1D-2D-3D Transformation Synthesis of Hierarchical Metal-Organic Framework Adsorbent for Multicomponent Alkane Separation

Supplementary Information

1D-2D-3D Transformation Synthesis of Hierarchical Metal-Organic Framework Adsorbent for Multicomponent Alkane Separation

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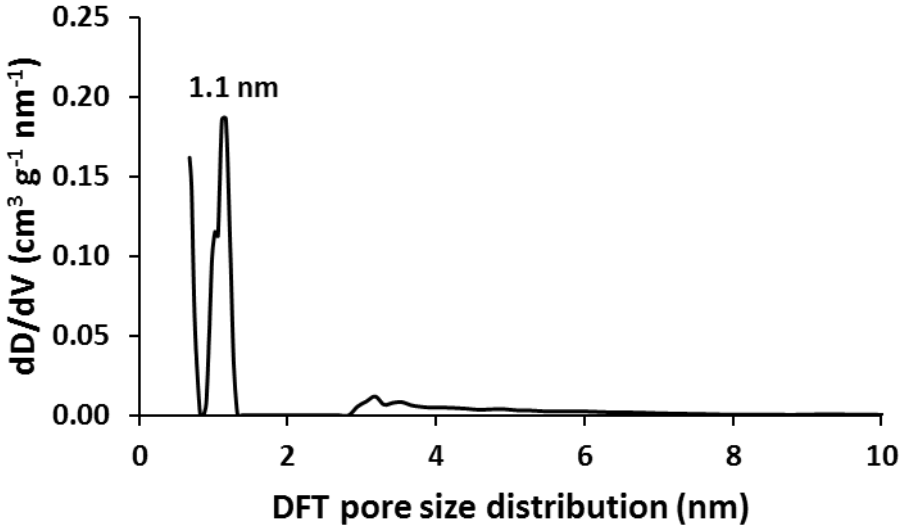

Figure S1. DFT pore size distribution curve of COK-18. Nitrogen adsorption isotherm was recorded on an Autosorb-1 instrument (Quantachrome, USA) at 77 K. The sample was evacuated at 423 K under vacuum for 12 h. The micropore size distribution of COK-18 was extracted from adsorption branch by the Nonlocal Density Functional Theory (NLDFT) adsorption branch.

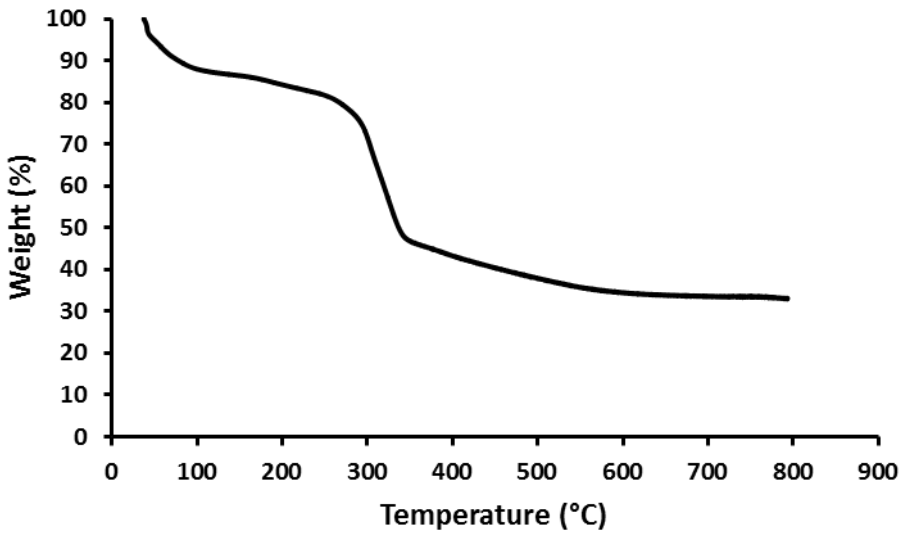

Figure S2. TGA profile of COK-18. TG analysis was performed using a thermogravimetric instrument (TGA, Q500) under N_2 atmosphere at a heating rate of 276 K min^{-1}.

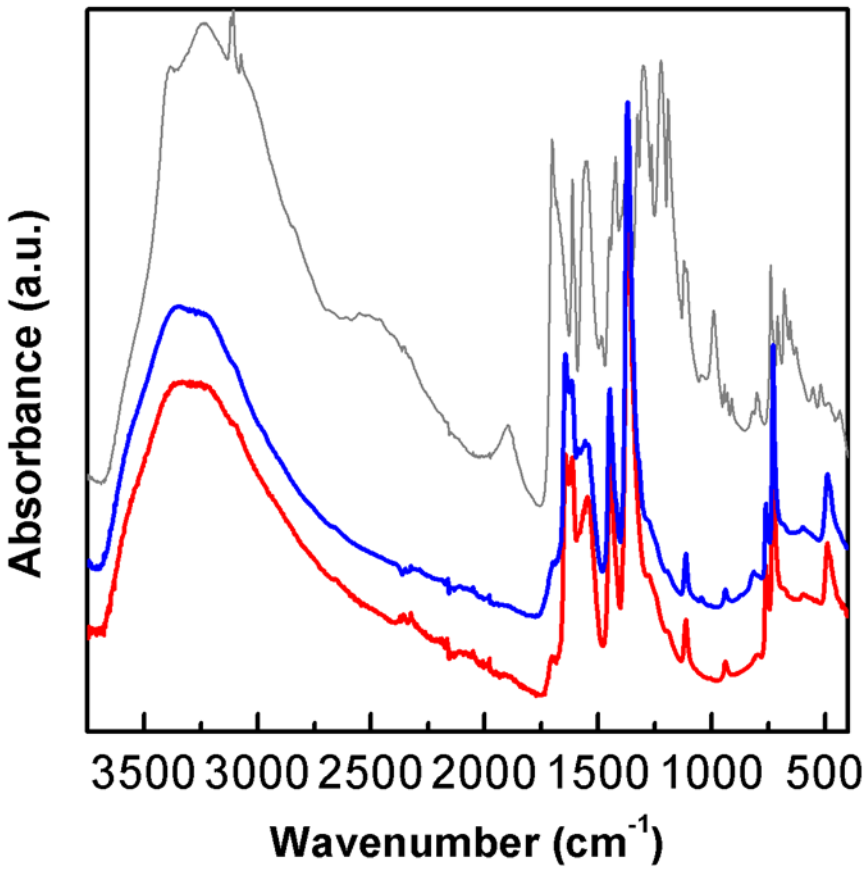

Figure S3. Mid-IR spectra in ATR mode of COK-18, blue curve), HKUST-1 (red curve) and dense H1 precursor (grey curve) in air.

