

Supporting Information

Design of Covalent Organic Frameworks for Methane Storage

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1 New COFs

Previous studies showed that the main topologies to be obtained given a connectivity of the three and four points of extension are **ctn** and **bor** [1],[2],[3], we designed new COFs with these characteristics but with different ligands. The proposed chemistry is same; condensation of boronic acids to give boroxine esters and borosilicates. The building blocks are shown in Figure S1 while the inset shows the type of condensations used.

2 Delivery amount

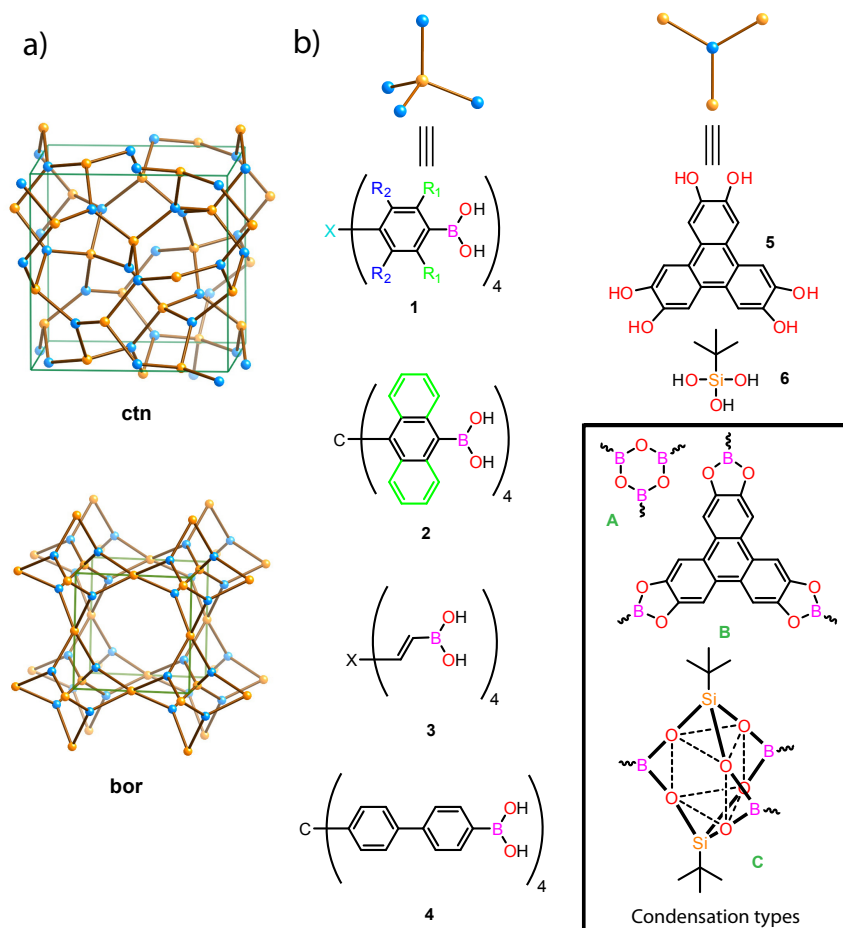
We have calculated $v(\text{CH}_4 \text{ STP}) v^{-1}$ delivery amount with respect to total volume of the framework. Here STP is the volume of methane at standard and pressure condition (STP; T = 298 K and P = 1.01 bar). In addition to the newly designed COFs, we have calculated the uptake amount of methane at room temperature from 0-300 bar for published COFs [2],[4] as well as for MOF-177 [5] and MOF-200 [6].

2.1 1 to 100 bar

We have calculated the methane delivery amount from 1 to 300 bar, and the results are shown in Figure S2. This is the theoretical upper limit for methane to be delivered if no kinetic affects are taken into account.

2.2 5 to 100 bar

We have calculated the methane delivery amount from 5 to 300 bar, and the results are shown in Figure S3. We have used 5 bar instead of 1 bar here in order to take into account possible kinetic effects. However, with this constraint we can see that none of the compounds presented in this work reach the DOE target. Also at 300 bar, COF-102-Ant performs worse than bulk methane.



Reactants	Type	X	R ₁	R ₂	Name	topology
1	A	X=C	—H	—H	COF-102	ctn
1	A	X=C	—CH ₂ CH ₃	—H	COF-102-Et-H	ctn
1	A	X=C	—CH(CH ₃) ₂	—H	COF-102-iPr-H	ctn
1	A	X=C	—(CH ₂) ₂ CH ₃	—H	COF-102-Pr-H	ctn
1	A	X=C	—C(CH ₃) ₃	—H	COF-102-tBu-H	ctn
1	A	X=C	—CH ₃	—CH ₃	COF-102-Me-Me	ctn
1	A	X=Si	—CH ₃	—CH ₃	COF-103-Me-Me	ctn
2	A	X=C	N/A	N/A	COF-102-Ant	ctn
3	A	X=C	N/A	N/A	COF-102-Eth-cis	ctn
3	A	X=Si	N/A	N/A	COF-103-Eth-cis	ctn
5+1	B	X=Si	—CH ₃	—CH ₃	COF-105-Me-Me	ctn
5+1	B	X=C	—H	—H	COF-108	bor
5+1	B	X=C	—(CH ₂) ₅ CH ₃	—H	COF-108-nHex-H	bor
5+1	B	X=C	—CH ₃	—CH ₃	COF-108-Me-Me	bor
5+3	B	X=C	N/A	N/A	COF-105-Eth-cis	ctn
6+1	C	X=C	—H	—H	COF-202	ctn
6+4	C	X=C	—H	—H	COF-212	ctn

Figure S1: New designed COFs. The inset shows the types of known condensation for COFs. We used these building blocks and condensation modes to design the new COFs.

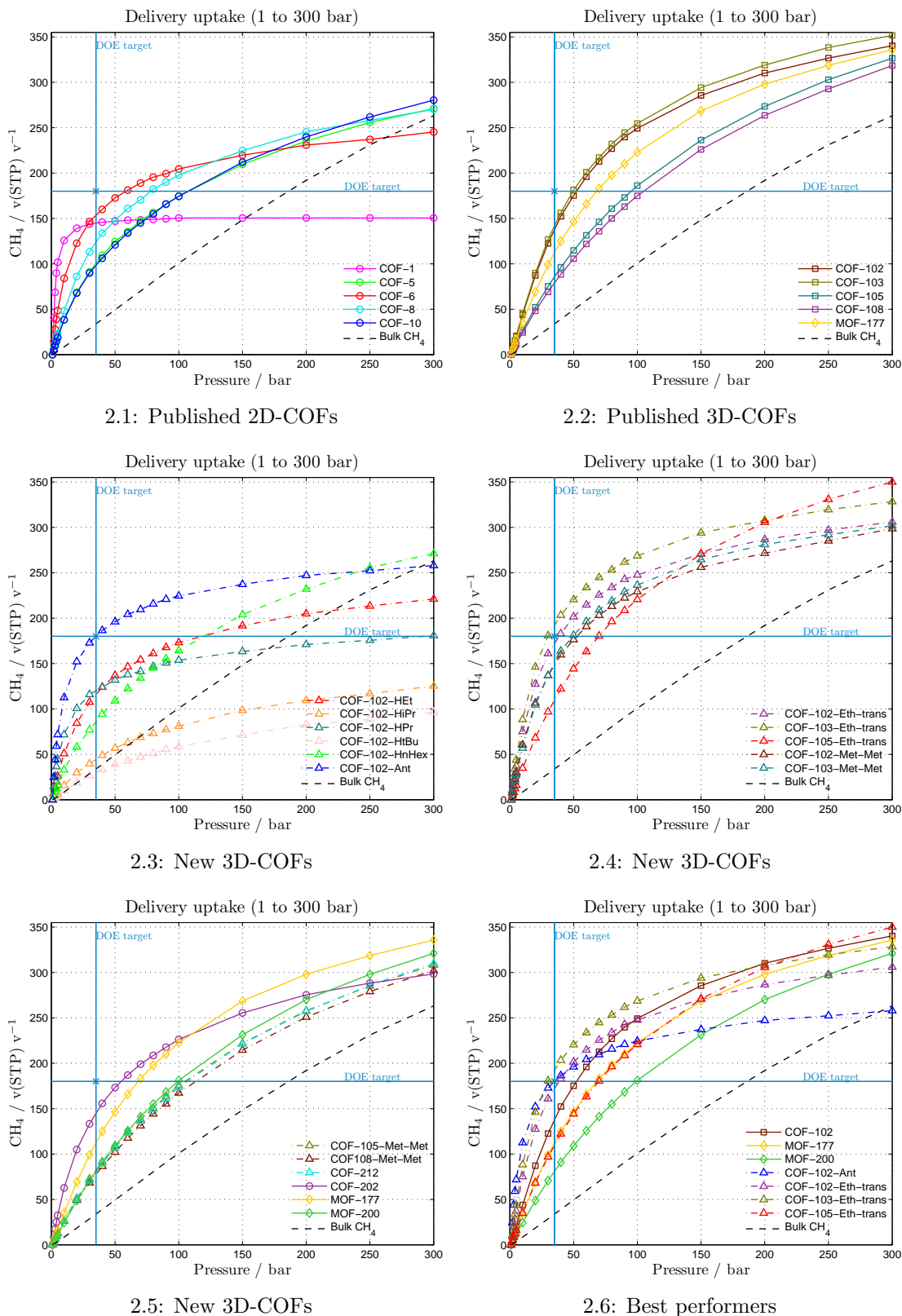
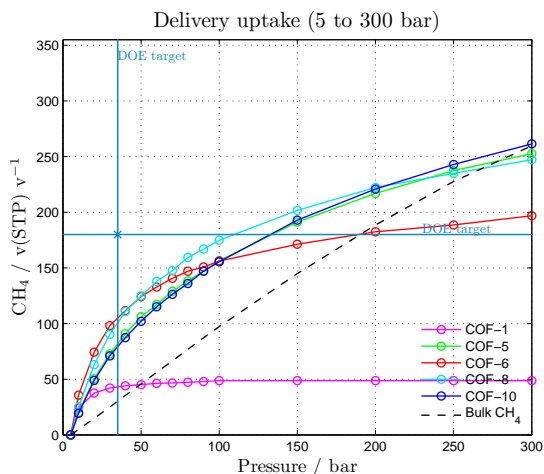
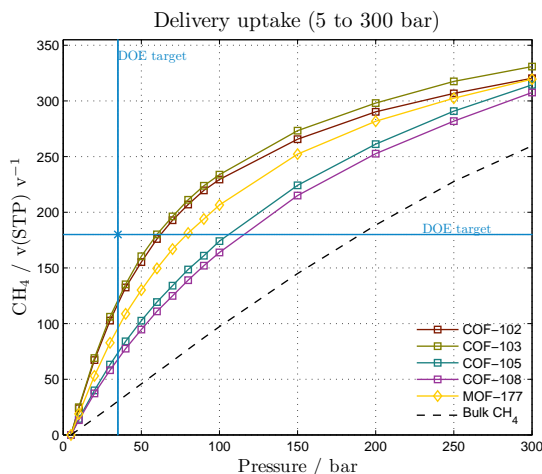


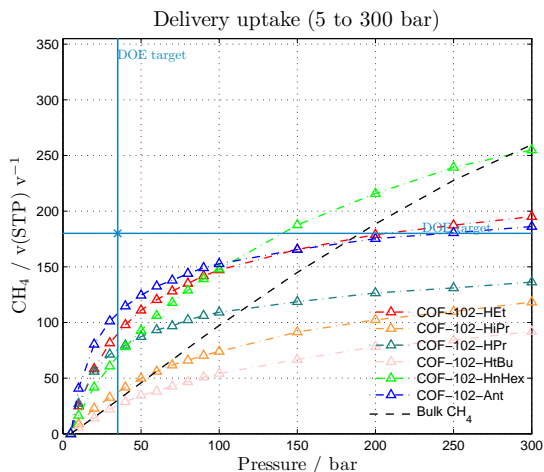
Figure S2: CH₄ delivery amount in v(STP)/v units (1-300 bar)



