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Supplementary Material

Supramolecular assemblies of cucurbit[10]uril based on outer surface interactions

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Experimental section

Table S1 Crystal data and structure refinement details for compounds **1**

Compound	**1**
Empirical formula	$C_{60}H_{60}Cd_2Cl_9N_{40}O_{20}$
Formula weight	2205.35
Crystal system	Tetragonal
Space group	P4(2)/mnm
a, Å	21.6484(3)
b, Å	21.6484(3)
c, Å	15.3828(4)
α, deg	90.00
β, deg	90.00
γ, deg	90.00
V, Å^3	7209.2(3)
Z	2
D_{calcd}, g cm^{-3}	1.016
T, K	223(2)
μ, mm^{-1}	4.372
Unique reflns	3228
Obsd reflns	1959
Params	162
R_{int}	0.0301
R [$I > 2\sigma$(I)][a]	0.0773
wR [$I > 2\sigma$(I)][b]	0.2563
R (all data)	0.1024
wR (all data)	0.2869
GOF on F^2	1.042

[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 $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$; $P = (F_o^2 + 2F_c^2)/3$.

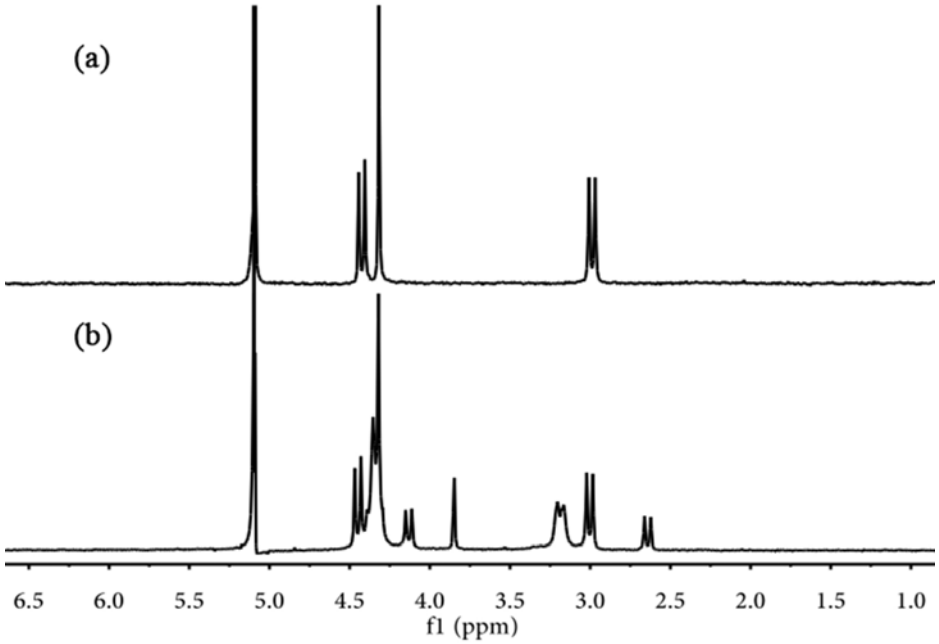

Fig. S1. ^{1}H NMR spectra in 4M DCl: (a) Pure Q[10]; (b) above pure Q[10] with excess Q[5].