ATR spectrum of H1 phase is very complex, showing very intense bands as in the ν(OH) region (above 2500 cm^{-1}) as in the framework range (below 1700 cm^{-1}), where beside modes due to the aromatic rings of the linker and carboxylate units, also bands ascribable to a large variety of OH bending modes, both related to the solvent and coordinated to some copper species can be considered. The IR profile does not exclude the presence of protonated water inside the cages. ATR spectra of both COK-18 and HKUST-1 are much simpler testifying a formation of a well-defined three dimensional network. The presence of larger pores in case of COK-18 is testified by the stronger absorption in the ν(OH) region observed in this case, due to a larger amount of adsorbed water.

Table S1. Physicochemical properties of COK-18 samples recovered at different solvothermal synthesis time.

COK-18 synthesis time (h)	BET surface area (cm^3 g^{-1})	Langmuir surface area (cm^3 g^{-1})	Total pore volume (cm^3 g^{-1})[a]	Micropore surface area (cm^2 g^{-1})[b]	Micropore volume (cm^3 g^{-1})[c]	Mesopore volume (cm^3 g^{-1})[d]	Mesopore surface area (cm^2 g^{-1})[e]	Average mesopore diamemter (nm)[f]
3	112	146	0.18	87	0.05	0.13	25	23
6	386	533	0.28	364	0.19	0.09	22	20
9	380	513	0.33	331	0.17	0.16	49	13
12	646	892	0.42	613	0.31	0.11	33	15
48	800	1098	0.45	735	0.38	0.07	65	12

[a] The total pore volume is determined by using the adsorption branch of the N_2 isotherm at P/P_0=0.99. [b] The micropore surface area is the t-plot specific micropore surface area calculated from the N_2 adsorption–desorption isotherm. [c] The micropore volume is calculated from t-plot. [d] The mesopore volume is calculated by subtracting the micropore volume from the total pore volume. [e] The mesopore surface area is determined from the external surface area. [f] The average mesopore diameter is determined from the BJH pore size distribution curve obtained in the adsorption branch of the N_2 isotherm.

Table S2. Listing of lattice parametres (refined) and atomic coordinates of H3.

Lattice parametres (refined) and atomic coordinates of H3

Spacegroup P 2_1

a/Å	b/Å	c/Å
18.819(7)	18.585(7)	18.934(4)

α/°	β/°	γ/°
90	100.374(20)	90

atom	x	y	z	occ	atom	x	y	z	occ
C1	0.12886	0.31513	0.9176	1	C30	0.34337	0.25	0.60004	1
C2	0.12886	0.18487	0.9176	1	C31	0.42654	0.31513	0.54692	1
C3	0.15657	0.25	0.89988	1	C32	0.42654	0.18487	0.54692	1
C4	0.07343	0.31513	0.95305	1	C33	0.45426	0.25	0.52921	1
C5	0.07343	0.18487	0.95305	1	C34	0.28266	0.25	0.63882	1
C6	0.04572	0.25	0.97077	1	C35	0.4569	0.38644	0.52753	1
C7	0.21726	0.25	0.86108	1	C36	0.4569	0.11356	0.52753	1
C8	0.04309	0.38644	0.97245	1	O19	0.25757	0.30895	0.65485	1
C9	0.04309	0.11356	0.97245	1	O20	0.50708	0.38644	0.49548	1
O1	0.24235	0.30895	0.84504	1	O21	0.50708	0.11356	0.49548	1
O2	0.99292	0.38644	0.00453	1	O22	0.25757	0.19105	0.65485	1
O3	0.99292	0.11356	0.00453	1	O23	0.4318	0.44539	0.54356	1
O4	0.24235	0.19105	0.84504	1	O24	0.4318	0.05461	0.54356	1
O5	0.06817	0.44539	0.95641	1	Cu1	0.03504	0.97255	0.9776	1
O6	0.06817	0.05461	0.95641	1	O25	0.11212	0.91217	0.92831	1
C10	0.6289	0.31513	0.91765	1	O26	0.10399	0.97255	0.07141	1
C11	0.6289	0.18487	0.91765	1	O27	0.96608	0.97255	0.88378	1
C12	0.65662	0.25	0.89994	1	Cu2	0.53505	0.97255	0.97761	1
C13	0.57345	0.31513	0.95307	1	O28	0.61215	0.91217	0.92835	1
C14	0.57345	0.18487	0.95307	1	O29	0.60398	0.97255	0.07144	1
C15	0.54573	0.25	0.97078	1	O30	0.46612	0.97255	0.88377	1
C16	0.71732	0.25	0.86116	1	Cu3	0.03502	0.02745	0.47757	1
C17	0.5431	0.38644	0.97246	1	O31	0.11206	0.08783	0.42823	1
C18	0.5431	0.11356	0.97246	1	O32	0.10402	0.02745	0.57136	1
O7	0.74241	0.30895	0.84512	1	O33	0.96602	0.02745	0.38378	1
O8	0.49292	0.38644	0.00453	1	Cu4	0.53505	0.02745	0.47761	1
O9	0.49292	0.11356	0.00453	1	O34	0.61216	0.08783	0.42836	1
O10	0.74241	0.19105	0.84512	1	O35	0.60397	0.02745	0.57145	1
O11	0.56819	0.44539	0.95643	1	O36	0.46613	0.02745	0.38377	1
O12	0.56819	0.05461	0.95643	1	Cu5	0.75	0.19511	0.75	1
C19	0.87121	0.31513	0.58249	1	O37	0.75	0.07434	0.75	1
C20	0.87121	0.18487	0.58249	1	O38	0.85625	0.19511	0.77512	1
C21	0.84351	0.25	0.60023	1	O39	0.64375	0.19511	0.72488	1
C22	0.92661	0.31513	0.54701	1	Cu6	0.25	0.19511	0.75	1
C23	0.92661	0.18487	0.54701	1	O40	0.25	0.07434	0.75	1
C24	0.9543	0.25	0.52927	1	O41	0.35625	0.19511	0.77512	1
C25	0.78285	0.25	0.63908	1	O42	0.14375	0.19511	0.72488	1
C26	0.95693	0.38644	0.52758	1					
C27	0.95693	0.11356	0.52758	1					
O13	0.75778	0.30895	0.65514	1					
O14	0.00708	0.38644	0.49547	1					
O15	0.00708	0.11356	0.49547	1					
O16	0.75778	0.19105	0.65514	1					
O17	0.93186	0.44539	0.54364	1					
O18	0.93186	0.05461	0.54364	1					
C28	0.37109	0.31513	0.58234	1					
C29	0.37109	0.18487	0.58234	1					

Table S3. Listing of lattice parametres (refined) and atomic coordinates of H6.

