Electronic Supplementary Information (ESI)

Covalent Triazine Frameworks for the Dynamic Adsorption/Separation of Benzene/Cyclohexane Mixtures

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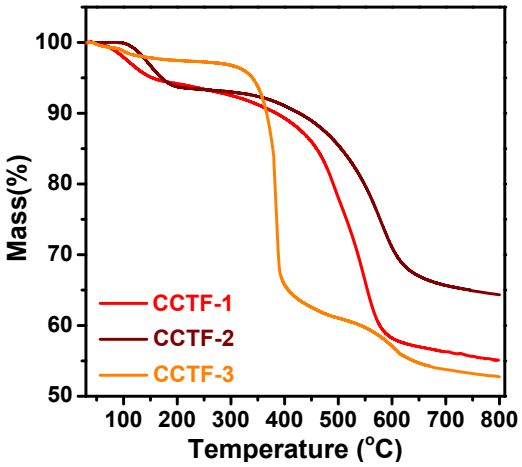

Fig. S1 The TGA curves of CCTF-1, CCTF-2, and CCTF-3.

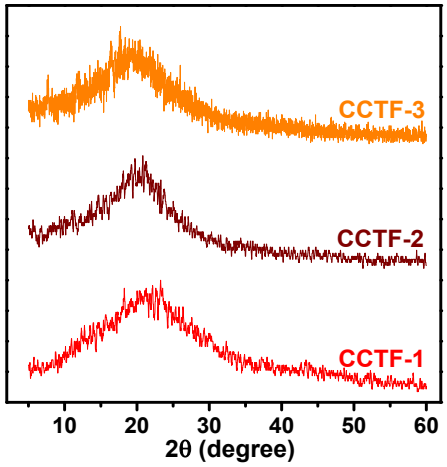

Fig. S2 X-ray diffractions of CCTFs.

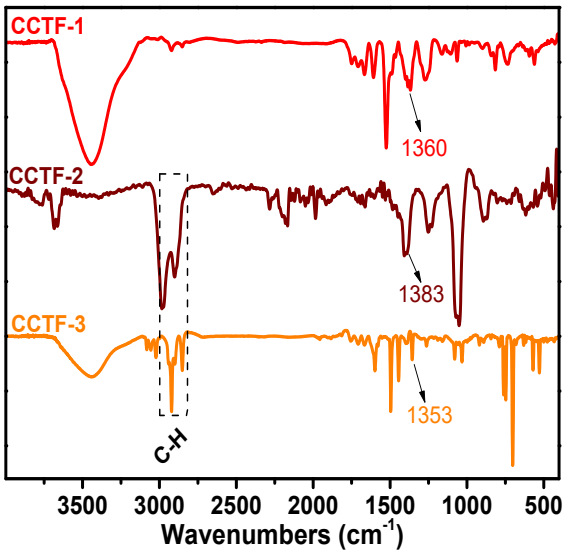

Fig. **S3** The FT-IR spectrum of CCTF-1, CCTF-2, and CCTF-3.

