	31	5.021530	-2.970545	0.120102	x
x	C	32	4.966506	-2.969771	0.155879	x
x	C	33	5.116482	-3.022994	-0.091016	x
x	C	34	5.194431	-2.988788	0.028429	x
x	C	35	5.231147	-3.047245	-0.072364	x
x	C	36	5.284307	-3.049833	-0.067418	x
x	C	37	5.302788	-2.994046	0.035553	x
x	C	38	5.266195	-2.935517	0.133650	x
x	C	39	5.212882	-2.933487	0.132598	x
x	C	40	5.359270	-2.998591	0.050848	x
x	C	41	5.383166	-3.069473	0.167807	x
x	C	42	5.435238	-3.074242	0.190546	x
x	C	43	5.465847	-3.008704	0.091686	x
x	C	44	5.442391	-2.937647	-0.028709	x
x	C	45	5.389683	-2.932593	-0.046040	x
x	C	46	5.521236	-3.017084	0.122717	x
x	N	1	5.138539	-2.984859	0.039727	x
x	N	2	5.555753	-2.963357	-0.013562	x
x	O	1	4.784769	-2.701002	-0.023123	x
x	O	2	4.879865	-2.713654	-0.081501	x
x	O	3	4.874966	-3.281760	0.051553	x
x	O	4	4.789475	-3.258632	-0.059032	x

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aniso-COF 4

Lattice parameters(A)		Cell Angles	
a =	26.500000	alpha =	75.000000
b =	22.000000	beta =	72.000000
c =	4.200000	gamma =	83.000000

Current cell volume = 2247.066701 A**3

Cell Contents

Total number of ions in cell = 90

Total number of species in cell = 5

Max number of any one species = 52

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x	Element	Atom Number	Fractional coordinates of atoms u	v	w	x
x	H	1	6.079095	-1.914065	0.661638	x
x	H	2	6.079918	-2.023250	0.628100	x
x	H	3	6.225195	-2.062883	0.920864	x
x	H	4	6.224861	-1.952728	0.943762	x
x	H	5	6.054572	-2.458857	0.816233	x
x	H	6	6.250134	-2.475357	0.543937	x
x	H	7	6.064222	-2.687053	0.677431	x
x	H	8	6.233590	-2.722838	0.979905	x
x	H	9	6.039381	-2.495307	0.390344	x
x	H	10	5.945906	-2.491596	0.411859	x
x	H	11	5.921064	-2.652803	1.273252	x
x	H	12	6.014254	-2.654714	1.255325	x
x	H	13	6.288663	-2.672567	0.467120	x
x	H	14	6.381072	-2.684206	0.463161	x
x	H	15	6.356509	-2.534358	0.988023	x
x	H	16	6.457699	-2.654768	0.589194	x
x	H	17	6.530646	-2.682558	0.757084	x
x	H	18	6.621647	-2.688111	0.782333	x
x	H	19	6.601964	-2.497988	0.916957	x
x	H	20	6.510322	-2.492350	0.888474	x
x	H	21	6.067047	-2.127487	0.922046	x
x	H	22	6.067475	-2.235918	0.874562	x
x	H	23	6.238531	-2.244056	0.542682	x
x	H	24	6.238497	-2.134755	0.577382	x
x	H	25	6.673120	-2.694909	1.163728	x
x	H	26	6.762936	-2.702298	1.216743	x
x	H	27	6.785449	-2.509465	0.646859	x
x	H	28	6.695002	-2.501727	0.593804	x
x	H	29	6.848237	-2.658318	1.123365	x
x	H	30	6.261413	-2.531973	1.059638	x
x	B	1	6.153014	-2.320407	0.680646	x
x	B	2	6.151026	-2.852217	0.820540	x
x	C	1	6.151942	-1.924348	0.804952	x
x	C	2	6.111194	-1.946116	0.719754	x
x	C	3	6.111459	-2.009306	0.703689	x
x	C	4	6.152470	-2.053197	0.773389	x
x	C	5	6.193278	-2.031031	0.859290	x
x	C	6	6.193017	-1.967653	0.874523	x
x	C	7	6.125605	-2.414032	0.721966	x
x	C	8	6.179553	-2.418455	0.645335	x
x	C	9	6.096996	-2.466280	0.764829	x