Lattice parametres (refined) and atomic coordinates of H6

Spacegroup P 2_1

a/Å	b/Å	c/Å
20.5883(32)	18.677(6)	19.1884(34)

α/°	β/°	γ/°
90	100.094(14)	90

atom	x	y	z	occ	atom	x	y	z	occ
C1	0.09881	0.31393	0.90009	1	C30	0.37994	0.25	0.6214	1
C2	0.09881	0.18607	0.90009	1	C31	0.44369	0.31393	0.55693	1
C3	0.12006	0.25	0.8786	1	C32	0.44369	0.18607	0.55693	1
C4	0.05631	0.31393	0.94307	1	C33	0.46495	0.25	0.53545	1
C5	0.05631	0.18607	0.94307	1	C34	0.33341	0.25	0.66845	1
C6	0.03506	0.25	0.96455	1	C35	0.46696	0.38393	0.53341	1
C7	0.16659	0.25	0.83155	1	C36	0.46696	0.11607	0.53341	1
C8	0.03304	0.38393	0.96659	1	O19	0.31417	0.30787	0.6879	1
C9	0.03304	0.11607	0.96659	1	O20	0.50543	0.38393	0.49451	1
O1	0.18582	0.30787	0.8121	1	O21	0.50543	0.11607	0.49451	1
O2	0.99457	0.38393	0.00549	1	O22	0.31417	0.19213	0.6879	1
O3	0.99457	0.11607	0.00549	1	O23	0.44773	0.4418	0.55286	1
O4	0.18582	0.19213	0.8121	1	O24	0.44773	0.0582	0.55286	1
O5	0.05227	0.4418	0.94714	1	Cu1	0.02687	0.97306	0.97283	1
O6	0.05227	0.0582	0.94714	1	O25	0.08597	0.91378	0.91307	1
C10	0.59881	0.31393	0.90009	1	O26	0.10597	0.97306	0.0528	1
C11	0.59881	0.18607	0.90009	1	O27	0.94776	0.97306	0.89286	1
C12	0.62006	0.25	0.8786	1	Cu2	0.52687	0.97306	0.97283	1
C13	0.55631	0.31393	0.94307	1	O28	0.58597	0.91378	0.91307	1
C14	0.55631	0.18607	0.94307	1	O29	0.60597	0.97306	0.0528	1
C15	0.53505	0.25	0.96455	1	O30	0.44776	0.97306	0.89286	1
C16	0.66659	0.25	0.83155	1	Cu3	0.02687	0.02694	0.47283	1
C17	0.53304	0.38393	0.96659	1	O31	0.08597	0.08622	0.41307	1
C18	0.53304	0.11607	0.96659	1	O32	0.10597	0.02694	0.5528	1
O7	0.68583	0.30787	0.8121	1	O33	0.94776	0.02694	0.39286	1
O8	0.49457	0.38393	0.00549	1	Cu4	0.52687	0.02694	0.47283	1
O9	0.49457	0.11607	0.00549	1	O34	0.58597	0.08622	0.41307	1
O10	0.68583	0.19213	0.8121	1	O35	0.60597	0.02694	0.5528	1
O11	0.55227	0.4418	0.94714	1	O36	0.44776	0.02694	0.39286	1
O12	0.55227	0.0582	0.94714	1	Cu5	0.75	0.19611	0.75	1
C19	0.90119	0.31393	0.59991	1	O37	0.75	0.07756	0.75	1
C20	0.90119	0.18607	0.59991	1	O38	0.8291	0.19611	0.82997	1
C21	0.87994	0.25	0.6214	1	O39	0.6709	0.19611	0.67003	1
C22	0.94369	0.31393	0.55693	1	Cu6	0.25	0.19611	0.75	1
C23	0.94369	0.18607	0.55693	1	O40	0.25	0.07756	0.75	1
C24	0.96494	0.25	0.53545	1	O41	0.3291	0.19611	0.82997	1
C25	0.83341	0.25	0.66845	1	O42	0.1709	0.19611	0.67003	1
C26	0.96696	0.38393	0.53341	1					
C27	0.96696	0.11607	0.53341	1					
O13	0.81417	0.30787	0.6879	1					
O14	0.00543	0.38393	0.49451	1					
O15	0.00543	0.11607	0.49451	1					
O16	0.81417	0.19213	0.6879	1					
O17	0.94773	0.4418	0.55286	1					
O18	0.94773	0.0582	0.55286	1					
C28	0.40119	0.31393	0.59991	1					
C29	0.40119	0.18607	0.59991	1					

Table S4. Listing of lattice parametres (refined) and atomic coordinates of H9.

Lattice parametres (refined) and atomic coordinates of H9

Spacegroup P 2_1

a/Å	b/Å	c/Å
35.712(5)	18.5569(28)	13.1994(20)