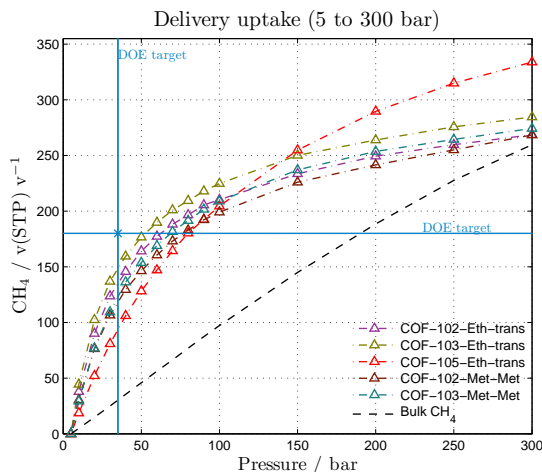
3.1: Published 2D-COFs



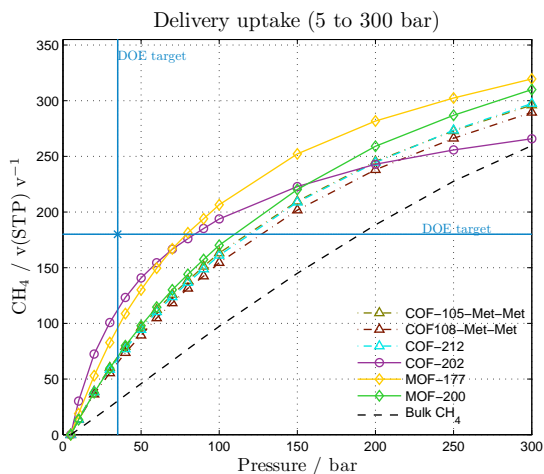
3.2: Published 3D-COFs



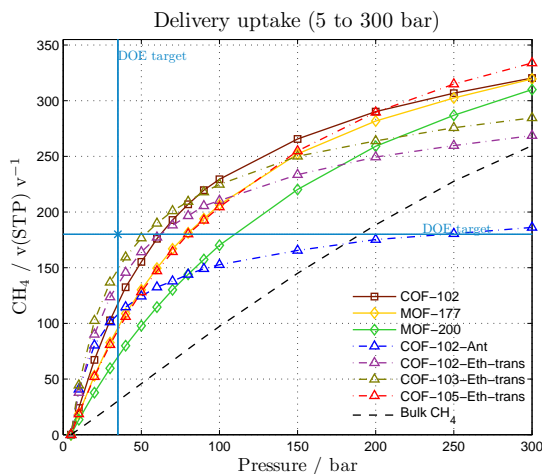
3.3: New 3D-COFs



3.4: New 3D-COFs



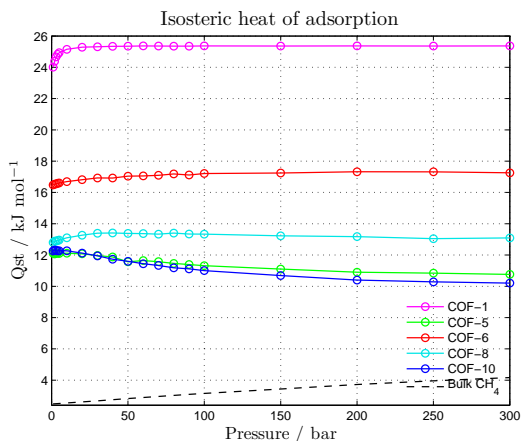
3.5: New 3D-COFs



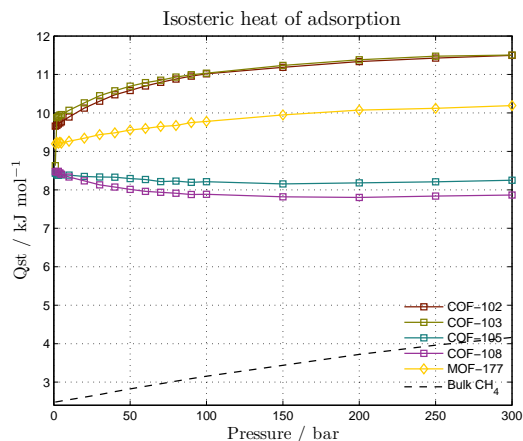
3.6: Best performers

Figure S3: CH₄ delivery amount in v(STP)/v units (5-300 bar)

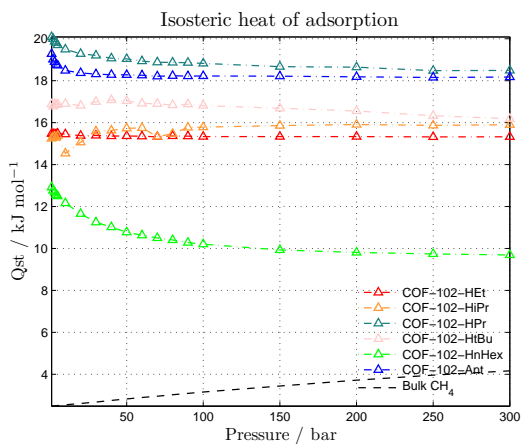
3 Heat of adsorption (Q_{st})



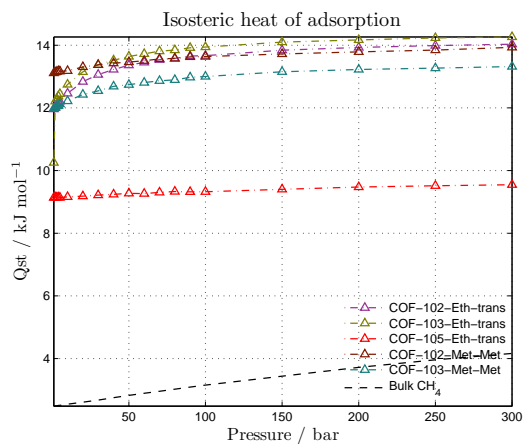
4.1: Published 2D-COFs



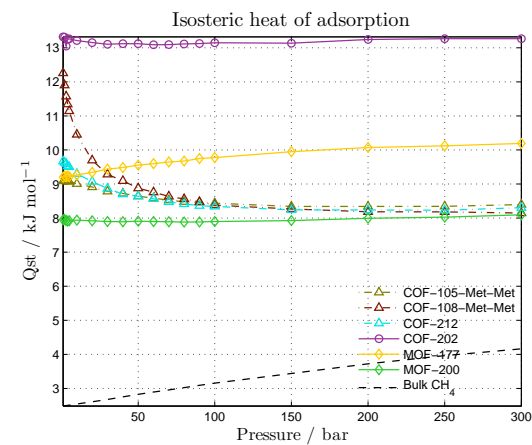
4.2: Published 3D-COFs



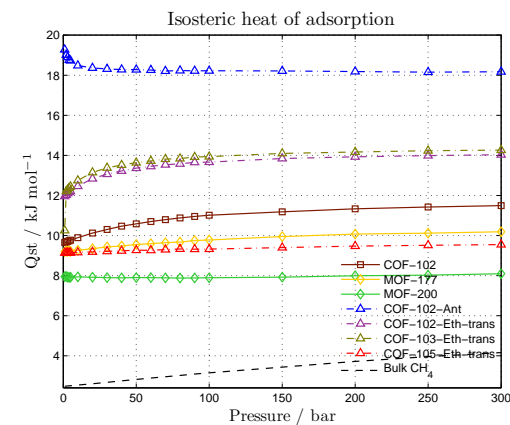
4.3: New 3D-COFs



4.4: New 3D-COFs



4.5: New 3D-COFs



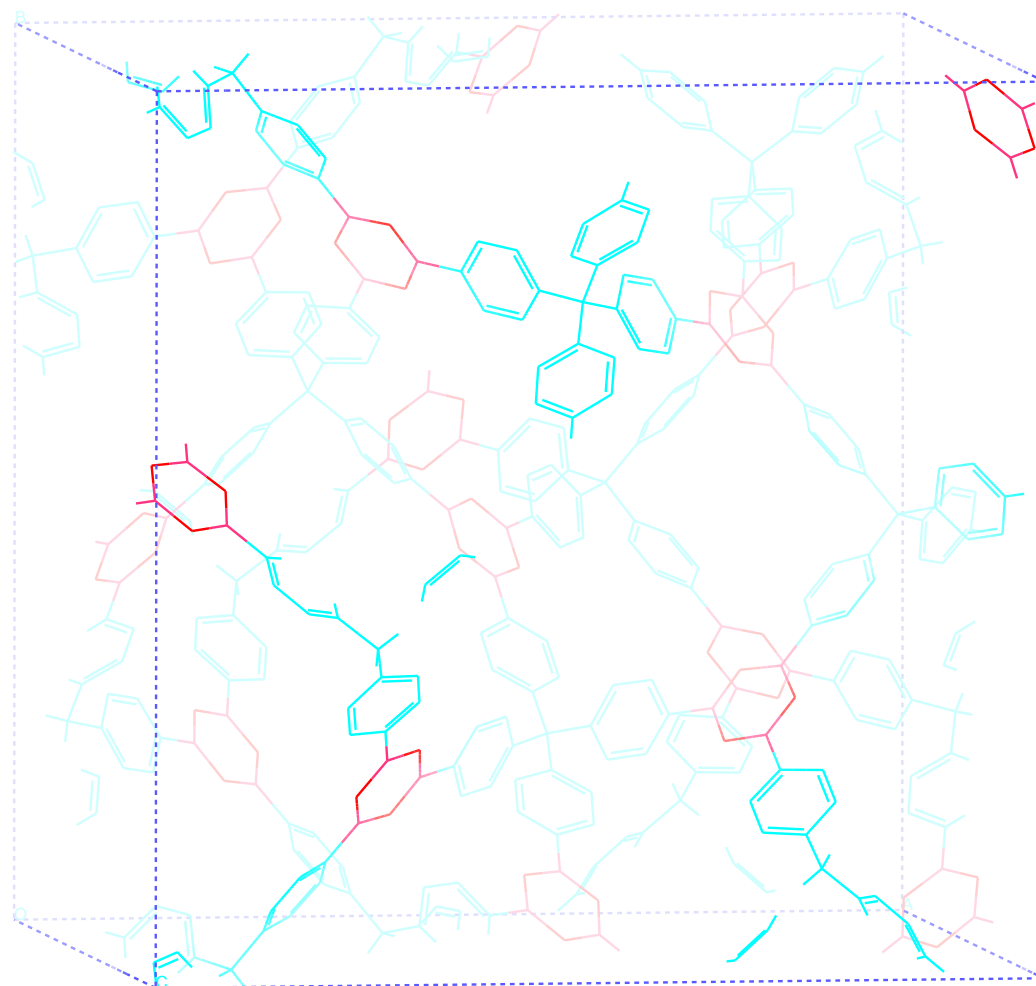
4.6: Best performers

Figure S4: Q_{st} for CH₄ adsorption for the range of 1 to 300 bar.

4 Surface area (S_A), pore volume (V_P) and density (ρ) for the studied frameworks.

Table 1: Properties of COFs. S_A and V_P were estimated from rolling an Ar molecule with diameter of 3.42 Å over the framework’s surface.

