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Supplementary Information

Self-assembly of guest-induced calix[4]arene nanocapsules into three-dimensional molecular architecture

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Experimental Section:

Synthesis

1: L_1 was treated with one equivalent of $AgNO_3$ in a mixture of ammonia aqueous and ethanol. The mixture was sonicated for around 5 minutes. After a few days, crystals of 1 were grown from the solutions by slow evaporation at room temperature in dark place. Yield: 28%. Anal. Calc. for 1: C, 59.48; H, 5.17; N, 4.95. Found: C, 59.98; H, 5.47; N, 4.45.

2: Aqueous solutions of $AgNO_3$, KCl, hmt and L_2, were combined in 14: 4: 1: 4 molar ratio, followed by adding the ammonia solution. The mixture was sonicated for around 3 minutes. After a few days, crystals of 2 were obtained in dark place. Yield: 22%. Anal. Calc. for 2: C, 37.33; H, 3.47; N, 2.32. Found: C, 37.96; H, 3.97; N, 2.05.

Measurement

Elemental analysis were carried out on Vario EL instrument. Data were collected on a Bruker SMART 1000 CCD diffractometer with Mo_{Ka} radiation using the w-scan mode. Data were corrected for absorption using the SADABS program, and solution and refinement of the structure were performed using the SHELX-97 software package.

Crystal data for 1: $C_{28}H_{29}AgN_2O_4$, Mr= 565.40, monoclinic, *P21/n*, a= 15.2273(15) Å, b= 9.6988(9) Å, c= 17.8475(17) Å, β= 110.874(2)°，V=2462.8(4) $Å^3$, Z=4, T= 193 K, λ=0.71073 Å, 13493 reflections , 4840 unique (2339 observed, R_{int}= 0.0705), $1.51<\theta<26.05$, GOF=0.957, R_1=0.0530, wR_2 (all data) = 0.1057. Crystal data for 2: $C_{75}H_{83}Ag_7ClK_2N_4O_{31.5}$, Mr= 2413.19, orthorhombic, *Pccn*, a= 27.1014(14) (15) Å,

b= 30.1316(15) Å, *c*= 19.7260 (10) Å, *V*=16108.4(14) Å^3, *Z*=8, *T*= 193 K, λ=0.71073 Å,; 81836 reflections, 14559 unique (10644 observed, R_{int} = 0.0487), 1.44<θ<25.38, GOF=1.039, R_1=0.0955, wR_2 (all data) = 0.2874. All non-hydrogen atoms and non-guest molecules were refined anisotropically, whereas the hydrogen atoms were included at geometrically calculated positions and allowed to ride on their parent atoms. The hydrogen atoms from water molecules were not assigned. CCDC-666196, 666197 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