α/°	β/°	γ/°
90	67.698(9)	90

atom	x	y	z	occ	atom	x	y	z	occ
C1	0.09631	0.06394	0.90909	1	C30	0.38298	0	0.61047	1
C2	0.09631	0.93607	0.90909	1	C31	0.44512	0.06394	0.55181	1
C3	0.11702	0	0.88953	1	C32	0.44512	0.93607	0.55181	1
C4	0.05488	0.06394	0.94819	1	C33	0.46583	0	0.53226	1
C5	0.05488	0.93607	0.94819	1	C34	0.33763	0	0.65328	1
C6	0.03417	0	0.96774	1	C35	0.4678	0.13394	0.5304	1
C7	0.16237	0	0.84672	1	C36	0.4678	0.86606	0.5304	1
C8	0.0322	0.13394	0.9696	1	O19	0.31888	0.05787	0.67098	1
C9	0.0322	0.86606	0.9696	1	O20	0.50529	0.13394	0.495	1
O1	0.18112	0.05787	0.82902	1	O21	0.50529	0.86606	0.495	1
O2	0.99471	0.13394	0.005	1	O22	0.31888	0.94213	0.67098	1
O3	0.99471	0.86606	0.005	1	O23	0.44905	0.19181	0.5481	1
O4	0.18112	0.94213	0.82902	1	O24	0.44905	0.80819	0.5481	1
O5	0.05095	0.19181	0.9519	1	Cu1	0.02619	0.72306	0.97528	1
O6	0.05095	0.80819	0.9519	1	O25	0.08379	0.66378	0.9209	1
C10	0.5963	0.56393	0.90909	1	O26	0.02418	0.72306	0.12873	1
C11	0.5963	0.43606	0.90909	1	O27	0.02819	0.72306	0.82183	1
C12	0.61702	0.5	0.88953	1	Cu2	0.52619	0.22306	0.97528	1
C13	0.55488	0.56393	0.94819	1	O28	0.58379	0.16378	0.9209	1
C14	0.55488	0.43606	0.94819	1	O29	0.52418	0.22306	0.12873	1
C15	0.53417	0.5	0.96774	1	O30	0.52819	0.22306	0.82183	1
C16	0.66237	0.5	0.84672	1	Cu3	0.02619	0.27695	0.47528	1
C17	0.5322	0.63394	0.9696	1	O31	0.08379	0.33622	0.4209	1
C18	0.5322	0.36606	0.9696	1	O32	0.02418	0.27695	0.62873	1
O7	0.68112	0.55787	0.82902	1	O33	0.02819	0.27695	0.32183	1
O8	0.49471	0.63394	0.005	1	Cu4	0.52619	0.77695	0.47528	1
O9	0.49471	0.36606	0.005	1	O34	0.58379	0.83622	0.4209	1
O10	0.68112	0.44213	0.82902	1	O35	0.52418	0.77695	0.62873	1
O11	0.55095	0.69181	0.9519	1	O36	0.52819	0.77695	0.32183	1
O12	0.55095	0.30819	0.9519	1	Cu5	0.75	0.44611	0.25	1
C19	0.9037	0.56393	0.59091	1	O37	0.75	0.32755	0.25	1
C20	0.9037	0.43606	0.59091	1	O38	0.74967	0.44611	0.4018	1
C21	0.88298	0.5	0.61047	1	O39	0.75033	0.44611	0.0982	1
C22	0.94512	0.56393	0.55181	1	Cu6	0.75	0.55389	0.75	1
C23	0.94512	0.43606	0.55181	1	O40	0.75	0.67245	0.75	1
C24	0.96583	0.5	0.53226	1	O41	0.74967	0.55389	0.9018	1
C25	0.83763	0.5	0.65328	1	O42	0.75033	0.55389	0.5982	1
C26	0.9678	0.63394	0.5304	1					
C27	0.9678	0.36606	0.5304	1					
O13	0.81888	0.55787	0.67098	1					
O14	0.00529	0.63394	0.495	1					
O15	0.00529	0.36606	0.495	1					
O16	0.81888	0.44213	0.67098	1					
O17	0.94905	0.69181	0.5481	1					

Table S5. Listing of lattice parametres (refined) and atomic coordinates of H12.

Lattice parametres (refined) and atomic coordinates of H12

Spacegroup P n $2_{1\,m}$

a/Å	b/Å	c/Å
26.059(5)	18.574(5)	19.751(4)

α/°	β/°	γ/°
90	90	90

atom	x	y	z	occ
C1	0.60363	0.81387	0.1645	1
C2	0.60363	0.68613	0.1645	1
C3	0.62592	0.75	0.14611	1
C4	0.55906	0.81387	0.20128	1
C5	0.55906	0.68613	0.20128	1
C6	0.53677	0.75	0.21967	1
C7	0.67473	0.75	0.10584	1
C8	0.53465	0.88381	0.22141	1
C9	0.53465	0.61619	0.22141	1
O1	0.6949	0.80781	0.0892	1
O2	0.49431	0.88381	0.2547	1
O3	0.49431	0.61619	0.2547	1
O4	0.6949	0.69219	0.0892	1
O5	0.55483	0.94162	0.20477	1
O6	0.55483	0.55838	0.20477	1
C10	0.88982	0.81387	0.81982	1
C11	0.88982	0.68613	0.81982	1
C12	0.86613	0.75	0.83483	1
C13	0.93722	0.81387	0.78979	1
C14	0.93722	0.68613	0.78979	1
C15	0.96091	0.75	0.77477	1
C16	0.81424	0.75	0.86771	1
C17	0.96316	0.88381	0.77334	1
C18	0.96316	0.61619	0.77334	1
O7	0.79279	0.80781	0.8813	1
O8	0.00605	0.88381	0.74616	1
O9	0.00605	0.61619	0.74616	1
O10	0.79279	0.69219	0.8813	1
O11	0.94171	0.94162	0.78694	1
O12	0.94171	0.55838	0.78694	1
Cu1	0.52818	0.47308	0.22675	1
O13	0.59017	0.41386	0.17561	1
O14	0.56887	0.47308	0.31262	1
O15	0.48749	0.47308	0.14089	1
Cu2	0.02996	0.52692	0.73102	1
O16	0.09587	0.58614	0.68925	1
O17	0.06319	0.52692	0.8223	1
O18	0.99673	0.52692	0.63973	1
Cu3	0.25	0.1922	0.47	0.5
Cu4	0.25	0.3078	0.47	0.5
O19	0.25	0.4178	0.47	0.5
O20	0.25	0.0822	0.47	0.5

Table S6. Listing of lattice parametres (refined) and atomic coordinates of as made COK-18.

Lattice parametres (refined) and atomic coordinates of as made COK-18

Spacegroup I m m m

a/Å	b/Å	c/Å
18.6756(26)	18.6311(26)	26.296(7)

α/°	β/°	γ/°
90	90	90

atom	x	y	z	occ	uiso
Cu1	0.791(8)	0.791(8)	0.291(8)	1	0.036(5)
Cu2	0.0742(17)	0.5	0	1	0.042(4)
C6	0.063528(0)	0.66054(24)	0.14129(11)	0.5	0.05714
C7	-0.0635280(0)	0.66054(24)	0.14129(11)	0.5	0.05714
C8	0	0.6407(5)	0.11938(22)	1	0.04679
C9	0.0635280(0)	0.70032(24)	0.18510(11)	0.5	0.05714
C10	-0.0635280(0)	0.70032(24)	0.18510(11)	0.5	0.05714
C11	0	0.7202(5)	0.20701(22)	1	0.04679
C12	0	0.5971(10)	0.0714(5)	1	0.05908
C13	0.1330830(0)	0.7221(5)	0.20909(23)	0.5	0.10449
C14	-0.1330830(0)	0.7221(5)	0.20909(23)	0.5	0.10449
O15	0.0574990(0)	0.5791(12)	0.0516(6)	0.5	0.07741
O16	0.1330830(0)	0.7581(9)	0.2488(4)	0.5	0.11434
O17	-0.1330830(0)	0.7581(9)	0.2488(4)	0.5	0.11434
O18	-0.0574990(0)	0.5791(12)	0.0516(6)	0.5	0.07741
O19	0.1905830(0)	0.70410(28)	0.18926(13)	0.5	0.16206
O20	-0.1905830(0)	0.70410(28)	0.18926(13)	0.5	0.16206
ocu1	0.839(3)	0.841(5)	0.353(7)	1	0.30862
ocu2	0.775(4)	0.853(8)	0.230(8)	1	0.53957
ocu4	0.200(2)	0.5	0	1	0.025
ocu3	0.289(3)	-0.208(6)	0.166(6)	0.942(5)	0.025
ow1	0.1206(30)	-0.098(4)	0.560(8)	0.992(14)	0.090(25)
ow2	0.587(5)	0.581(10)	0.368(11)	0.964(12)	0.0620(8)
ow3	0.4075(11)	0.873(5)	0.088(3)	0.912(14)	0.041(10)
ow4	0.5	0	0	0.994(6)	0.0920(9)

Table S7. Listing of lattice parametres (refined) and atomic coordinates of activated COK-18.