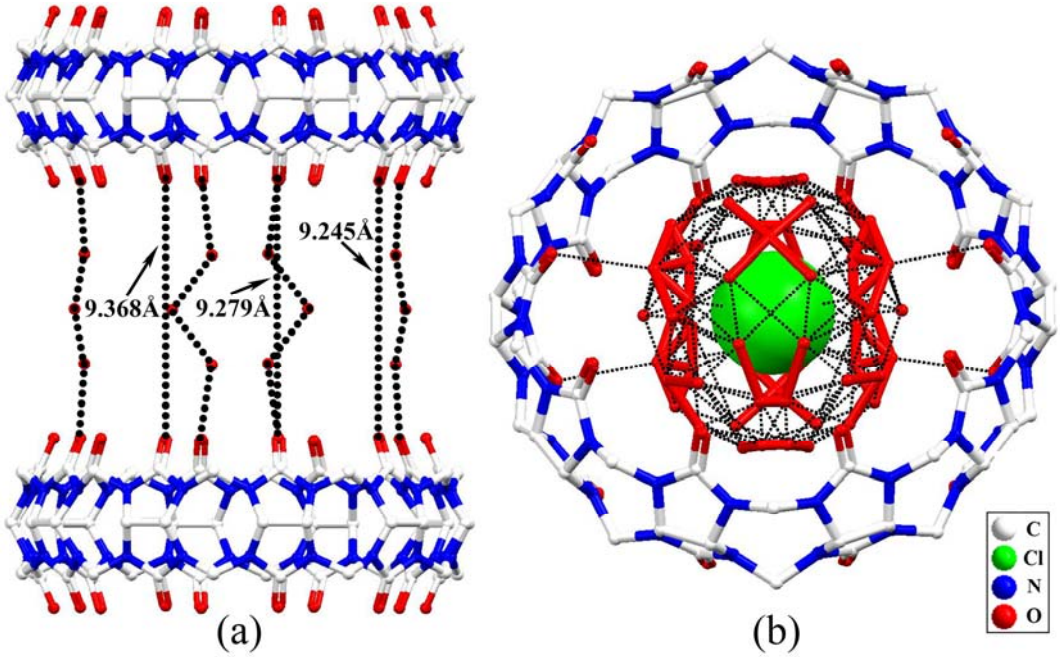

Fig. S2. Crystal structure of compound **1**: (a) Interaction of neighbouring Q[10] carbonyl oxygens through water molecules in the Q[10]-based columnar channel; (b) Q[10]-based inclusion complex in which a disordered water surrounds chloride anion Cl2.

Synthesis of compound 2. $CdCl_2$(5.00 mg, 0.027 mmol) and Q[10]·50H2O (9.2mg, 0.004 mmol) were dissolved in 3.0 mL of 3.0 M HNO_3 with stirring and heating. The solution was left to stand in air at room temperature to allow slow evaporation. Colorless crystals were obtained from the solution within four days. Elemental analysis (%) found C, 27.78; H, 5.22; N, 22.05. Melting point: 388°C (decomposed).

In the presence of HNO_3, Cd^{2+} cations can not form structure-directing $[Cd(NO_3)_4]^{2-}$ anions, thus, the interaction of NO_3^- anions with the electrostatically positive outer surface of Q[10] in the compound **2** could be different with that of $[CdCl_4]^{2\bullet}$ anions with the electrostatically positive outer surface of Q[10] in the compound **1**, therefore, using different synthetic strategies could give different Q[10]-based supramolecular assemblies and there was no equivalent structure-directing effect in compound **2**, and outer surface interactions between different Q[10] molecules were instead observed to form a porous layer constructed of Q[10] molecules (Fig. S3a). Each Q[10] molecule is situated almost vertically on top of the portal of two neighboring Q[10] molecules, meanwhile two portals of a Q[10] molecule are covered by two Q[10] molecules in the same manner, and four orthogonal Q[10] molecules together create a square hole. The driving force could undoubtedly be attributed to the outer surface interaction of Q[10]. Fig. S3b shows a detailed view of interactions between the orthogonal Q[10] molecules. Thus, outer surface interactions of Q[10] result in the formation of a Q[10]-based sheet with numerous square holes. Figs S3c and S3d show the supramolecular arrangement of the Q[10]-based layers. One can see the neighboring layers overlap with a slight shift, whereas alternating layers are exactly overlapped, and this stacking leads to a narrowing of the channels in compound **2**.