Compound	$S_A / (\text{m}^2 \text{ g}^{-1})$	$V_P / (\text{cm}^3 \text{ g}^{-1})$	$\rho / (\text{g cm}^{-3})$	Topology
COF-1	1230	0.38	0.91	gra
COF-5	1520	1.17	0.58	bnn
COF-6	1050	0.55	1.03	bnn
COF-8	1320	0.87	0.71	bnn
COF-10	1830	1.65	0.49	bnn
COF-102	4940	1.81	0.42	ctn
COF-103	5230	2.05	0.38	ctn
COF-105	6450	4.94	0.18	ctn
COF-108	6280	5.40	0.17	ctn
COF-102-H-Et	3970	0.95	0.64	ctn
COF-102-H-iPr	1420	0.63	0.76	ctn
COF-102-H-Pr	2590	0.72	0.75	ctn
COF-102-H-tBu	900	0.50	0.87	ctn
COF-108-H-nHex	5250	2.54	0.31	bor
COF-102-Ant	2720	0.75	0.76	ctn
COF-102-Eth-trans	4640	1.20	0.57	ctn
COF-103-Eth-trans	4920	1.36	0.57	ctn
COF-105-Eth-trans	6350	3.62	0.26	ctn
COF-102-Met-Met	3500	1.04	0.63	ctn
COF-103-Met-Met	3550	1.17	0.57	ctn
COF-105-Met-Met	5420	3.72	0.23	ctn
COF-108-Met-Met	5340	4.01	0.22	bor
COF-202	4500	1.37	0.53	ctn
COF-212	6460	4.13	0.21	ctn
MOF-177	4800	1.93	0.43	qom
MOF-200	5730	4.04	0.22	qom



15.00 Angstroms

5.1: COF-102

Figure S5: 3D-representation

Name

COF-102

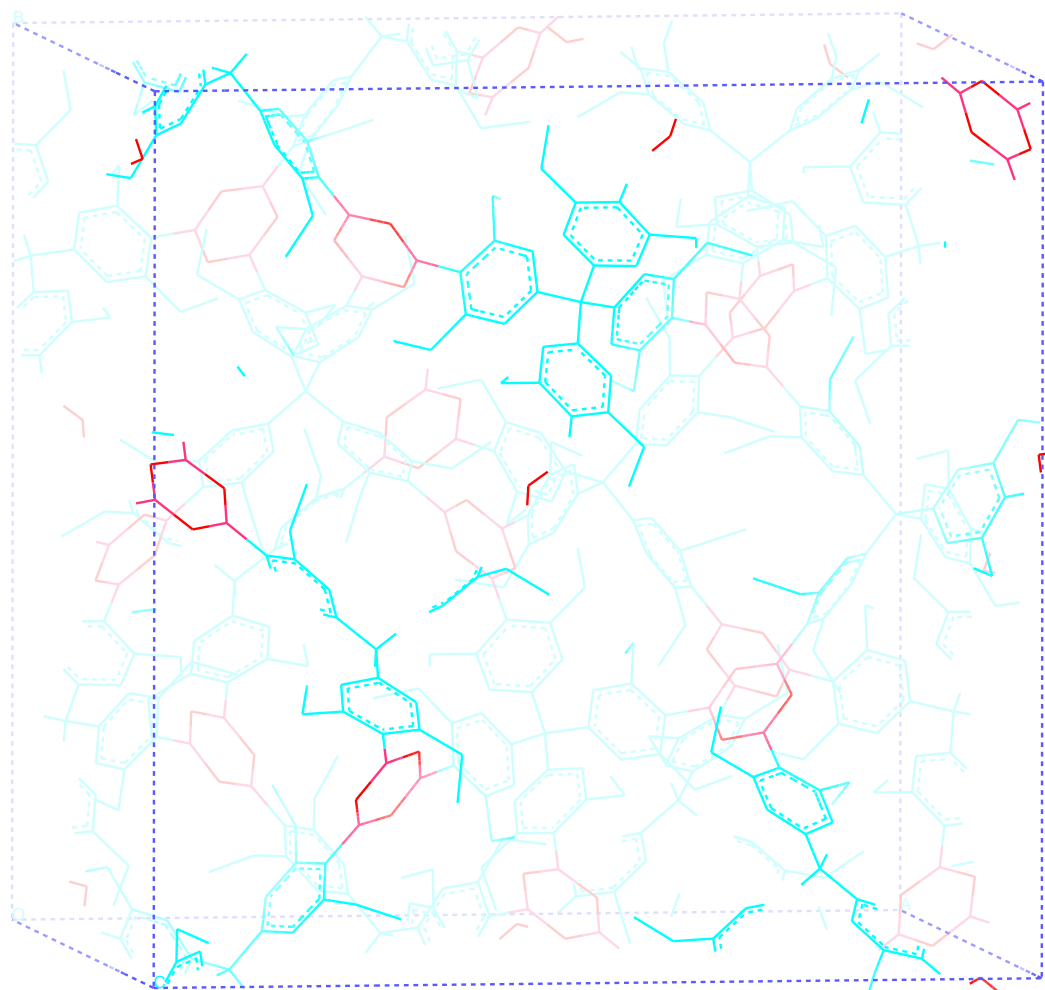
Space group symmetry

I -4 3 d

a = b = c = 27.177 27.177 27.177 Å

alpha = betha = gamma = 90

Atom	x	y	z
O1	0.82850	0.74693	0.30298
B1	0.83533	0.71325	0.26216
C1	0.90490	0.76629	0.22758
C2	0.87894	0.72231	0.22630
C3	0.93120	0.69419	0.16049
C4	0.95634	0.73930	0.15960
C5	0.89252	0.68630	0.19272
C6	0.94306	0.77459	0.19484
C7	1.00000	0.75000	0.12500
H1	0.89552	0.79460	0.25352
H2	0.94125	0.66415	0.13717
H3	0.87377	0.65150	0.19176
H4	0.96223	0.80911	0.19660



15.00 Angstroms

5.2: COF-102-Et-H

Figure S5: 3D-representation

Name

COF-102-Et-H

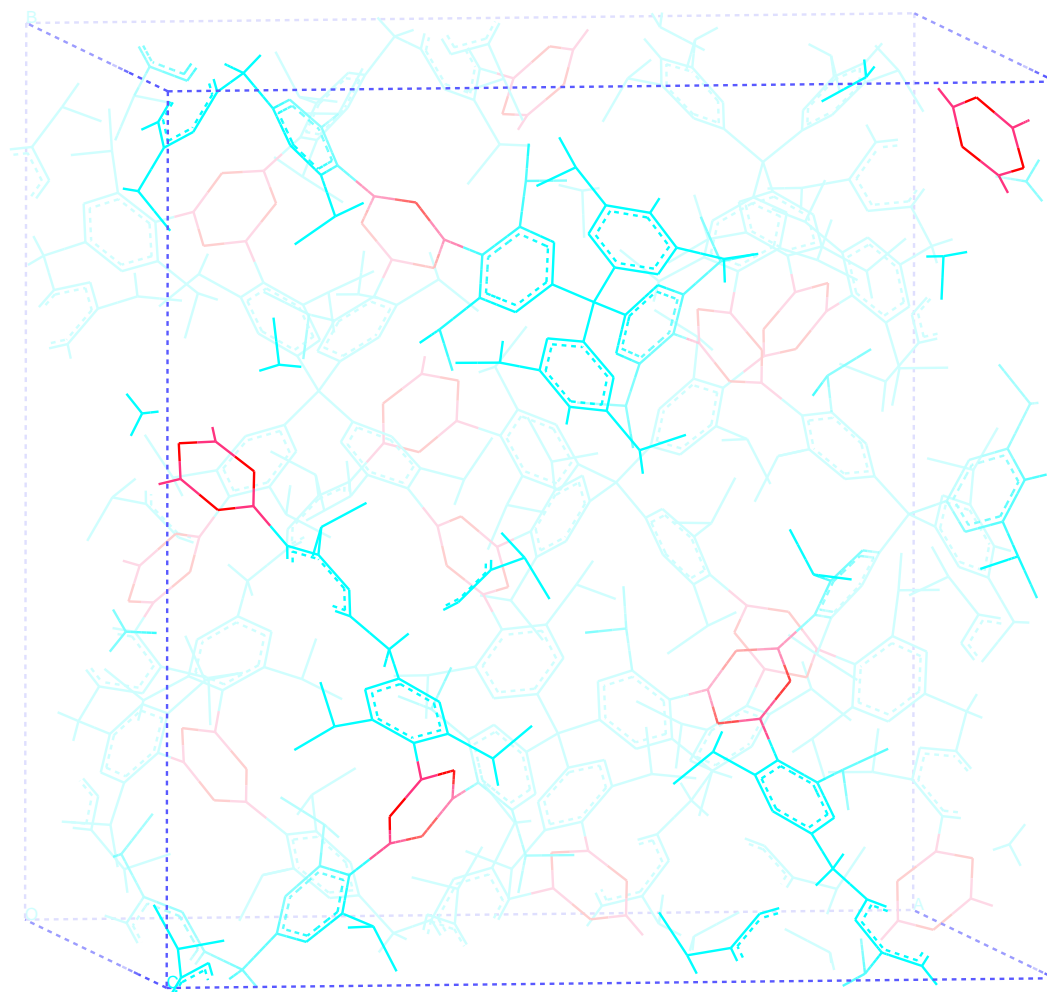
Space group symmetry

I -4 3 d

a = b = c = 27.190 27.190 27.190 A

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.37500	0.00000	0.25000
C2	0.31112	0.04591	0.19819
C3	0.33861	0.04238	0.24232
C4	0.32806	0.07808	0.27871
C5	0.29562	0.11798	0.27095
C6	0.27052	0.12130	0.22500
B7	0.23723	0.16369	0.21498
C8	0.27739	0.08429	0.18850
O9	0.19568	0.17363	0.24651
H10	0.17547	0.09495	0.16865
H11	0.17799	0.06639	0.11033
H12	0.19265	0.03217	0.16382
H13	0.31569	0.22849	0.33156
H14	0.35854	0.19516	0.29550
H15	0.30559	0.22132	0.26773
H16	0.34458	0.07507	0.31228
H17	0.31604	0.01922	0.17213
C18	0.25009	0.08307	0.14049
C19	0.29081	0.15525	0.31143
H20	0.25257	0.11864	0.12214
H21	0.26664	0.05672	0.11498
C22	0.19548	0.06826	0.14642
H23	0.25223	0.16372	0.31827
H24	0.30479	0.14081	0.34629
C25	0.31951	0.20316	0.30064