Lattice parametres (refined) and atomic coordinates of activated COK-18

Spacegroup I m m m

a/Å	b/Å	c/Å
18.5853(24)	18.5547(8)	26.382(4)

α/°	β/°	γ/°
90	90	90

atom	x	y	z	occ	uiso
Cu1	0.2841(5)	0.78774(32)	0.19192(29)	1	0.0119(9)
Cu2	0.0677(9)	0.5	0	1	0.0361(5)
C3	0.063837(0)	0.66080(30)	0.14505(25)	1	0.0276(7)
C4	0	0.6370(4)	0.12522(28)	1	0.0263(6)
C5	0.063837(0)	0.70847(29)	0.18471(25)	1	0.0276(7)
C6	0	0.7323(4)	0.20454(28)	1	0.0263(6)
C7	0	0.5848(6)	0.0818(4)	1	0.03072(9)
O8	0.05777(0)	0.5632(7)	0.0639(4)	1	0.03537(11)
O9	0.133735(0)	0.7346(4)	0.20642(28)	1	0.042(5)
O10	0.1567(4)	0.7087(7)	0.2466(4)	1	0.092(7)
O11	0.1685(4)	0.7820(6)	0.1842(5)	1	0.092(7)
oh	0.2769(5)	0.69613(34)	0.2418(5)	1	0.058(8)

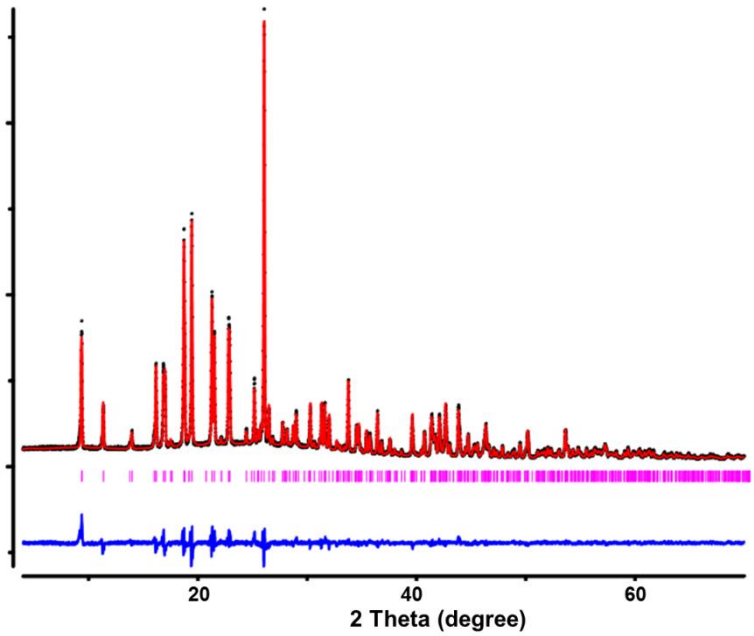

Figure S4a. Rietveld refinement of H1 phase. Observed (dots) and calculated (solid line) patterns and positions for Bragg-reflections (vertical bars).

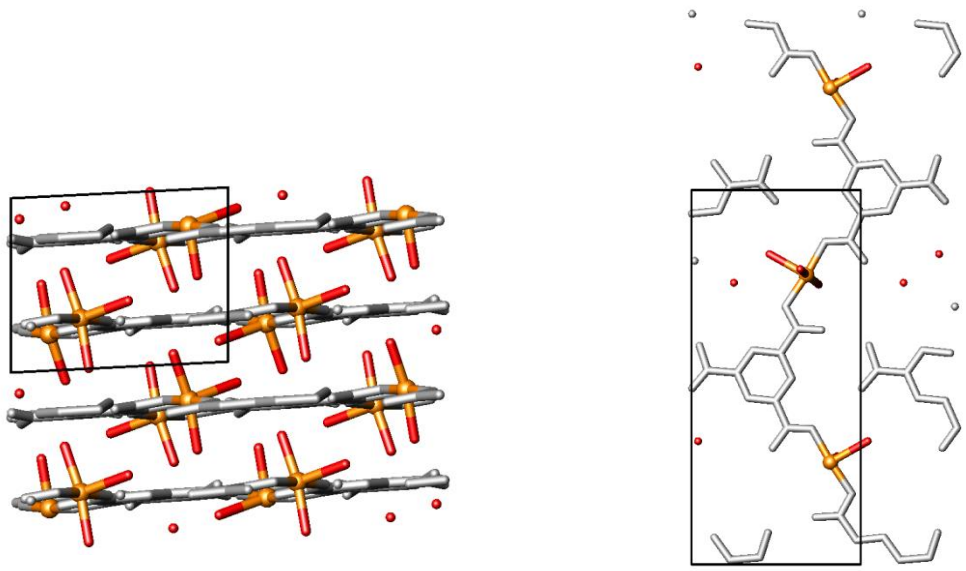

Figure S4b. Structure of H1.

