Electronic Supplementary Material (ESI) for RSC Advances.

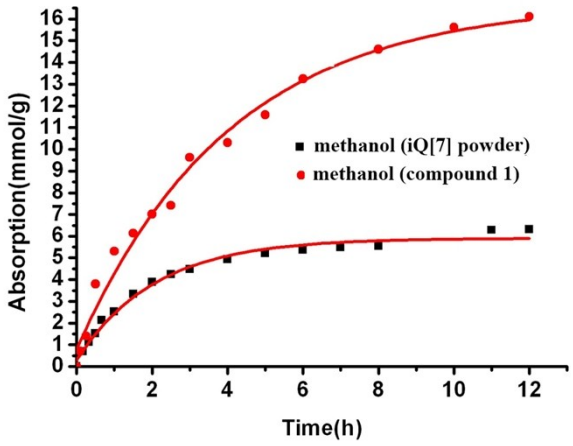
Supporting Information

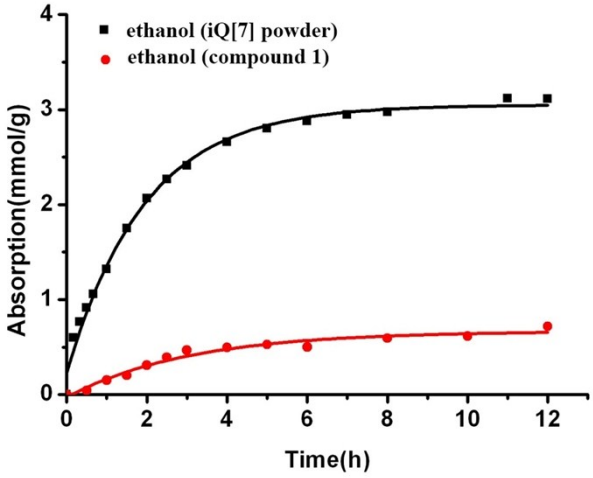
Supramolecular Assemblies Constructed from Inverted Cucurbit[7]uril and Lanthanide Cations: Synthesis, structure and sorption properties.

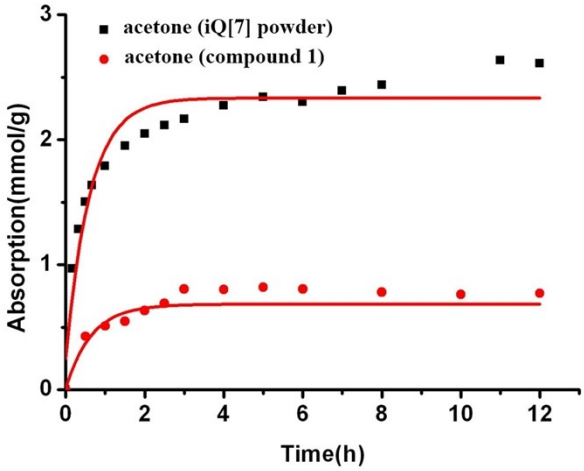
Qing Li,[a] Sheng-Chao Qiu,[a] Yun-Qian Zhang,[a] Sai-Feng Xue,[a] Zhu Tao,[a] Timothy J. Prior,[b] Carl Redshaw,[b*] Qian-Jiang Zhu,*[a] Xin Xiao *[a]

[a]Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China

[b]Department of Chemistry, University of Hull, Hull, HU6 7RX, U.K.


methanol (iQ[7] powder)
methanol (compound 1)
Absorption(mmol/g)
Time(h)


ethanol (iQ[7] powder)
ethanol (compound 1)
Absorption(mmol/g)
Time(h)


acetone (iQ[7] powder)
acetone (compound 1)
Absorption(mmol/g)
Time(h)