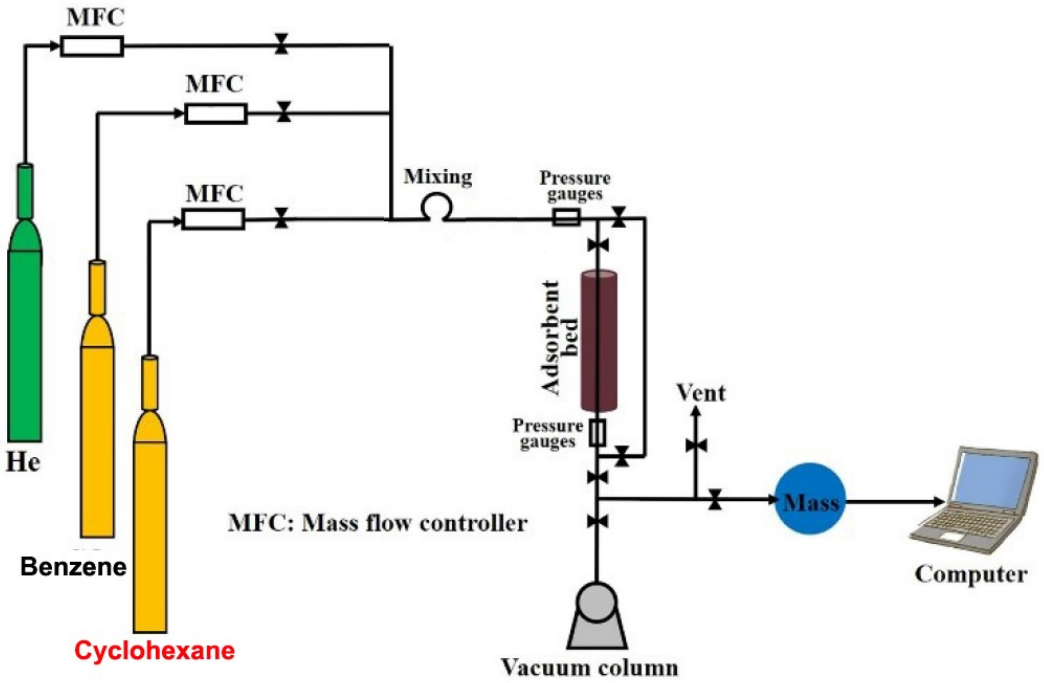

Fig S4. Scheme of the dynamic breakthrough apparatus.

The adsorption amount of adsorbent n is calculated according to the equation S1 as:

$$Q_{nad} = Q_{nin} - Q_{nout} = q_{in} \times C_{n0} \times \Delta T - \int_0^t [(q/(1 - \sum_1^N C_{nt}))] * C_{nt} dt \qquad \text{S1}$$

Q_{nad} is the adsorption amount of adsorbent n; Q_{nin} is total flow rate of adsorbent n flowing in of the penetrating column at ΔT; Q_{nout} is total flow rate of adsorbent n flowing out of the penetrating column at ΔT; q_{in} is total flow rate of gas through the column inlet; C_{n0} is the total flow rate of gas through the outlet of the column; ΔT is the total adsorption time (min); q is the flow rate of carrier gas; C_{nt} is the percentage concentration of adsorbent N at the entrance of the penetrating column;

The selectivity of gas (1) over gas (2) is calculated according to the equation S2 as:

$$\mathrm{S} = (\frac{X_1}{Y_1}) \div (\frac{X_2}{Y_2}) \qquad \text{S2}$$

X_1/Y_1: Molar fraction of component 1 in the adsorbed phase/molar fraction of component 1 in the gas phase

X_2/Y_2: Molar fraction of component 2 in the adsorbed phase/molar fraction of component 2 in the gas phase

The diffusion coefficient of vapor

$$\mathrm{D} = \frac{L^2}{6t_{eq}} \quad \text{S3}$$

D is the diffusion coefficient of vapor; L is the loading length; t_{eq} is the delay time.

Table S1. Comparison of uptakes of benzene and cyclohexane vapors, Bz/Cy selectivity between CCTFs, and other porous materials reported in the literature

Samples	S_{BET} (m^2/g)	Bz (mg/g)	Cy (mg/g)	Ideal Bz/Cy Selectivity	Ref
CCTF-1	512	878	441	1.99	This work
CCTF-2	538	650	311	2.09	This work
CCTF-3	207	136	61	2.23	This work
PAF-2	891	138	7	19.71	[1]
Hybrid[3]arene	0.9	80.4	7.5	10.72	[2]
MALP-1	1179	585	492	1.19	[3]
MALP-2	1126	545	472	1.15	[3]
MALP-3	1141	571	488	1.17	[3]
MALP-4	1093	558	465	1.20	[3]
CE-P1	630	478	-	-	[4]
CE-P2	195	151	-	-	[4]
PAN-1	925	726	527	1.38	[5]
PAN-2	1242	692	383	1.81	[5]
PAN-F	702	544	433	1.26	[6]
PAN-T	795	570	518	1.10	[6]
CMP-S-1	873	647.4	378	1.71	[7]
MP1	1020	765	440	1.74	[8]
PCN-AD	843	980	574	1.71	[9]
PBI-Ad-1	1023	980	536	1.83	[10]
PBI-Ad-2	926	765	463	1.65	[10]
PCN-TPC	686	176	74	2.38	[11]
PCN-TPPC	662	778	107	7.27	[11]
UMC-600	1980	663	527	1.26	[12]
UMC-700	2212	735	605	1.21	[12]
UMC-800	2406	868	734	1.18	[12]
FJU-P6	1066	630.4	313.6	2.01	[13]
FJU-P7	1425	768.6	640.4	1.20	[13]
PCN-TA	721	1009	206	4.90	[14]
PCN-TC	674	867	244	3.55	[14]
PCN-DC	393	635	129	4.92	[14]
POP-1	486	1020	658	1.55	[15]
MPI-1	1454	1198	501	2.39	[16]
MPI-2	814	766	448	1.71	[16]
MPI-3	586	549	415	1.32	[16]
sPI-1	1108	1597	851	1.88	[17]
sPI-2	900	1760	778	2.26	[17]

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