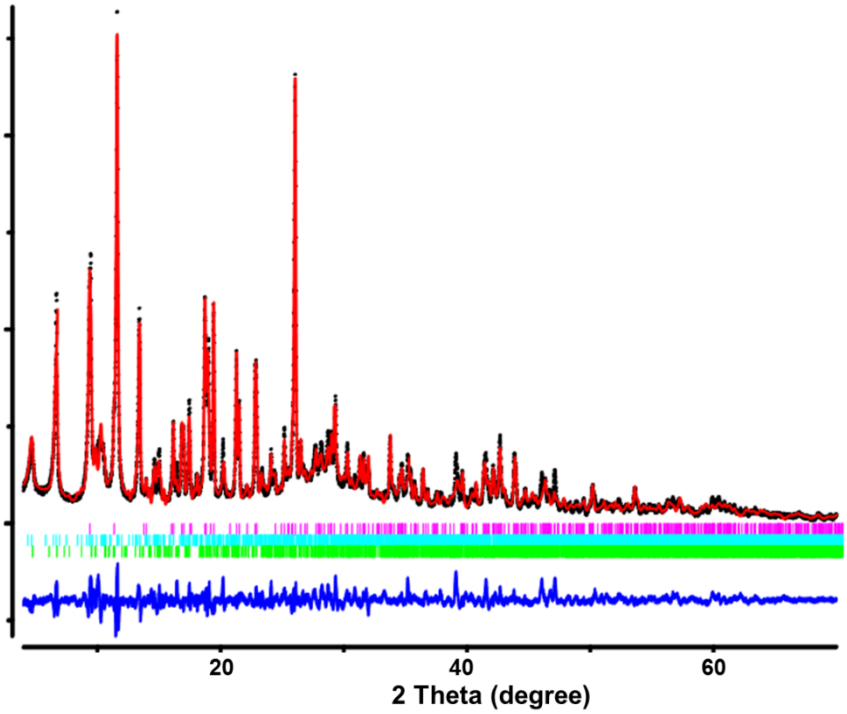

Figure S5a. Rietveld refinement after 3h.. Observed (dots) and calculated (solid line) patterns and positions for Bragg-reflections (vertical bars).

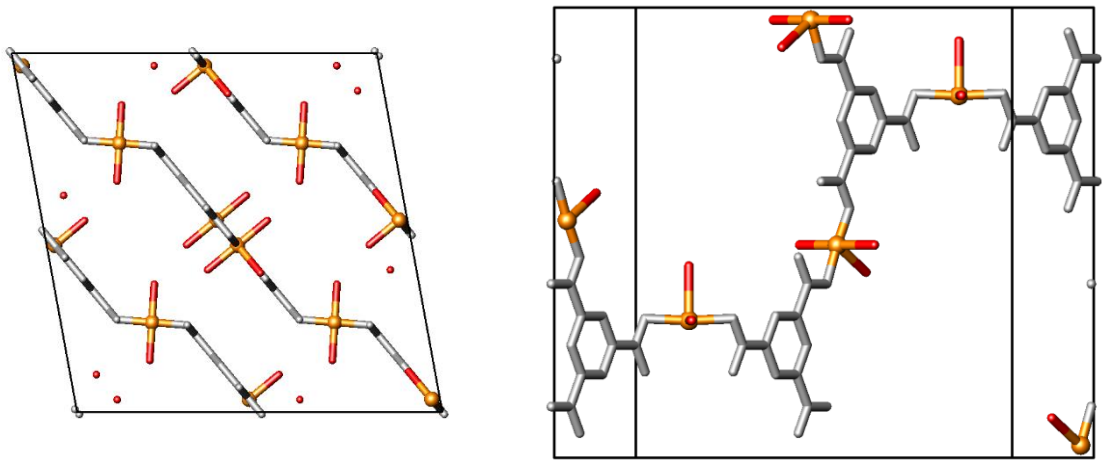

Figure S5b. Structure of H3, dominant phase after 3h

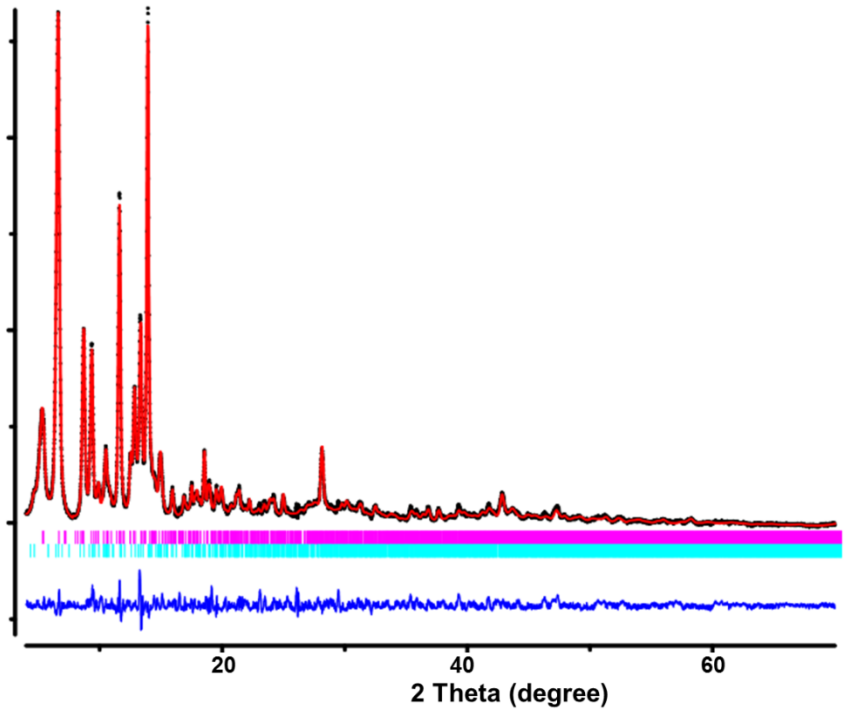

Figure S6a. Rietveld refinement after 6h. Observed (dots) and calculated (solid line) patterns and positions for Bragg-reflections (vertical bars).