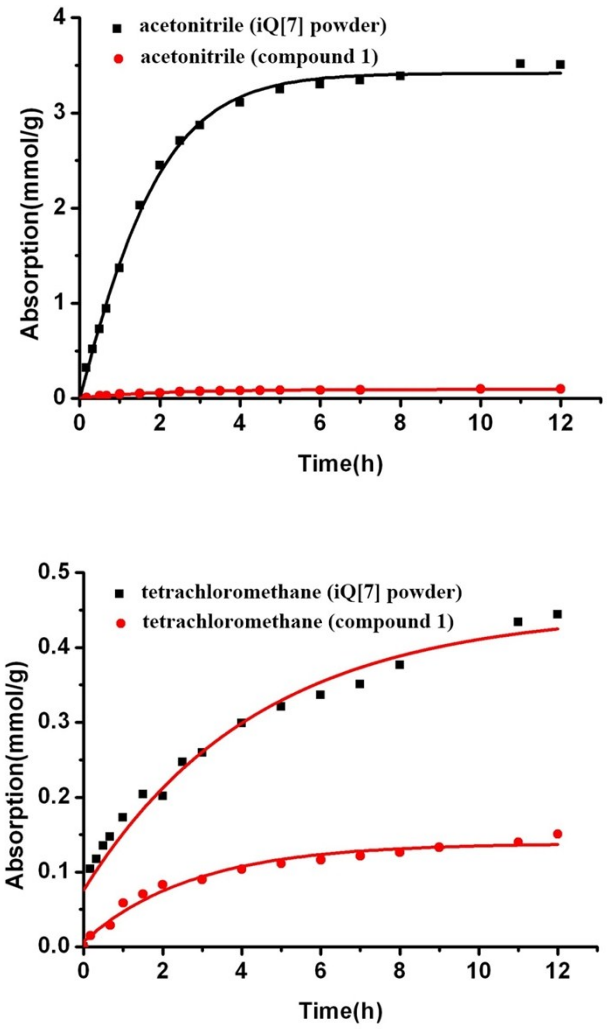
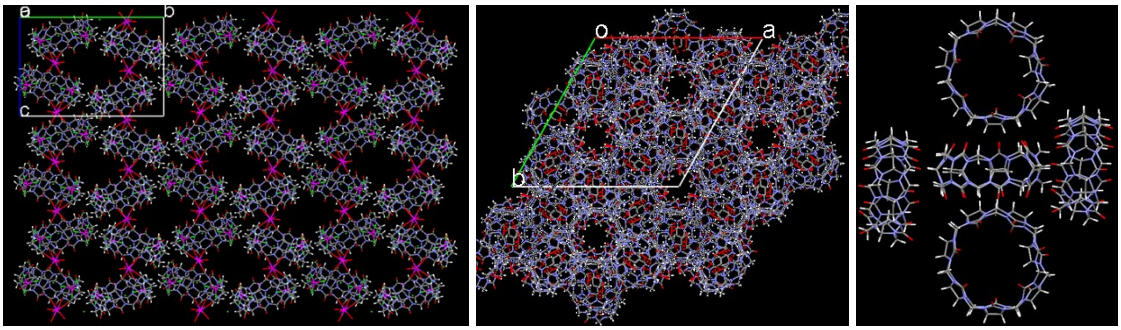


Figure S1. Sorption profiles of volatile materials on the *i*Q[7]-based porous supramolecular assembly compound **1** and *i*Q[7] powder: methanol, ethanol, acetone, acetonitrile and tetrachloromethane at 298 K.

Note: All the experiments were conducted at least 3 times and the variation of the results measured. The error margins observed were 1.2 %, 2.3 %, 2.5 %, 1.8 % or 2.1 %, for methanol, ethanol, acetone, acetonitrile and tetrachloromethane, respectively.

Inspection of crystal structures of the porous *i*Q[7] and the metal free *i*Q[7] (Isaacs: *J. Am. Chem. Soc*. 2005, 127, 18000) revealed that the portals of *i*Q[7] were sealed by Ln^{3+} cations (Figure S2a) or neighboring *i*Q[7] molecules through the outer surface interaction (Figure S2c), thus, absorption for the volatile materials of both porous *i*Q[7] and *i*Q[7] could be mainly dependent upon the free space in porous *i*Q[7] and *i*Q[7]. The crystal structure of the porous *i*Q[7] shows that the supramolecular assembly has numerous channels constructed of zig-zag *i*Q[7]−Ln^{3+}-based coordination polymers along the *c*-axis (Figure 1a). The aperture of each channel is constructed from four *i*Q[7] molecules, and has dimensions of length ~8 Å × width ~4 Å or with cross-sectional area of 32 $Å^2$ along the *a* axis (Figure S2a). By contrast, the supramolecular assembly of the metal-free *i*Q[7] along the *c*-axis exhibits fewer and smaller channels with a radius of ~2.4 Å and with cross-sectional area of ~18 $Å^2$ (Figure S2b). Moreover, the aperture is constructed of four portals from four *i*Q[7] molecules, therefore the channels should be polar in the porous *i*Q[7], while the channels are constructed from the rears of *i*Q[7] molecules in the metal-free *i*Q[7]. Thus, the porous *i*Q[7] and the metal-free *i*Q[7] show not only different selectivity but also differing sorption capacity towards volatile materials.



a b c

Figure S2 Supramolecular assemblies constructed of (a) Zig-zag *i*Q[7]−Ln^{3+}-based coordination polymers ("bee pupa") along the *a* axis; (b) metal free *i*Q[7] molecules along the *c* axis, (c) basic arrangement of *i*Q[7] molecules in the metal free *i*Q[7].