15.00 Angstroms

5.3: COF-102-iPr-H

Figure S5: 3D-representation

Name

COF-102-iPr-H

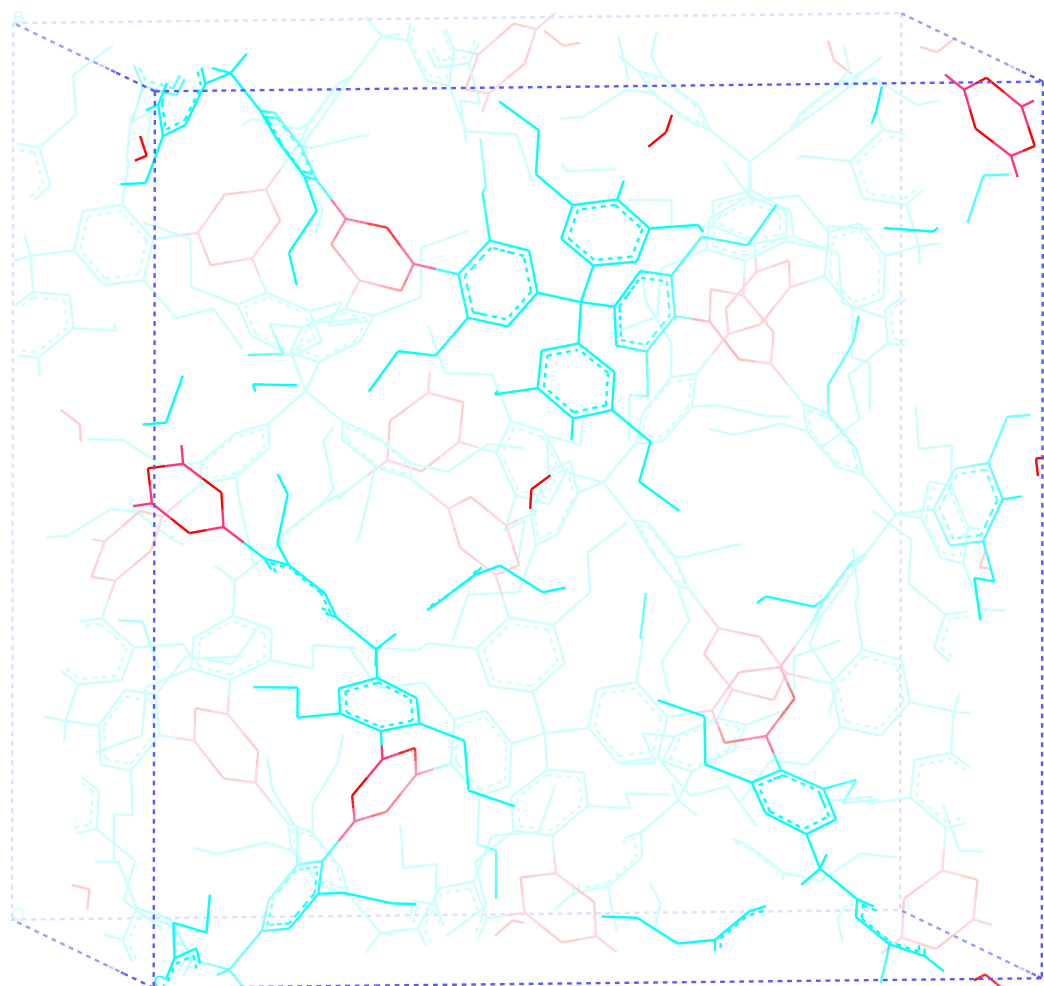
Space group symmetry

I -4 3 d

a = b = c = 27.085 27.085 27.085 A

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.62500	0.50000	0.25000
C2	0.56088	0.44691	0.29471
C3	0.58823	0.49138	0.29206
C4	0.57619	0.52793	0.32734
C5	0.54239	0.52025	0.36643
C6	0.51723	0.47390	0.36839
B7	0.48360	0.46282	0.41038
C8	0.52445	0.43754	0.33092
O9	0.44161	0.49390	0.42088
C10	0.50739	0.60599	0.37974
H11	0.49928	0.63389	0.40771
H12	0.52921	0.62327	0.35059
H13	0.47239	0.59356	0.36400
C14	0.52659	0.34360	0.33544
H15	0.50320	0.31077	0.33674
H16	0.55354	0.33867	0.30593
H17	0.54609	0.34644	0.37062
H18	0.44345	0.42068	0.27190
H19	0.44069	0.35570	0.27746
H20	0.49041	0.38342	0.24561
H21	0.57641	0.60375	0.45880
H22	0.60839	0.59752	0.40238
H23	0.60382	0.54654	0.44338
H24	0.59244	0.56174	0.32432
H25	0.56748	0.42056	0.26853
C26	0.49468	0.39040	0.32661
C27	0.53541	0.56177	0.40325
H28	0.46590	0.38901	0.35475
C29	0.46563	0.38740	0.27711
H30	0.51260	0.54992	0.43416
C31	0.58426	0.57846	0.42838



15.00 Angstroms

5.4: COF-102-Pr-H

Figure S5: 3D-representation

Name

COF-102-Pr-H

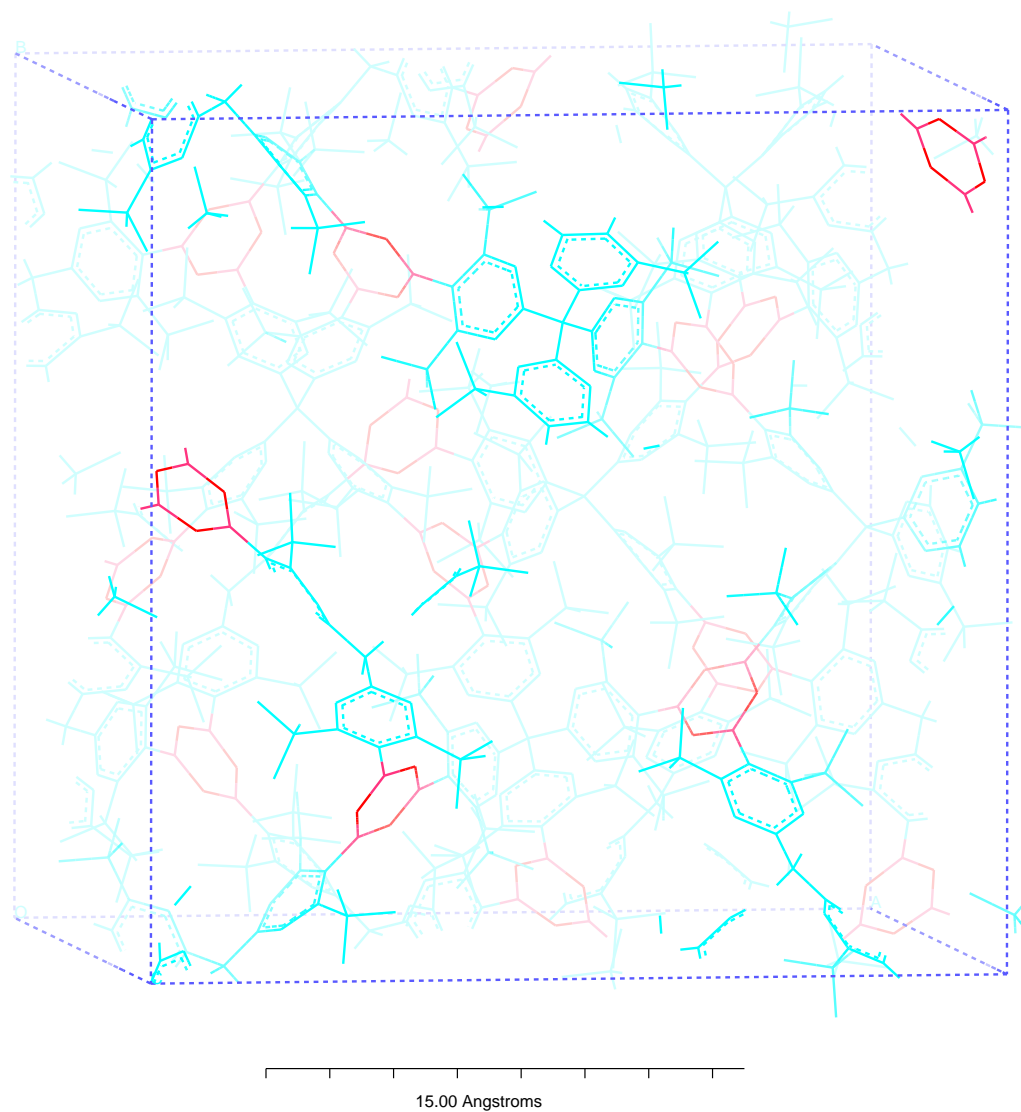
Space group symmetry

I -4 3 d

a = b = c = 27.234 27.234 27.234 Å

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.62500	0.50000	0.25000
H2	0.58221	0.43555	0.18606
H3	0.57787	0.58397	0.22238
C4	0.51945	0.61858	0.15387
C5	0.52720	0.43368	0.10717
H6	0.52837	0.63103	0.11689
H7	0.54008	0.64308	0.17814
C8	0.46416	0.62738	0.16495
H9	0.48766	0.42978	0.10266
H10	0.53881	0.39979	0.12536
C11	0.55324	0.43507	0.05639
H12	0.44128	0.60468	0.14123
C13	0.44880	0.68149	0.15727
H14	0.45647	0.61705	0.20298
H15	0.45741	0.69337	0.11996
H16	0.46791	0.70530	0.18325
H17	0.40934	0.68537	0.16296
C18	0.54394	0.38849	0.02541
H19	0.59284	0.43888	0.06193
H20	0.54070	0.46665	0.03519
H21	0.56232	0.39212	-0.01000
H22	0.50468	0.38346	0.01904
H23	0.55841	0.35609	0.04405
C24	0.56826	0.55599	0.19929
C25	0.58840	0.50900	0.20835
C26	0.57075	0.47045	0.17844
C27	0.53874	0.47789	0.13824
C28	0.52122	0.52649	0.12877
B29	0.48781	0.53574	0.08629
C30	0.53587	0.56614	0.15995
O31	0.49591	0.57662	0.05357



5.5: COF-102-tBu-H

Figure S5: 3D-representation

Name

COF-102-tBu-H

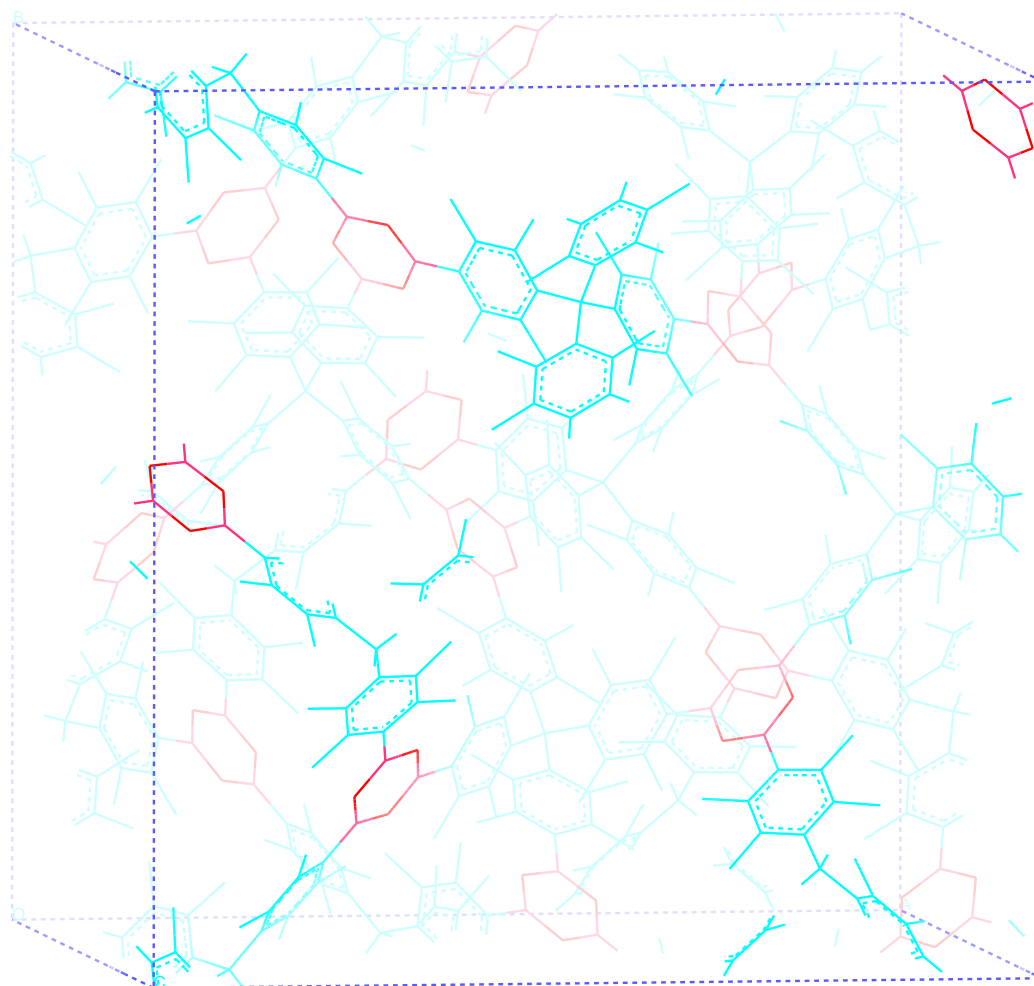
Space group symmetry

I -4 3 d

a = b = c = 27.178 27.178 27.178 Å

alpha = beta = gamma = 90

Atom	x	y	z
C1	0.62500	0.50000	0.25000
C2	0.50042	0.62198	0.18408
C3	0.52586	0.43986	0.10725
H4	0.57783	0.44216	0.18865
H5	0.58372	0.58799	0.22396
C6	0.44311	0.61779	0.18066
H7	0.43084	0.61531	0.14284
H8	0.43009	0.58557	0.20087
H9	0.42406	0.65007	0.19507
C10	0.50822	0.64257	0.23787
H11	0.48522	0.67469	0.24542
H12	0.49905	0.61447	0.26506
H13	0.54577	0.65511	0.24433
C14	0.51856	0.66461	0.15012
H15	0.55862	0.66739	0.15035
H16	0.50668	0.65950	0.11242
H17	0.50362	0.70021	0.16160
C18	0.47480	0.41476	0.11564
H19	0.46077	0.39807	0.08197
H20	0.47612	0.38606	0.14376
H21	0.44781	0.44113	0.12825
C22	0.53296	0.45542	0.05273
H23	0.56725	0.47581	0.04756
H24	0.53202	0.42451	0.02707
H25	0.50267	0.47788	0.04211
C26	0.56427	0.39636	0.11106
H27	0.60171	0.41054	0.10812
H28	0.56083	0.37584	0.14548
H29	0.55967	0.36881	0.08204
C30	0.56790	0.56087	0.20374
C31	0.58788	0.51351	0.20986
C32	0.56704	0.47681	0.18049
C33	0.53346	0.48489	0.14165
C34	0.51192	0.53400	0.13900
B35	0.47587	0.54645	0.09900
C36	0.52638	0.57196	0.17378
O37	0.48366	0.58775	0.06647