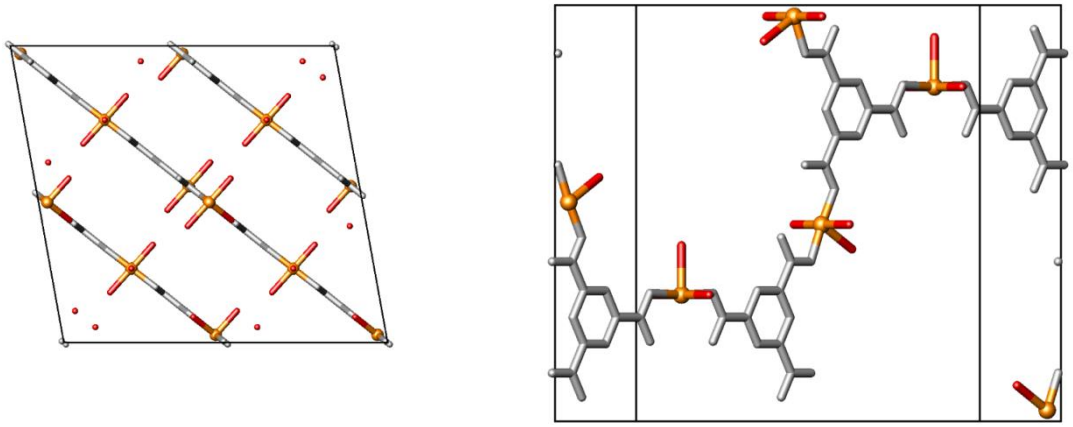

Figure S6b. Structure of H6, dominant phase after 6h

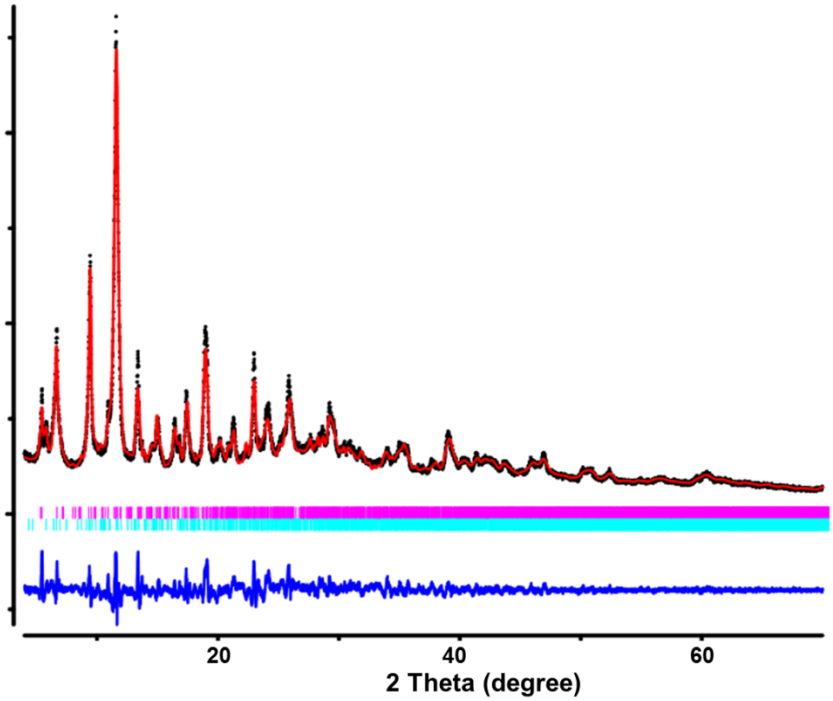

Figure S7a. Rietveld refinement after 9h. Observed (dots) and calculated (solid line) patterns and positions for Bragg-reflections (vertical bars).

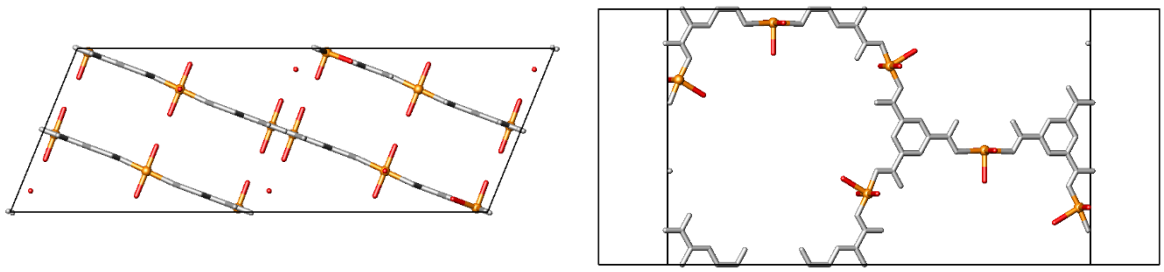

Figure S7b. Structure of H9, dominant phase after 9h

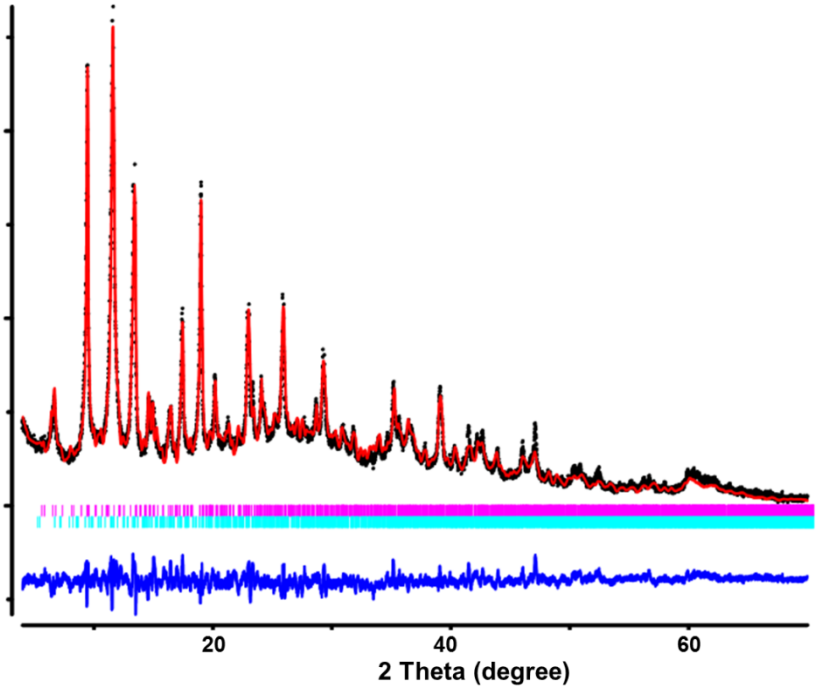

Figure S8a. Rietveld refinement after 12h. Observed (dots) and calculated (solid line) patterns and positions for Bragg-reflections (vertical bars).

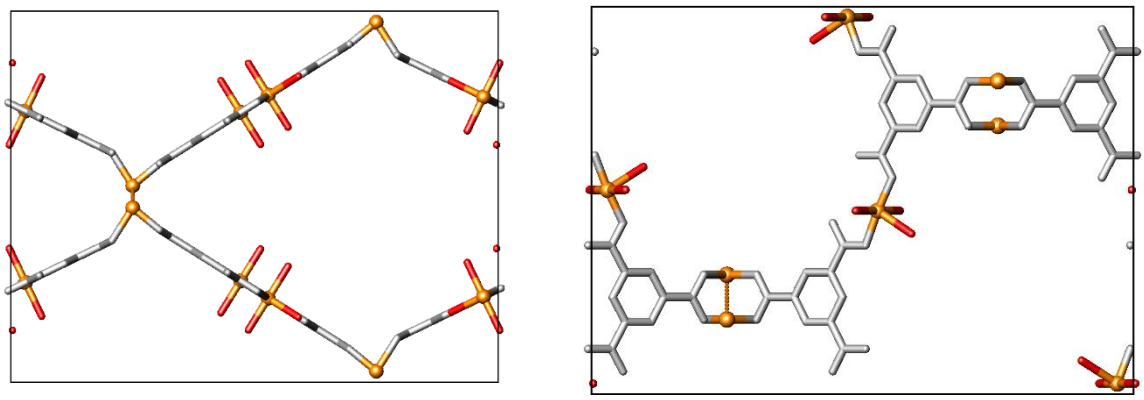

Figure S8b. Structure of H12, dominant phase after 12h

Table S8. Reliability factor and phase content of COK-18 at different synthesis times.

