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Supplementary Information

Highly Selective Absorption of Polychloromethanes in Perhydroxylated Cucurbit[6]uril-based Supramolecular Assemblies

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EXPERIMENTAL SECTION

Vapour absorption studies for A and B

The required solid compounds (**A** or **B**; 0.5 – 1.0 g) contained in a tared open glass phial was added to a sealed glass vessel which was then evacuated with the aid of a vacuum pump. Pumping was continued until the sample achieved constant weight. A second open container containing a few mL of the volatile liquid, chosen in turn from acetonitrile, methanol, ethanol, acetone, ethoxyethane, dichloromethane, trichloromethane or tetrachloromethane, was then added and the vessel resealed. The weight change of the sample was then determined at ~0.25-1h intervals within 15 hours to obtain the vapour absorption profile.

Table S1 Volatile compounds absorption profile of the porous compounds **A** and **B**

Absorption capacities (gram/per gram)	**A**	**B**
tetrachloromethane	0.44	0.06
trichloromethane	0.30	0.30
acetonitrile	0.23	0.02
dichloromethane	0.22	0.34
ethoxyethane	0.20	0.12
ethanol	0.14	0.30
acetone	0.10	0.03
methanol	0.06	0.16

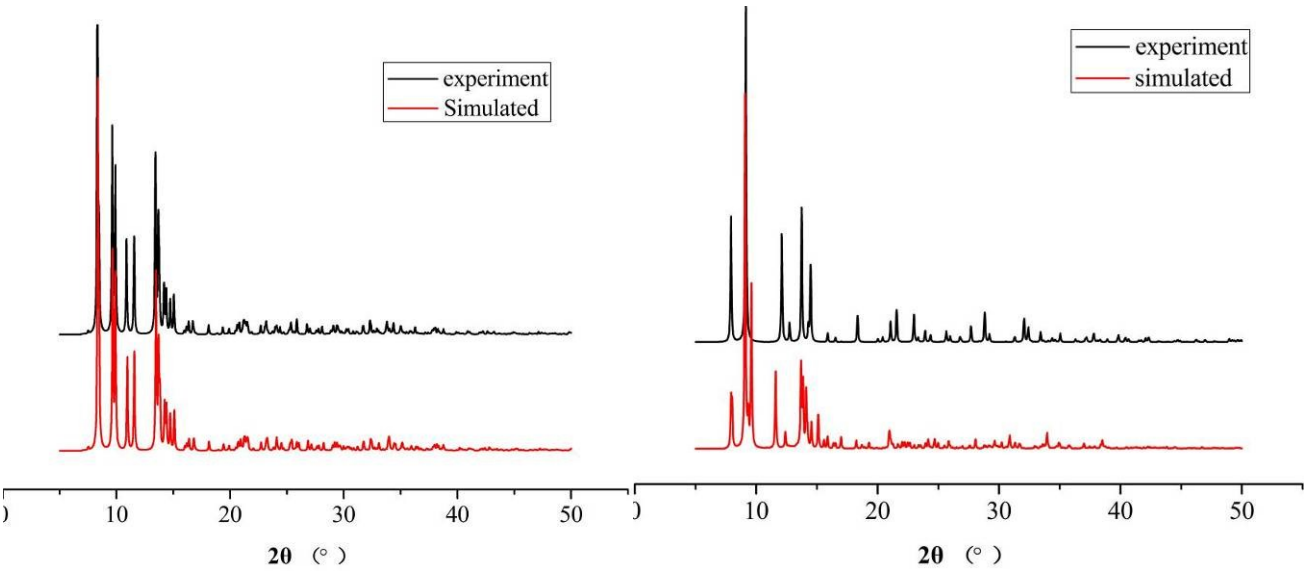
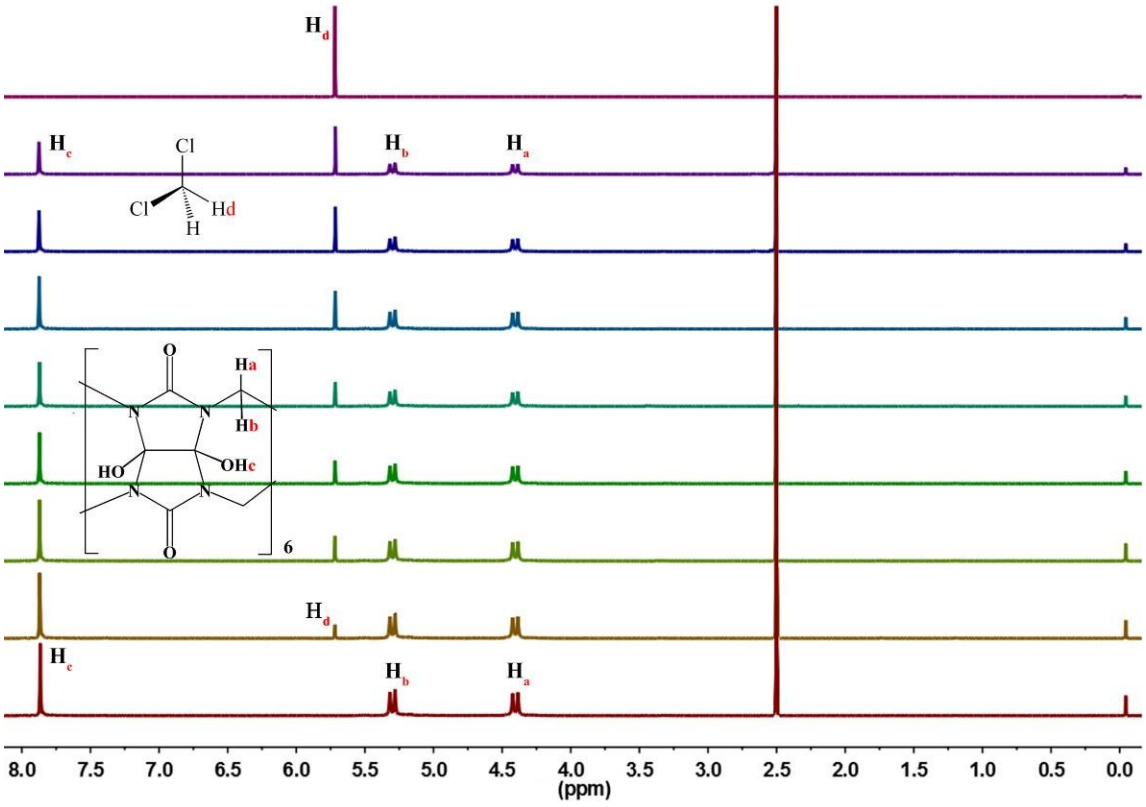