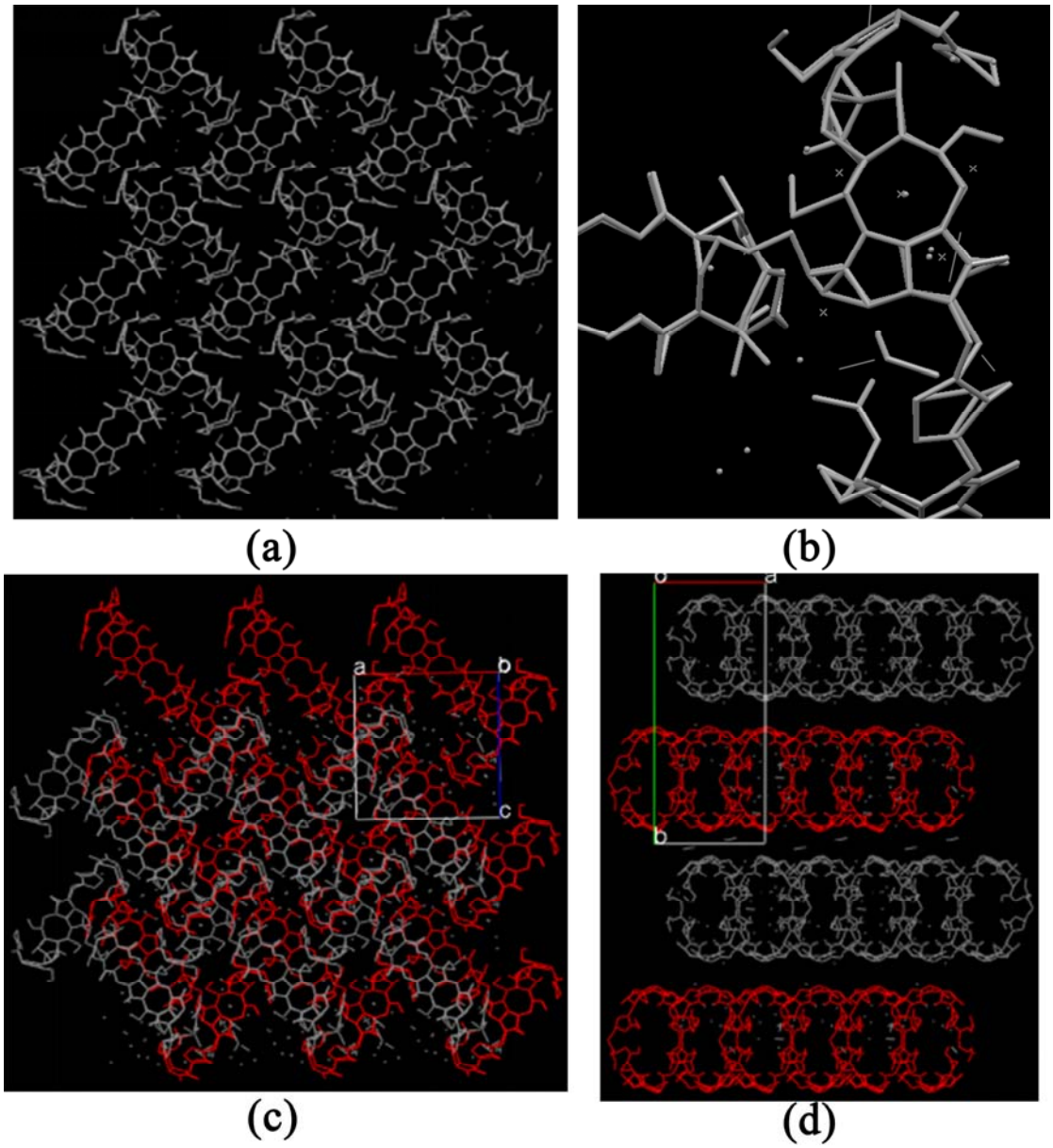

Fig. S3. Crystal structure of compound **2**: (a) Q[10]-based layer constructed of orthogonal Q[10] molecules; (b) Detailed interactions between two orthogonal Q[10] molecules; (c and d) Overall views of the supramolecular assemblies constructed from Q[10]-based layers.

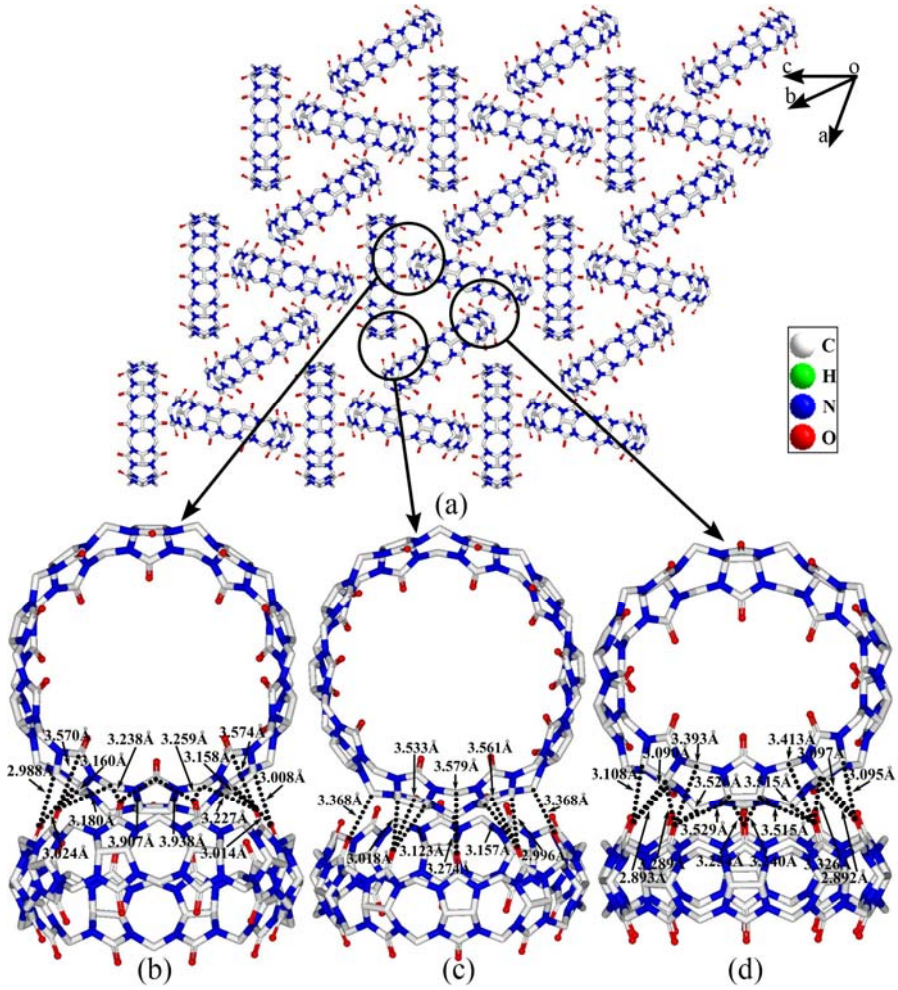

Fig. S4. Crystal structure of the compound previously reported by the Isaacs group: (a) Q[10]-based layer; (b, c and d) Detailed interactions between two neighboring Q[10] molecules.