15.00 Angstroms

5.7: COF-102-Me-Me

Figure S5: 3D-representation

Name

COF-102-Me-Me

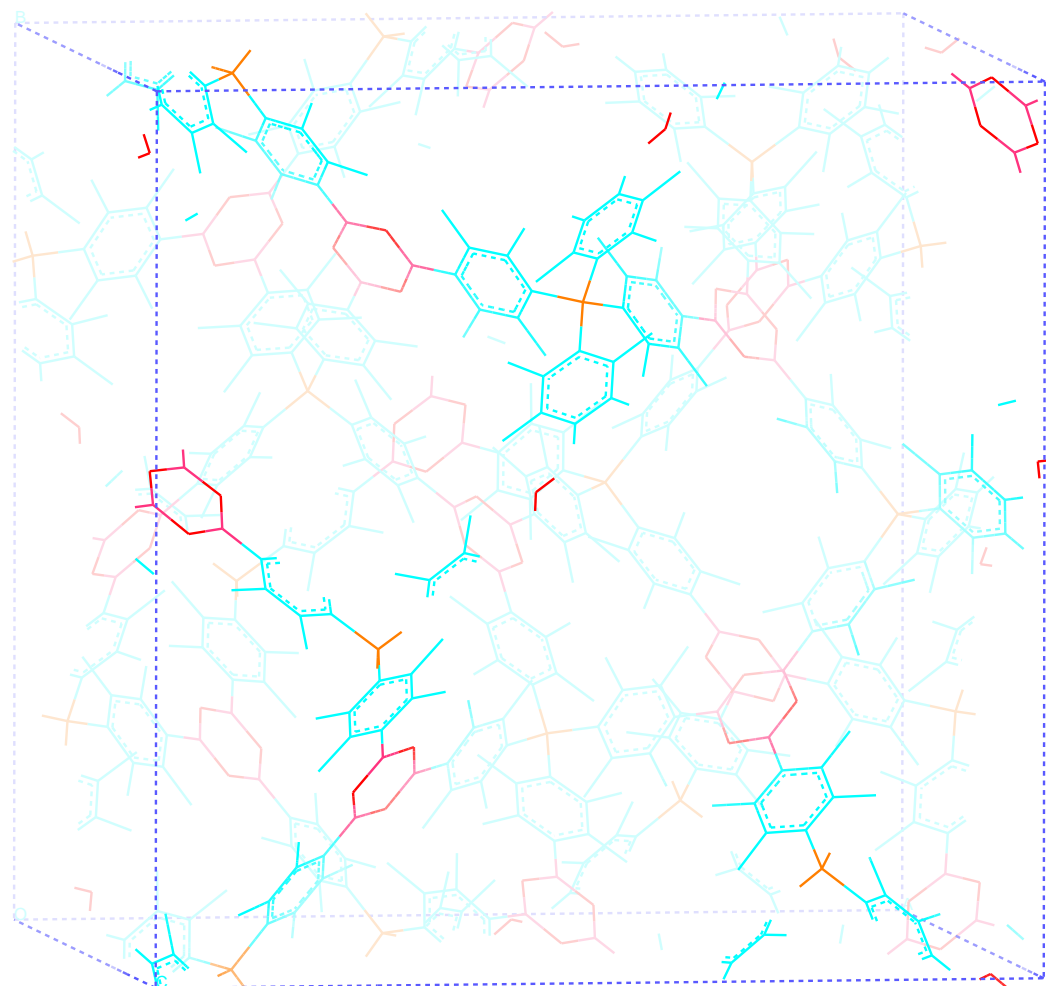
Space group symmetry

I -4 3 d

a = b = c = 27.408 27.408 27.408 A

alpha = betha = gamma = 90

Atom	x	y	z
O1	0.19700	0.17173	0.24691
C2	0.00000	0.25000	0.37500
C3	0.06876	0.19417	0.33948
C4	0.04365	0.23929	0.34040
C5	0.05696	0.27460	0.30517
C6	0.09512	0.26629	0.27244
C7	0.12105	0.22229	0.27369
B8	0.16465	0.21323	0.23782
C9	0.10744	0.18627	0.30725
C10	0.02776	0.32244	0.30734
C11	0.05409	0.15687	0.37854
C12	0.13601	0.13886	0.30639
C13	0.10968	0.30443	0.23519
H14	0.03951	0.34933	0.27959
H15	-0.01144	0.31442	0.30101
H16	0.03179	0.33969	0.34378
H17	0.08536	0.14849	0.40289
H18	0.02352	0.16995	0.40171
H19	0.04186	0.12307	0.35985
H20	0.17521	0.14688	0.31272
H21	0.12426	0.11197	0.33414
H22	0.13198	0.12161	0.26995
H23	0.07841	0.31280	0.21084
H24	0.12191	0.33823	0.25388
H25	0.14025	0.29135	0.21202



15.00 Angstroms

5.8: COF-103-Me-Me

Figure S5: 3D-representation

Name

COF-103-Me-Me

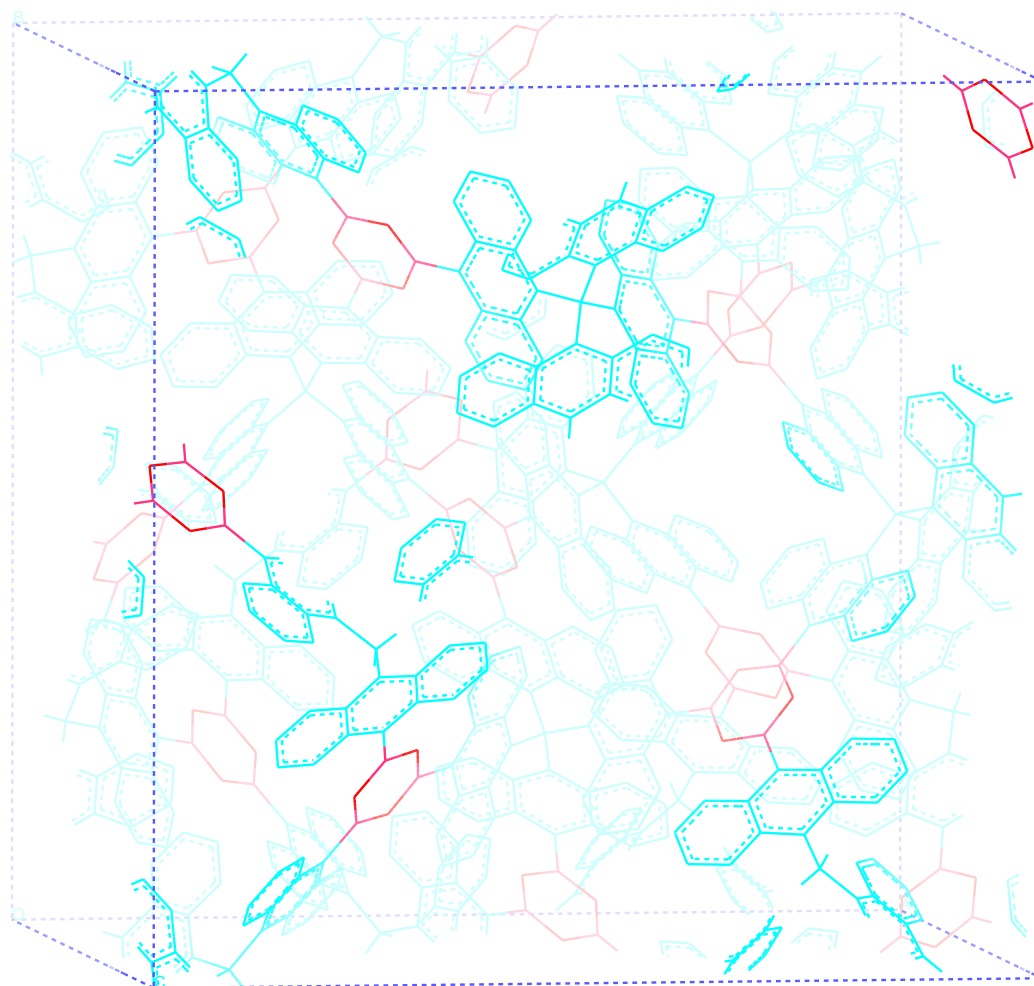
Space group symmetry

I -4 3 d

a = b = c = 28.454 28.454 28.454 Å

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.13828	0.48062	0.45080
C2	0.10068	0.56512	0.59988
C3	0.18314	0.63062	0.58358
C4	0.22075	0.54612	0.43449
H5	0.16194	0.47831	0.42000
H6	0.13978	0.44644	0.46958
H7	0.10197	0.48608	0.43758
H8	0.08362	0.60021	0.60024
H9	0.07245	0.53815	0.59983
H10	0.12166	0.56033	0.63243
H11	0.18164	0.66479	0.56479
H12	0.15949	0.63292	0.61438
H13	0.21945	0.62516	0.59680
H14	0.23781	0.51103	0.43414
H15	0.19977	0.55090	0.40194
H16	0.24898	0.57309	0.43454
Si17	0.25000	0.62500	0.50000
C18	0.17034	0.59070	0.54999
C19	0.19861	0.58591	0.50993
C20	0.18875	0.55021	0.47747
C21	0.15079	0.51989	0.48467
C22	0.12212	0.52496	0.52451
B23	0.07948	0.49102	0.53269
C24	0.13217	0.56062	0.55710
O25	0.04827	0.49979	0.57262