Figure S1 Powder X-ray diffraction (PXRD) of **A** and **B**, respectively



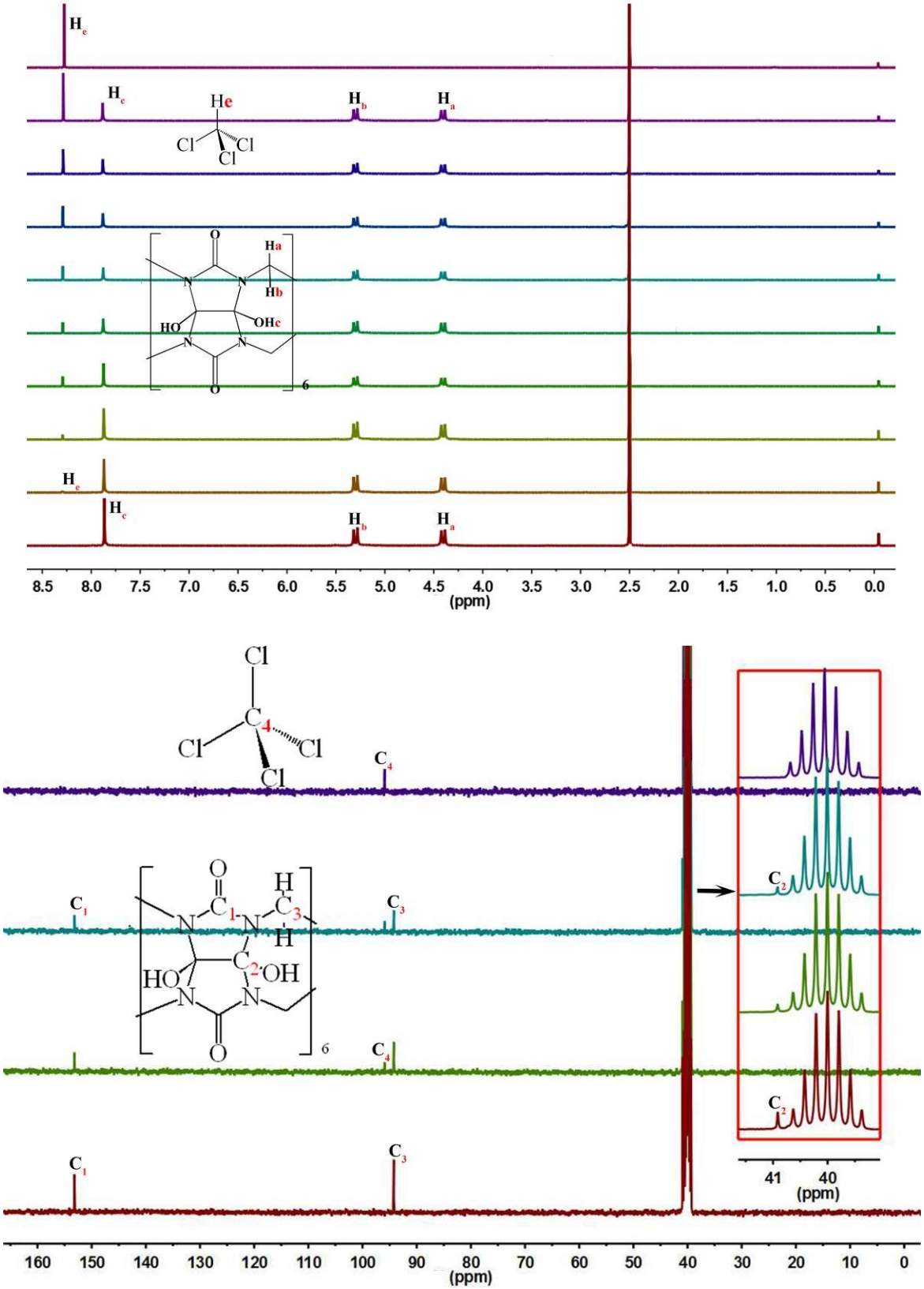


Figure S2 Titration ^{1}H NMR spectra of $(HO)_{12}Q[6]$ with increasing amount of (a) dichloromethane; (b) trichloromethane; (c) titration ^{13}C NMR spectra of $(HO)_{12}Q[6]$ with increasing amount of tetrachloromethane in $DMSO_{d6}$ at 20°C.