x	C	10	6.123322	-2.526871	0.756367	x
x	C	11	6.179656	-2.532910	0.718547	x
x	C	12	6.207431	-2.476152	0.627757	x
x	C	13	6.095049	-2.580542	0.783183	x
x	C	14	6.123921	-2.639861	0.781948	x
x	C	15	6.176754	-2.648302	0.819171	x
x	C	16	6.206460	-2.594309	0.772984	x
x	C	17	6.101053	-2.691978	0.742952	x
x	C	18	6.126717	-2.751430	0.781462	x
x	C	19	6.173224	-2.761575	0.866885	x
x	C	20	6.198171	-2.711560	0.897180	x
x	C	21	6.265355	-2.601440	0.767455	x
x	C	22	6.035673	-2.575919	0.813472	x
x	C	23	6.014293	-2.530009	0.582292	x
x	C	24	5.960403	-2.527651	0.597023	x
x	C	25	5.925824	-2.572570	0.836695	x
x	C	26	5.946299	-2.618270	1.075694	x
x	C	27	6.000133	-2.619275	1.066294	x
x	C	28	6.301442	-2.644341	0.601536	x
x	C	29	6.355436	-2.649821	0.589052	x
x	C	30	6.376786	-2.609883	0.721677	x
x	C	31	6.341933	-2.565463	0.877532	x
x	C	32	6.286989	-2.563710	0.915201	x
x	C	33	6.434695	-2.617465	0.701846	x
x	C	34	6.512976	-2.586098	0.813274	x
x	C	35	6.545571	-2.641344	0.785928	x
x	C	36	6.598073	-2.644830	0.804509	x
x	C	37	6.620046	-2.593301	0.848271	x
x	C	38	6.587306	-2.538250	0.875449	x
x	C	39	6.534603	-2.535031	0.860918	x
x	C	40	6.676076	-2.597646	0.874989	x
x	C	41	6.152756	-2.121106	0.752902	x
x	C	42	6.104941	-2.151667	0.834031	x
x	C	43	6.105100	-2.214352	0.809073	x
x	C	44	6.153014	-2.248898	0.704392	x
x	C	45	6.200824	-2.218992	0.625057	x
x	C	46	6.200730	-2.156156	0.648159	x
x	C	47	6.697054	-2.654011	1.046954	x
x	C	48	6.748690	-2.658202	1.079131	x
x	C	49	6.781689	-2.606587	0.936715	x
x	C	50	6.761241	-2.550185	0.761486	x
x	C	51	6.709133	-2.545721	0.732614	x
x	C	52	6.836738	-2.613735	0.975407	x
x	N	1	6.457764	-2.580920	0.810804	x

x	N	2	6.871203	-2.569786	0.825391	x
x	O	1	6.104420	-2.353712	0.749284	x
x	O	2	6.201334	-2.361506	0.608490	x
x	O	3	6.108907	-2.805680	0.746442	x
x	O	4	6.192204	-2.824348	0.900751	x

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aniso-COF 5

Lattice parameters(A) Cell Angles

a =	29.300000	alpha =	75.000000
b =	18.000000	beta =	72.000000
c =	4.650000	gamma =	83.000000

Current cell volume = 2250.563117 A**3

Cell Contents

Total number of ions in cell = 82

Total number of species in cell = 5

Max number of any one species = 48

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x	Element	Atom Number	Fractional coordinates of atoms u	v	w	x
x	H	1	4.254976	-3.690059	-0.038500	x
x	H	2	4.254931	-3.825333	-0.060364	x
x	H	3	4.393182	-3.868210	0.108328	x
x	H	4	4.393658	-3.732586	0.123869	x
x	H	5	4.247744	-4.109868	-0.133024	x
x	H	6	4.402693	-4.156400	0.118148	x
x	H	7	4.236743	-4.413158	0.124427	x
x	H	8	4.410488	-4.437578	0.019717	x
x	H	9	4.195528	-4.182519	0.289371	x
x	H	10	4.112063	-4.177111	0.284243	x
x	H	11	4.150064	-4.336112	-0.312053	x
x	H	12	4.234013	-4.330826	-0.350504	x
x	H	13	4.414029	-4.385540	0.450670	x
x	H	14	4.496243	-4.395651	0.485340	x
x	H	15	4.536134	-4.216933	-0.354731	x
x	H	16	4.453063	-4.207990	-0.387886	x
x	H	17	4.578923	-4.357516	0.304879	x
x	H	18	4.651420	-4.367965	0.353313	x