15.00 Angstroms

5.9: COF-102-Ant

Figure S5: 3D-representation

Name

COF-102-Ant

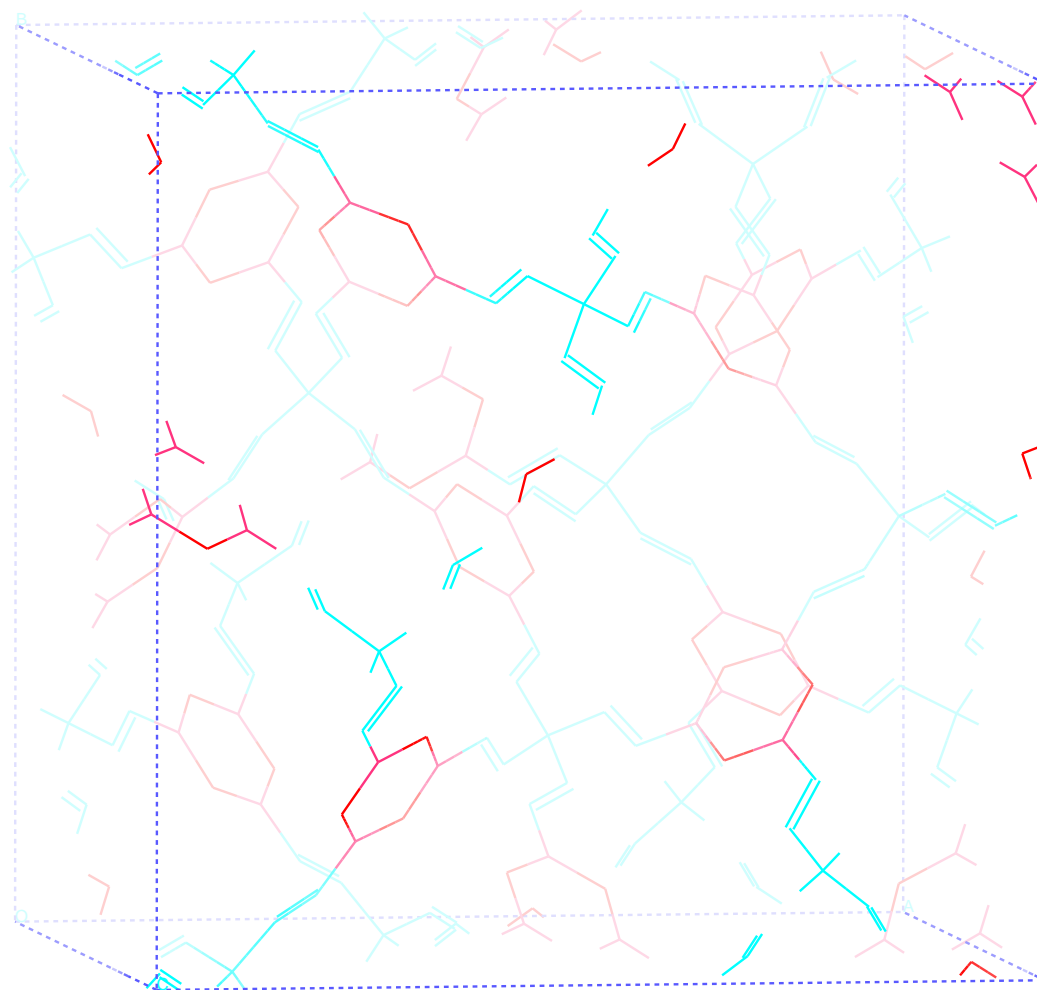
Space group symmetry

I -4 3 d

a = b = c = 27.821 27.821 27.821 A

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.82285	0.54942	0.68100
C2	0.83516	0.53805	0.73079
C3	0.80008	0.55693	0.76493
C4	0.75548	0.57867	0.75152
C5	0.74858	0.59413	0.70392
B6	0.71152	0.63670	0.69205
C7	0.78010	0.57598	0.66850
O8	0.66988	0.65218	0.72003
C9	0.87500	0.50000	0.75000
C10	0.77224	0.58631	0.61978
H11	0.74036	0.60605	0.60923
C12	0.80466	0.57106	0.58452
H13	0.79775	0.57904	0.54707
C14	0.84600	0.54554	0.59748
H15	0.87095	0.53384	0.57002
C16	0.85520	0.53508	0.64578
H17	0.88736	0.51529	0.65530
C18	0.72554	0.59596	0.78777
H19	0.69339	0.61577	0.77825
C20	0.73475	0.58552	0.83609
H21	0.70979	0.59722	0.86355
C22	0.77609	0.56000	0.84905
H23	0.78300	0.55203	0.88649
C24	0.80852	0.54475	0.81378
H25	0.84039	0.52500	0.82433



10.00 Angstroms

5.10: COF-102-Eth-trans

Figure S5: 3D-representation

Name

COF-102-Eth-trans

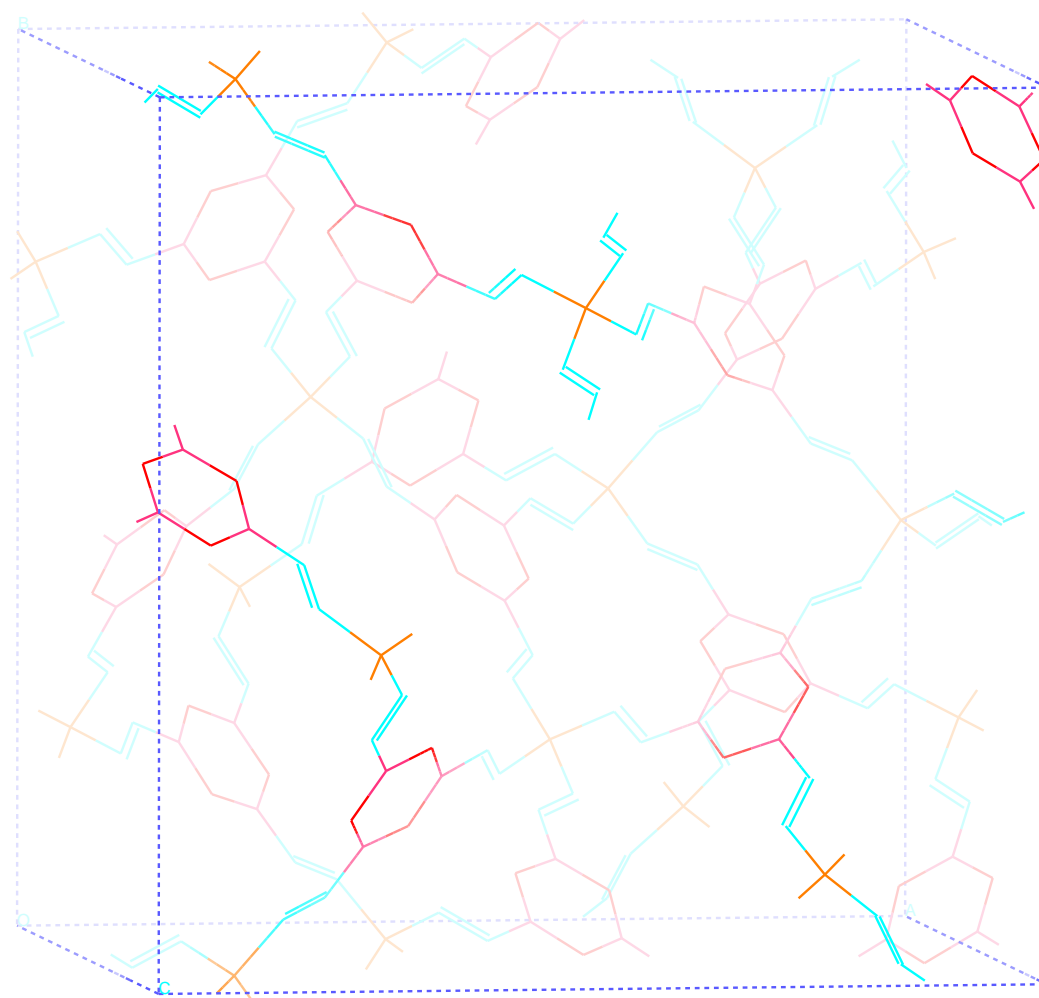
Space group symmetry

I -4 3 d

a = b = c = 19.779 19.779 19.779 Å

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.62500	0.50000	0.25000
B2	0.75957	0.35463	0.22886
O3	0.73610	0.31890	0.16958
C4	0.66738	0.44350	0.22168
C5	0.72293	0.41460	0.25535
H6	0.65373	0.42238	0.17633
H7	0.73873	0.43456	0.30031



10.00 Angstroms

5.11: COF-103-Eth-trans

Figure S5: 3D-representation

Name

COF-103-Eth-trans

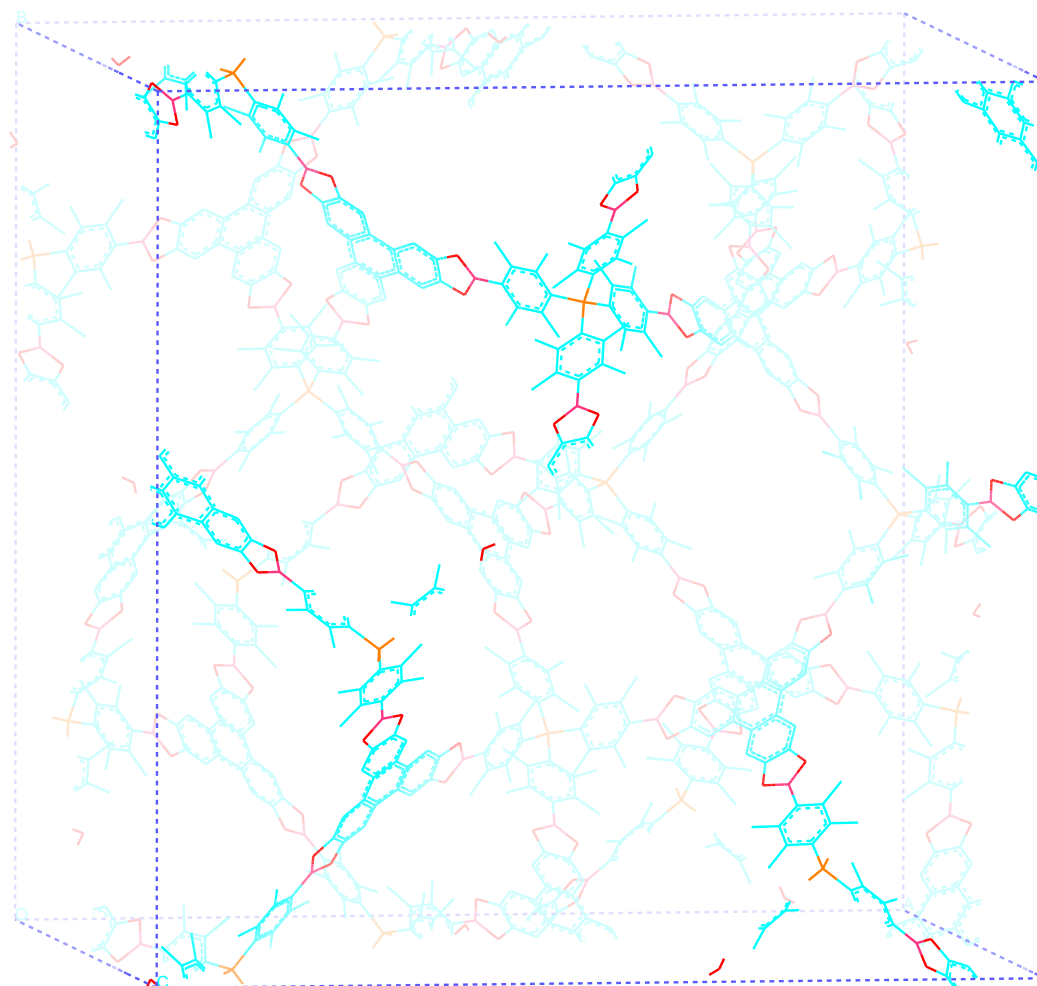
Space group symmetry

I -4 3 d

a = b = c = 20.250 20.250 20.250 Å

alpha = betha = gamma = 90

Atom	x	y	z
Si1	0.50000	0.25000	0.62500
B2	0.47711	0.39586	0.48890
O3	0.41924	0.43099	0.51157
C4	0.46984	0.31043	0.57967
C5	0.50270	0.33728	0.52489
H6	0.42597	0.33078	0.59423
H7	0.54616	0.31712	0.50884