		synthesis time					
		0 h	**3 h**	**6 h**	**9 h**	**12 h**	**48 h**
reliability factors/%	**R_p**	5.5	7.19	6.74	7.65	8.42	4.21
	R_{wp}	7.81	9.55	8.8	9.35	10.03	6.56
phase content/%	**H1**	100					
	H3	66	16	18			
	H6			85	15		
	H9			22	78		
	H12				24	76	
	COK-18						100

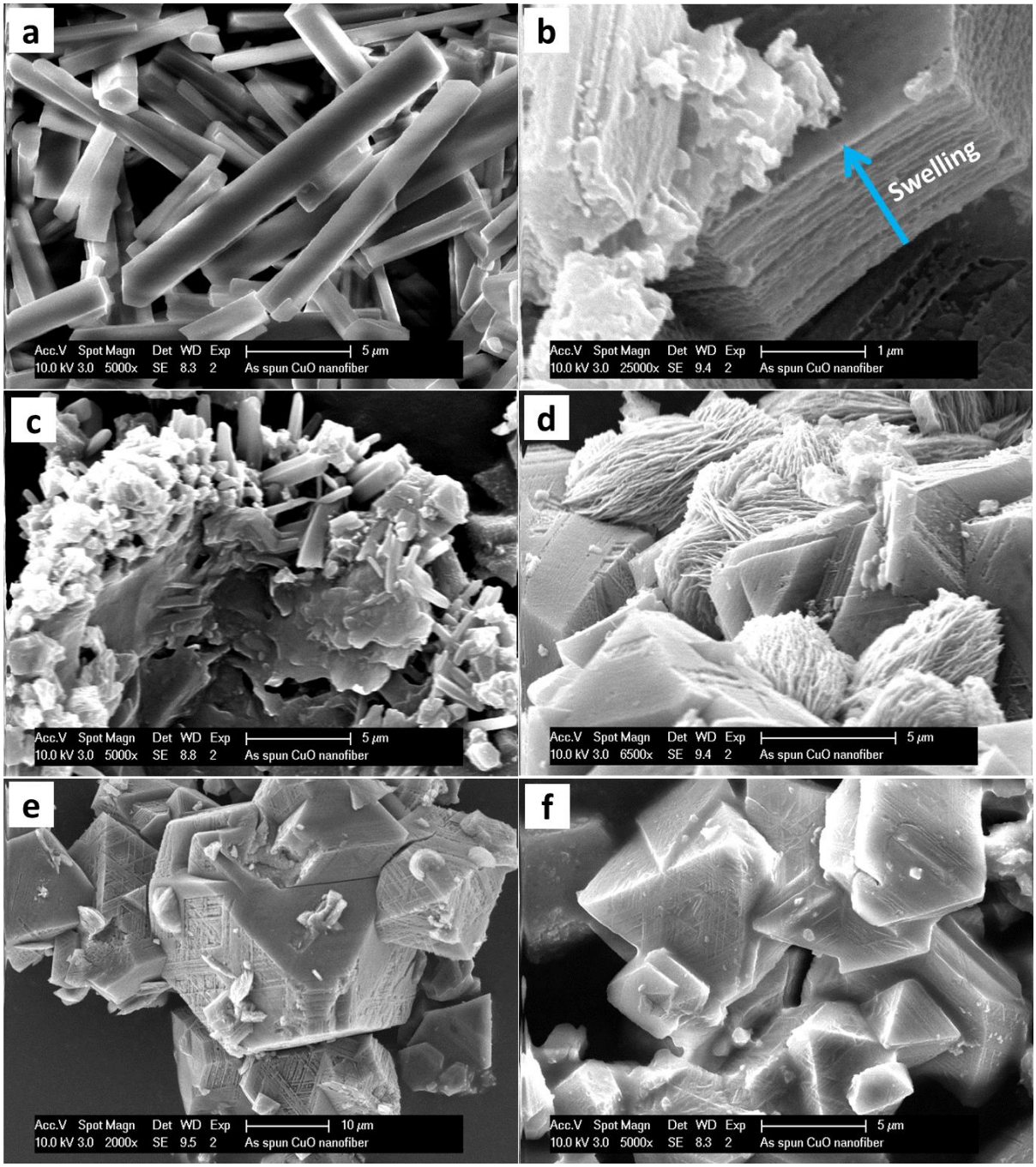

Figure S9. SEM images of (a) H1= dense crystalline CuBTC precursor phase, (b) H3= CuBTC intermediate phase obtained after 3h, (c) H6= CuBTC intermediate phase obtained after 6h, (d) H9= CuBTC intermediate phase obtained after 9h, (e) H12= CuBTC intermediate phase obtained after 12h and (f) H48= COK-18 obtained after 48h.

Table S9. Values of enthalpy, entropy and free Gibbs adsorption energies and partition coefficients $\alpha_{hexane/X}$ of the studied alkanes obtained from the variable temperature pulse gas chromatographic studies using HKUST-1 as chromatographic bed. The free energy was calculated using $\Delta G = \Delta H_{iso} - T\Delta S$.

Studied alkanes	$-\Delta H_{diff}$ (kJ mol^{-1})	$-\Delta H_{iso}$ (kJ mol^{-1})	$-\Delta S$ (J K^{-1} mol^{-1})	$-\Delta G$ (kJ mol^{-1})	$\alpha_{hexane/X}$ (x)
propane	13.4	16.8	48.9	-3.35	15.7
butane	25.5	28.9	72.4	-1.01	8.15
pentane	34.4	37.8	86.7	2.04	3.28
2-methylbutane	35.4	38.8	89.0	2.07	3.28
n-hexane	35.2	38.6	78.7	6.13	1.00
2-methylpentane	38.6	42.1	88.0	5.74	1.12
3-methylpentane	34.9	38.3	78.4	5.90	1.07
2,2-dimethylbutane	40.9	44.3	93.6	5.64	1.15
2,3-dimethylbutane	29.9	33.3	67.1	5.58	1.18