x	H	19	4.734475	-4.367682	0.360508	x
x	H	20	4.762275	-4.180596	-0.453887	x
x	H	21	4.678659	-4.180310	-0.463762	x
x	H	22	4.918696	-4.371229	-0.295350	x
x	H	23	5.003952	-4.377994	-0.323209	x
x	H	24	4.978548	-4.194723	0.155922	x
x	H	25	4.892574	-4.188023	0.182344	x
x	H	26	5.072881	-4.335831	-0.234251	x
x	B	1	4.324051	-3.950673	0.011035	x
x	B	2	4.324321	-4.607552	0.056915	x
x	C	1	4.324355	-3.698578	0.044456	x
x	C	2	4.285535	-3.728012	-0.005951	x
x	C	3	4.285505	-3.806345	-0.018832	x
x	C	4	4.324020	-3.859539	0.022207	x
x	C	5	4.362707	-3.830201	0.074471	x
x	C	6	4.363013	-3.751638	0.083352	x
x	C	7	4.303042	-4.063117	-0.032053	x
x	C	8	4.345706	-4.076110	0.037174	x
x	C	9	4.280400	-4.124265	-0.065881	x
x	C	10	4.300634	-4.202214	-0.015918	x
x	C	11	4.348096	-4.213559	0.024625	x
x	C	12	4.368968	-4.149709	0.063293	x
x	C	13	4.275095	-4.267886	-0.004936	x
x	C	14	4.299296	-4.343924	0.035405	x
x	C	15	4.349025	-4.352791	0.033529	x
x	C	16	4.373742	-4.287354	0.028269	x
x	C	17	4.275041	-4.412953	0.079633	x
x	C	18	4.300269	-4.484522	0.071548	x
x	C	19	4.347949	-4.492073	0.049283	x
x	C	20	4.372718	-4.428184	0.037781	x
x	C	21	4.426130	-4.295603	0.033138	x
x	C	22	4.222985	-4.258676	-0.025376	x
x	C	23	4.186868	-4.214072	0.145724	x
x	C	24	4.138332	-4.212010	0.148567	x
x	C	25	4.123152	-4.256571	-0.009448	x
x	C	26	4.158921	-4.301111	-0.181847	x
x	C	27	4.207883	-4.298552	-0.202644	x
x	C	28	4.440119	-4.348242	0.275221	x
x	C	29	4.487583	-4.354186	0.292518	x
x	C	30	4.523247	-4.306677	0.070020	x
x	C	31	4.509842	-4.254121	-0.176642	x
x	C	32	4.462098	-4.249000	-0.195414	x
x	C	33	4.573131	-4.314233	0.108197	x
x	C	34	4.657548	-4.273670	-0.058149	x

x	C	35	4.674607	-4.326442	0.174307	x
x	C	36	4.722667	-4.326512	0.179305	x
x	C	37	4.755101	-4.274004	-0.045396	x
x	C	38	4.738233	-4.221484	-0.276009	x
x	C	39	4.690285	-4.221329	-0.281523	x
x	C	40	4.805471	-4.274649	-0.042717	x
x	C	41	4.847600	-4.275843	-0.044700	x
x	C	42	4.898705	-4.279212	-0.054470	x
x	C	43	4.931179	-4.332551	-0.194751	x
x	C	44	4.980184	-4.336274	-0.210715	x
x	C	45	4.998609	-4.287107	-0.085583	x
x	C	46	4.966020	-4.233489	0.056173	x
x	C	47	4.916687	-4.229679	0.071538	x
x	C	48	5.051592	-4.294116	-0.111418	x
x	N	1	4.608446	-4.270999	-0.078661	x
x	N	2	5.072214	-4.253556	0.007115	x
x	O	1	4.286050	-3.985636	-0.055243	x
x	O	2	4.362329	-4.009393	0.068973	x
x	O	3	4.366874	-4.567687	0.041812	x
x	O	4	4.281566	-4.553602	0.078590	x

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aniso-COF 6

Lattice parameters(A) Cell Angles

a = 29.300000 alpha = 75.000000

b = 22.000000 beta = 72.000000

c = 4.250000 gamma = 83.000000

Current cell volume = 2514.069909 A**3

Cell Contents

Total number of ions in cell = 92

Total number of species in cell = 5

Max number of any one species = 54

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x	Element	Atom Number	Fractional coordinates of atoms u	v	w	x
x----------						----x
x	H	1	0.511874	0.996063	0.008874	x
x	H	2	0.513285	0.889895	-0.068055	x
x	H	3	0.648865	0.847719	0.164471	x