20.00 Angstroms

5.12: COF-105-Me-Me

Figure S5: 3D-representation

Name

COF-105-Me-Me

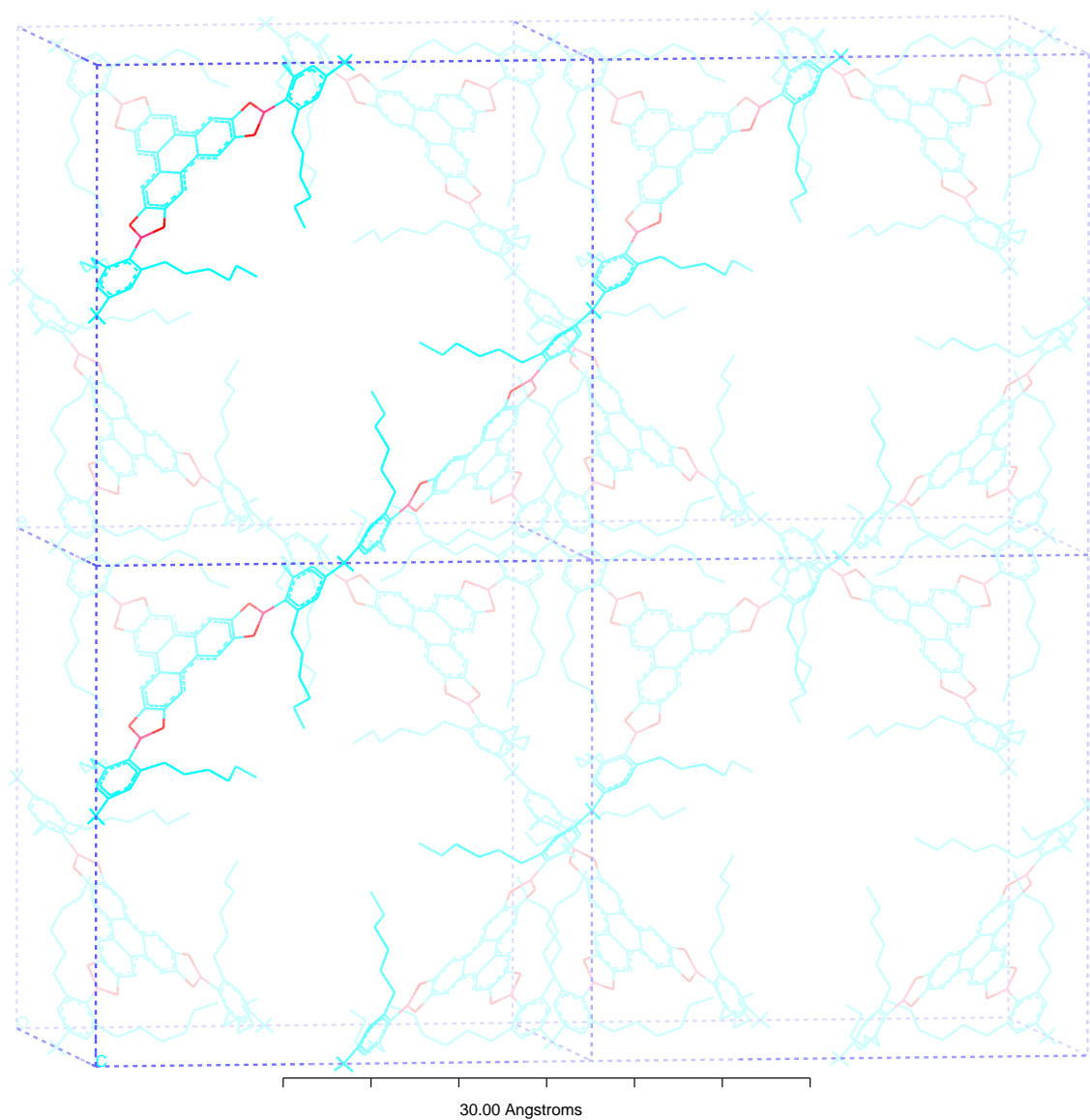
Space group symmetry

I -4 3 d

a = b = c = 44.382 44.382 44.382 A

alpha = betha = gamma = 90

Atom	x	y	z
Si1	0.37500	0.00000	0.25000
C2	0.21781	0.18335	0.22645
C3	0.23477	0.19174	0.20018
C4	0.22787	0.15826	0.24387
H5	0.21763	0.15114	0.26464
C6	0.25261	0.14166	0.23455
O7	0.26434	0.11672	0.24923
C8	0.26778	0.14873	0.20882
O9	0.29149	0.12931	0.20284
C10	0.25958	0.17328	0.19137
H11	0.27270	0.17680	0.17131
B12	0.28905	0.10906	0.22877
C13	0.35228	0.05035	0.21728
C14	0.34987	0.03288	0.24348
C15	0.32755	0.03978	0.26475
C16	0.30811	0.06410	0.26008
C17	0.31075	0.08180	0.23403
C18	0.33294	0.07478	0.21265
C19	0.28355	0.07305	0.28230
H20	0.28749	0.09649	0.29010
H21	0.26129	0.07200	0.27093
H22	0.28253	0.05838	0.30244
C23	0.32563	0.01996	0.29285
H24	0.30311	0.00913	0.29397
H25	0.32933	0.03390	0.31329
H26	0.34285	0.00179	0.29278
C27	0.33515	0.09429	0.18468
H28	0.35767	0.10512	0.18356
H29	0.31793	0.11246	0.18475
H30	0.33145	0.08035	0.16423
C31	0.37722	0.04150	0.19525
H32	0.39946	0.04266	0.20665
H33	0.37820	0.05618	0.17510
H34	0.37339	0.01804	0.18744



5.14: COF-108-nHex-H

Figure S5: 3D-representation

Name

COF-108-nHex-H

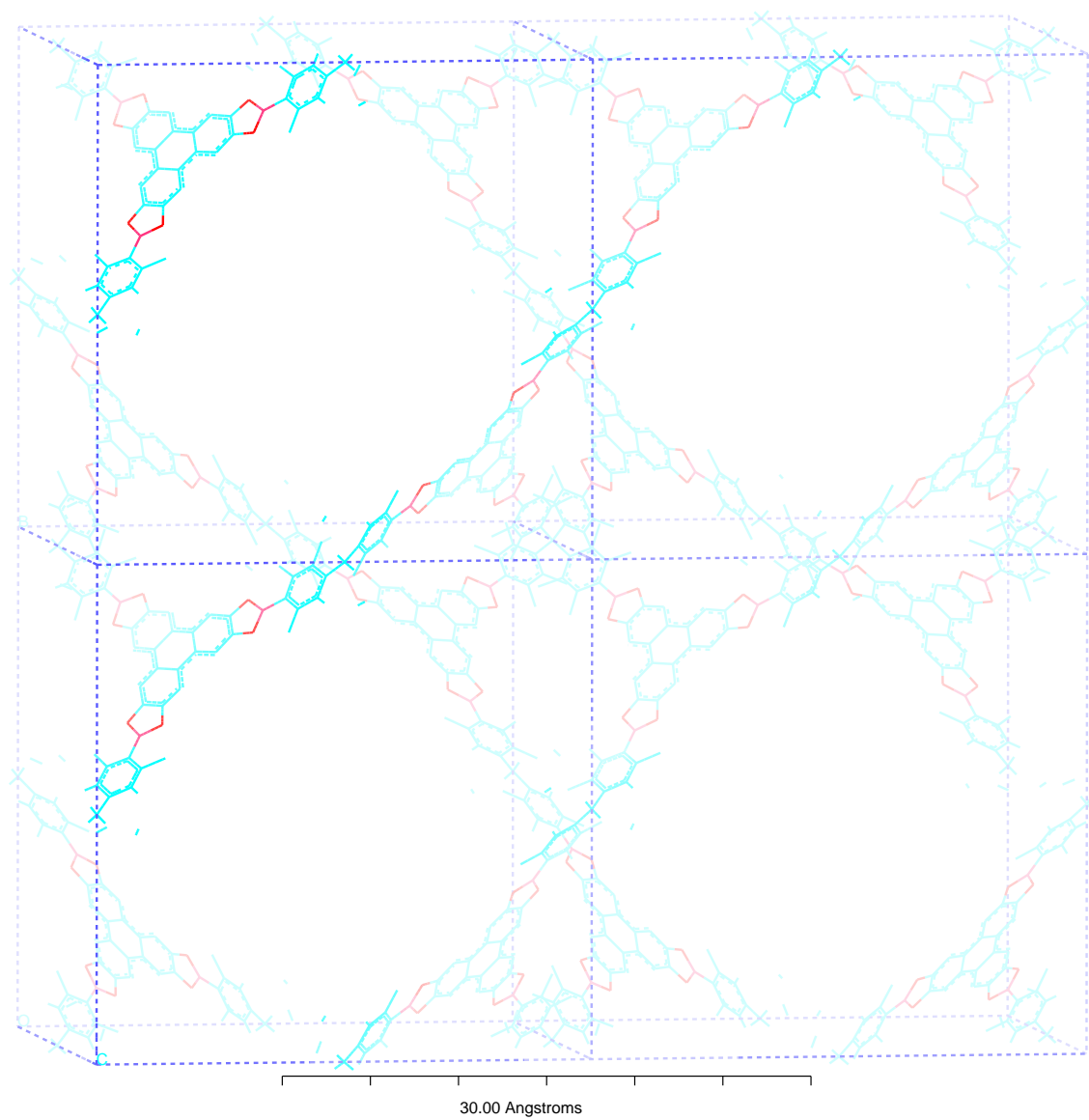
Space group symmetry

P -4 3 m

a = b = c = 28.589 28.589 28.589 A

alpha = betha = gamma = 90

Atom	x	y	z
B1	0.64596	0.89336	0.10664
C2	0.60575	0.92134	0.07866
C3	0.58778	0.90432	0.03511
C4	0.55277	0.92945	0.01140
C5	0.53289	0.97056	0.02944
C6	0.77050	0.80583	0.15859
C7	0.70201	0.84295	0.12351
H8	0.73217	0.78277	0.09509
O9	0.66764	0.84984	0.09004
C10	0.73506	0.80743	0.12331
C11	0.50000	0.00000	0.00000
C12	0.01128	0.85980	0.60423
H13	-0.02685	0.86161	0.59649
H14	0.01253	0.85620	0.64272
H15	-0.02221	0.91663	0.54095
C16	1.03135	1.42100	0.18315
H17	1.03056	1.45941	0.17691
H18	1.06830	1.41048	0.18844
C19	0.77297	0.40999	0.99756
C20	0.72916	0.43453	0.97837
H21	0.77875	0.42247	1.03395
H22	0.70261	0.43601	1.00677
H23	0.73773	0.47111	0.96834
C24	0.70803	0.40862	0.93639
H25	0.73349	0.40757	0.90708
H26	0.69933	0.37208	0.94648
H27	0.76718	0.37154	0.99911
C28	0.66356	0.43279	0.91951
H29	0.63680	0.43303	0.94767
H30	0.67130	0.46935	0.90885
H31	0.64924	0.41374	0.88886



5.15: COF-108-Me-Me

Figure S5: 3D-representation

Name

COF-108-Me-Me

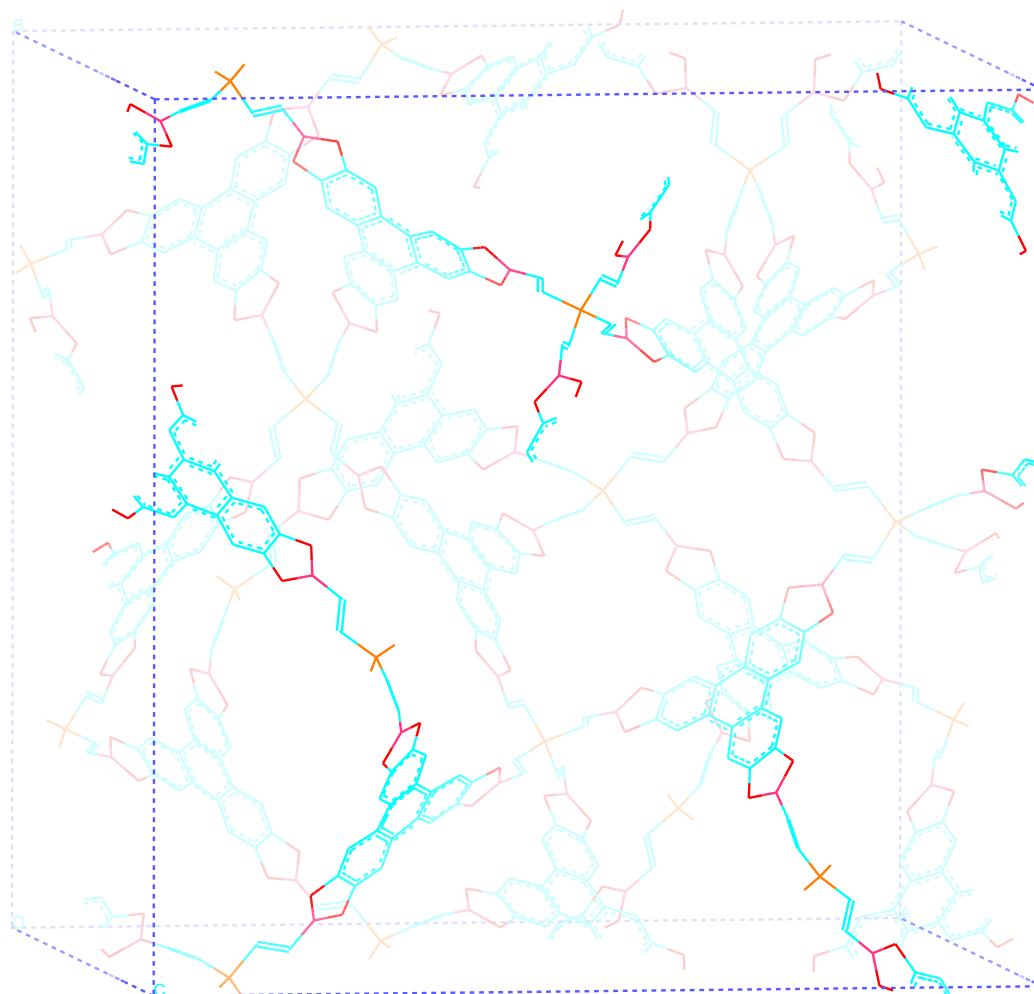
Space group symmetry

P -4 3 m

a = b = c = 28.441 28.441 28.441 Å

alpha = betha = gamma = 90

Atom	x	y	z
B1	0.64886	0.89710	0.10290
C2	0.60702	0.92264	0.07736
C3	0.58884	0.90473	0.03528
C4	0.55309	0.92861	0.01135
C5	0.53295	0.97038	0.02962
C6	0.77691	0.81243	0.15180
C7	0.70726	0.84893	0.11722
H8	0.73800	0.78882	0.08839
O9	0.67143	0.85456	0.08457
C10	0.74101	0.81373	0.11663
C11	0.50000	0.00000	0.00000
C12	0.01729	0.85899	0.61001
H13	-0.01608	0.84640	0.59442
H14	0.01147	0.86392	0.64830
H15	0.04413	0.83109	0.60490
C16	-0.03469	0.91013	0.53223
H17	-0.06178	0.90786	0.56025
H18	-0.02892	0.87483	0.51658
H19	-0.04850	0.93351	0.50416