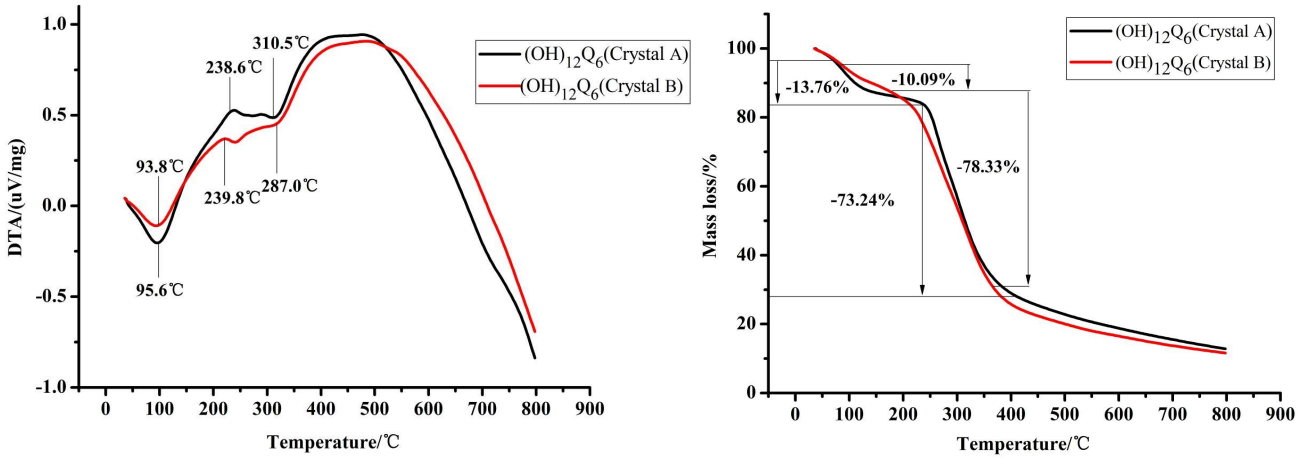


Figure S3 DTA (left) and TG (right) curves of compounds **A**，**B** in N_2 respectively.

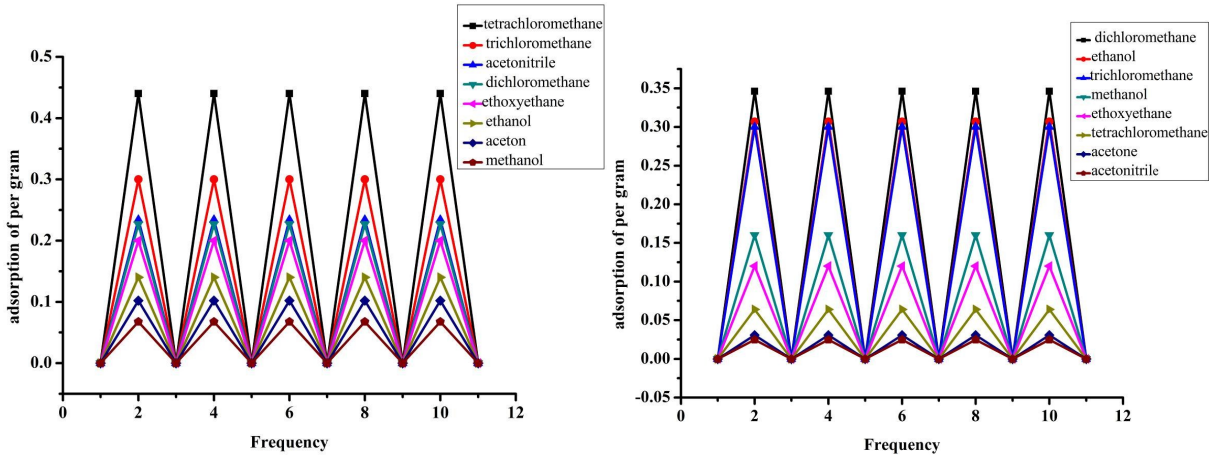


Figure S4 lifetime experiments for the selected absorbates on **A** and **B** in five cycles

Table S2 Crystallographic data forcompounds **A** and **B**

Compounds	A	B
empirical formula	$C_{36}H_{80}N_{24}O_{46}$	$C_{36}H_{86}N_{24}O_{49}$
formula weight	1585.24	1639.29
crystal system	triclinic	monoclinic
space group	*P*–1	*C* 2/c
a(Å)	11.3453(13)	15.359(12)
b(Å)	12.5873(15)	21.896(12)
c (Å)	13.3419(16)	18.644(12)
α(°)	61.922(4)	90.00
β(°)	83.098(4)	100.105(12)
γ (°)	69.125(4)	90.00
V(Å^3)	1568.1(3)	6172(7)
Z	1	4
D_{calcd}(g·cm^{-3})	1.641	1.706
μ(MoKα)(mm^{-1})	0.151	0.157
T(K)	223(2)	223(2)
Unique reflns	5505	5494
Obsd reflns	4508	3217
Params	379	381
R_{int}	0.0365	0.1298
R [I > 2σ(I)][a]	0.0956	0.0998
wR[I>2σ(I)][b]	0.3087	0.3802
R [all data][a]	0.1074	0.1694
*w*R[all data][b]	0.3280	0. 4026
GOF on F^2	1.479	1.478

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = |\Sigma w(|F_o|^2 - |F_c|^2)|/\Sigma|w(F_o)^2|^{1/2}$, where $w = 1/[^2(F_o^2) + (aP)^2 + bP]$; $P = (F_o^2 + 2F_c^2)/3$.