x	H	4	0.648281	0.955608	0.220963	x
x	H	5	0.500712	0.459791	-0.143599	x
x	H	6	0.671256	0.437998	-0.204890	x
x	H	7	0.491898	0.212991	0.202669	x
x	H	8	0.660881	0.191752	0.180799	x
x	H	9	0.451766	0.405594	0.318003	x
x	H	10	0.368262	0.411248	0.314218	x
x	H	11	0.401489	0.266241	-0.245803	x
x	H	12	0.485675	0.271110	-0.308143	x
x	H	13	0.707128	0.244161	-0.321181	x
x	H	14	0.791277	0.234108	-0.337566	x
x	H	15	0.768202	0.379771	0.209692	x
x	H	16	0.681846	0.379995	0.292658	x
x	H	17	0.861182	0.265389	-0.228913	x
x	H	18	0.933298	0.244435	-0.158520	x
x	H	19	1.017047	0.243495	-0.162429	x
x	H	20	0.988244	0.415403	0.183517	x
x	H	21	0.903860	0.417018	0.186374	x
x	H	22	0.504268	0.785409	0.132499	x
x	H	23	0.505741	0.679701	0.045684	x
x	H	24	0.660146	0.669420	-0.220639	x
x	H	25	0.659404	0.776418	-0.154209	x
x	H	26	1.168565	0.235874	-0.171219	x
x	H	27	1.253464	0.227298	-0.188905	x
x	H	28	1.235453	0.398256	0.162319	x
x	H	29	1.149888	0.406713	0.178549	x
x	H	30	1.323956	0.264825	-0.128235	x
x	B	1	5.584019	-3.405278	-0.137751	x
x	B	2	5.578902	-3.943877	0.159196	x
x	C	1	5.580009	-3.015081	0.120511	x
x	C	2	5.542028	-3.035918	0.043896	x
x	C	3	5.542701	-3.097700	0.002849	x
x	C	4	5.581088	-3.141789	0.042510	x
x	C	5	5.618932	-3.120606	0.123136	x
x	C	6	5.618548	-3.058352	0.158714	x
x	C	7	5.560550	-3.498488	-0.125523	x
x	C	8	5.608034	-3.504567	-0.146716	x
x	C	9	5.535917	-3.550416	-0.109796	x
x	C	10	5.557537	-3.613052	-0.053178	x
x	C	11	5.607778	-3.619507	-0.062383	x
x	C	12	5.632867	-3.562834	-0.143329	x
x	C	13	5.530694	-3.667902	0.006224	x
x	C	14	5.555019	-3.729215	0.070375	x
x	C	15	5.604934	-3.735700	0.068027	x

x	C	16	5.632063	-3.680788	0.000645	x
x	C	17	5.530194	-3.785951	0.146553	x
x	C	18	5.555036	-3.844190	0.155164	x
x	C	19	5.601803	-3.850691	0.153133	x
x	C	20	5.626106	-3.798469	0.138287	x
x	C	21	5.685725	-3.687055	-0.010628	x
x	C	22	5.477579	-3.662165	0.002280	x
x	C	23	5.442379	-3.622398	0.173952	x
x	C	24	5.393623	-3.620524	0.182694	x
x	C	25	5.376993	-3.661248	0.040908	x
x	C	26	5.411422	-3.702184	-0.123741	x
x	C	27	5.460674	-3.699539	-0.159553	x
x	C	28	5.718771	-3.728158	-0.185871	x
x	C	29	5.767866	-3.732804	-0.204254	x
x	C	30	5.787120	-3.693582	-0.068339	x
x	C	31	5.755138	-3.650896	0.097344	x
x	C	32	5.705230	-3.650328	0.141367	x
x	C	33	5.840010	-3.699784	-0.099020	x
x	C	34	5.911280	-3.668256	0.010217	x
x	C	35	5.944312	-3.717397	-0.085938	x
x	C	36	5.992650	-3.718260	-0.086984	x
x	C	37	6.009389	-3.670478	0.008436	x
x	C	38	5.976604	-3.621798	0.105759	x
x	C	39	5.928298	-3.620912	0.107516	x
x	C	40	6.059711	-3.671857	0.009907	x
x	C	41	5.581747	-3.208622	-0.003232	x
x	C	42	5.538851	-3.238244	0.048977	x
x	C	43	5.539538	-3.299649	0.001545	x
x	C	44	5.583030	-3.334392	-0.094785	x
x	C	45	5.625854	-3.305546	-0.145238	x
x	C	46	5.625291	-3.243827	-0.102853	x
x	C	47	6.101707	-3.673859	0.009924	x
x	C	48	6.152460	-3.678172	0.005284	x
x	C	49	6.182634	-3.728519	-0.096354	x
x	C	50	6.231370	-3.733304	-0.106535	x
x	C	51	6.251656	-3.688047	-0.014431	x
x	C	52	6.221354	-3.637440	0.088622	x
x	C	53	6.172316	-3.632604	0.098092	x
x	C	54	6.304184	-3.695660	-0.033751	x
x	N	1	5.860747	-3.665123	0.021083	x
x	N	2	6.326130	-3.657774	0.058739	x
x	O	1	5.541482	-3.437076	-0.121743	x
x	O	2	5.627040	-3.448162	-0.164374	x
x	O	3	5.536535	-3.900288	0.163697	x

x O 4 5.620562 -3.912642 0.163306 x
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