20.00 Angstroms

5.16: COF-105-Eth-trans

Figure S5: 3D-representation

Name

COF-105-Eth-trans

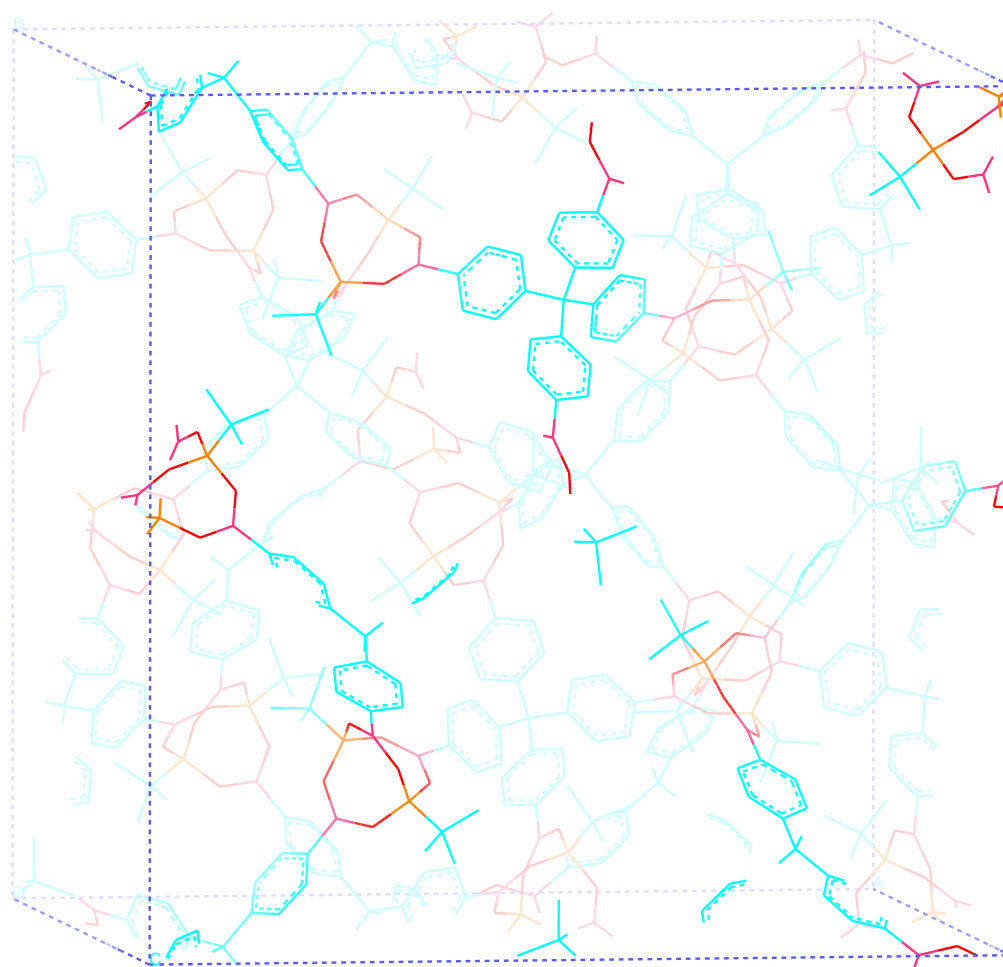
Space group symmetry

I -4 3 d

a = b = c = 35.925 35.925 35.925 A

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.21281	0.20244	0.15966
C2	0.18156	0.22454	0.17137
C3	0.22048	0.24370	0.10564
O4	0.23430	0.25627	0.07309
C5	0.19296	0.26722	0.11898
C6	0.17354	0.25807	0.15143
H7	0.15378	0.27661	0.15964
C8	0.23080	0.21192	0.12549
H9	0.25131	0.19622	0.11389
O10	0.18863	0.29710	0.09647
B11	0.21457	0.29056	0.06656
Si12	0.25000	0.37500	0.00000
C13	0.23661	0.34996	0.03620
C14	0.22094	0.31430	0.03344
H15	0.24032	0.36123	0.06209
H16	0.21538	0.30269	0.00809



15.00 Angstroms

5.17: COF-202

Figure S5: 3D-representation

Name

COF-202

Space group symmetry

I -4 3 d

a = b = c = 29.927 29.927 29.927 Å

alpha = betha = gamma = 90

Atom	x	y	z
C1	0.92551	0.69796	0.21730
C2	0.88866	0.72727	0.21939
C3	0.88889	0.76530	0.19154
C4	0.92449	0.77333	0.16199
C5	0.96088	0.74313	0.15750
C6	0.96063	0.70584	0.18707
H7	0.86329	0.78795	0.19268
H8	0.92703	0.67032	0.23736
H9	0.98650	0.68350	0.18658
H10	0.92318	0.80226	0.14407
C11	0.37500	0.00000	0.25000
Si12	0.73964	0.73964	0.73964
C13	0.82206	0.77388	0.75464
O14	0.74019	0.76139	0.69121
B15	0.71851	0.74997	0.64964
O16	0.68931	0.71237	0.64158
C17	0.66633	0.62131	0.59801
H18	0.83675	0.74044	0.75434
H19	0.84331	0.79501	0.77549
H20	0.67868	0.64878	0.57734
H21	0.69495	0.60130	0.60870
H22	0.64546	0.60015	0.57679
Si23	0.67243	0.67243	0.67243
C24	0.63895	0.63895	0.63895
C25	0.77313	0.77313	0.77313
H26	0.82331	0.78719	0.72066

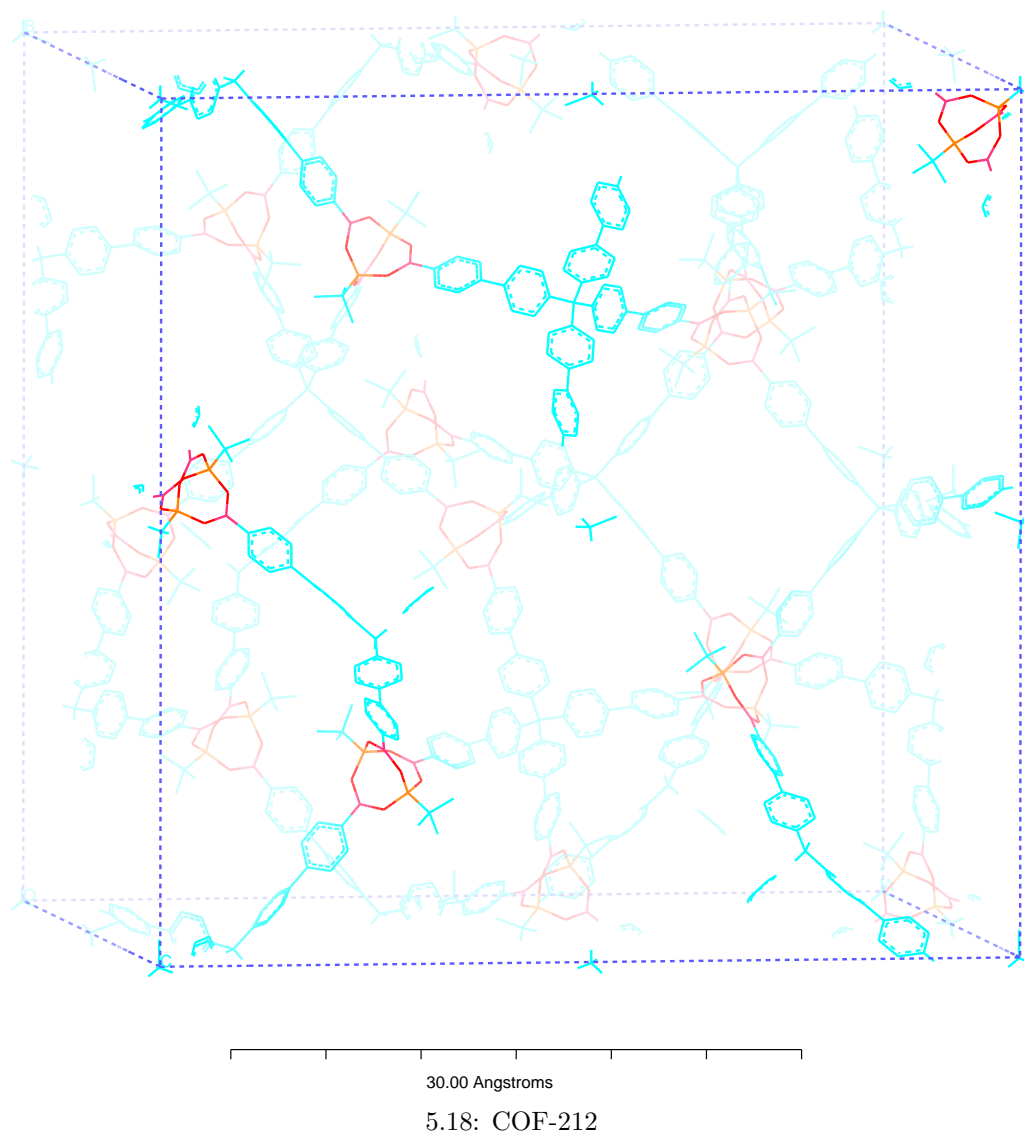


Figure S5: 3D-representation

Name

COF-212

Space group symmetry

I -4 3 d

a = b = c = 45.779 45.779 45.779 A

alpha = betha = gamma = 90

Atom	x	y	z
B1	0.83185	0.71326	0.26588
O2	0.83698	0.69455	0.29078
Si3	0.81669	0.68331	0.31669
C4	0.83857	0.66143	0.33857
C5	0.85418	0.73759	0.22158
C6	0.90523	0.72925	0.20740
C7	0.90817	0.71056	0.23184
C8	0.85707	0.71881	0.24595
C9	0.87782	0.74271	0.20265
Si10	0.77296	0.72704	0.27296
C11	0.75108	0.74892	0.25108
O12	0.80449	0.72709	0.25838
C13	0.88451	0.70543	0.25078
C14	0.94537	0.71082	0.17669
C15	0.92882	0.73425	0.18808
C16	0.93654	0.76288	0.17947
C17	0.95940	0.76773	0.15955
C18	0.97528	0.74434	0.14673
C19	0.96823	0.71584	0.15680
C20	0.76371	0.78068	0.24986
C21	0.85068	0.63508	0.32045
H22	0.88766	0.69174	0.26815
H23	0.92769	0.70056	0.23620
H24	0.92564	0.78056	0.18776
H25	0.83480	0.74780	0.21719
H26	0.87470	0.75627	0.18514
H27	0.94081	0.68974	0.18262
H28	0.97982	0.69813	0.14972
H29	0.96438	0.78888	0.15443
H30	0.86392	0.64249	0.30202
H31	0.83301	0.62146	0.31194
H32	0.86451	0.62119	0.33409
H33	0.78576	0.78097	0.24071
H34	0.75005	0.79459	0.23610
H35	0.76451	0.79061	0.27156
C36	1.00000	0.75000	0.12500

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