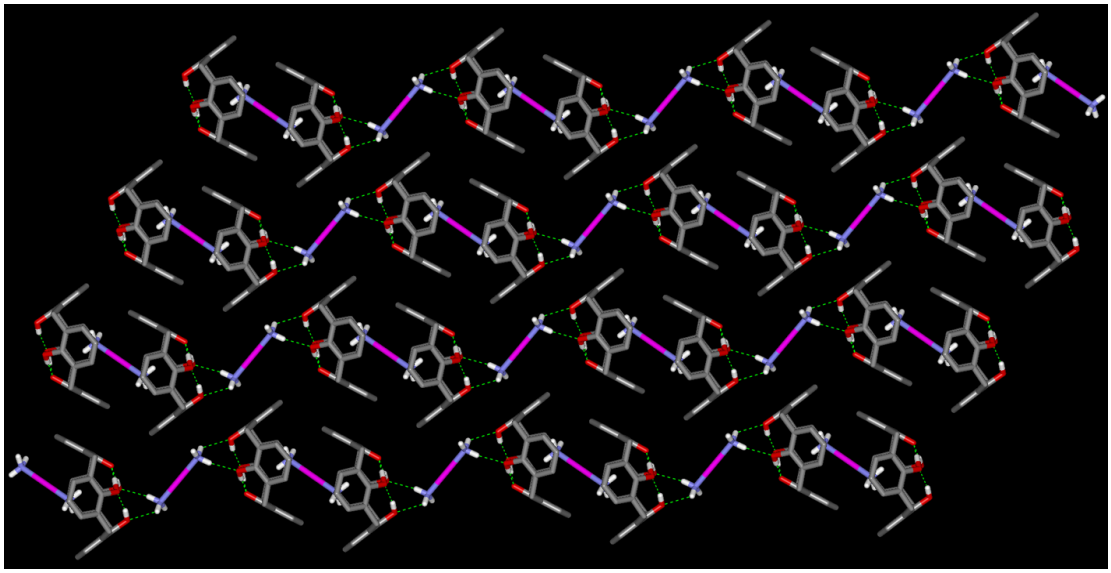

Fig. S1 The capsules are bridged by N-H···O bonds forming a chain structure.

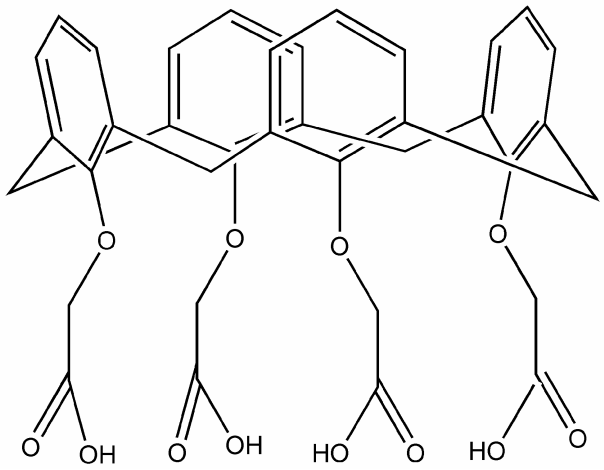

Fig. S2　25，26，27，28-tetrakis(carboxymethoxy)-calix[4]arene (L_2).

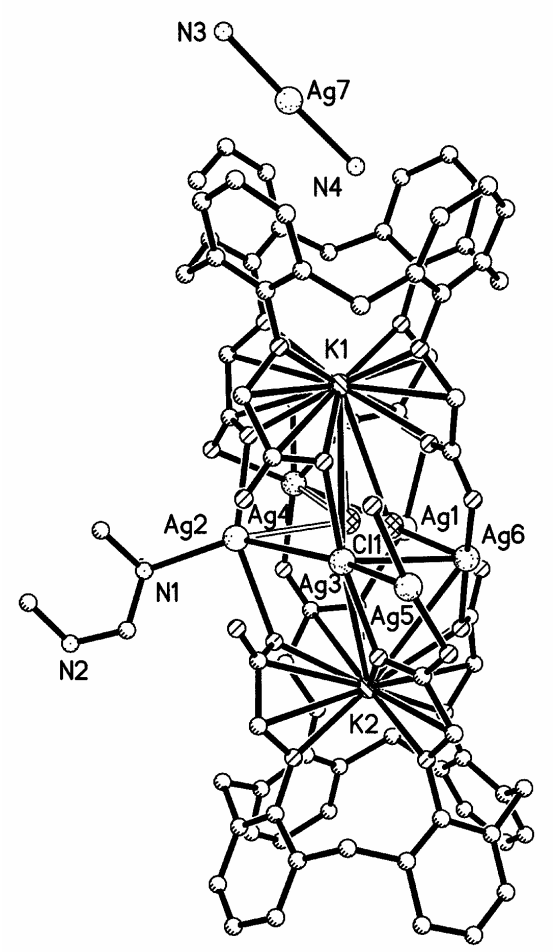

Fig. S3 The columelliform structure showing the interactions of metal (Ag, K) cations to the ligands.

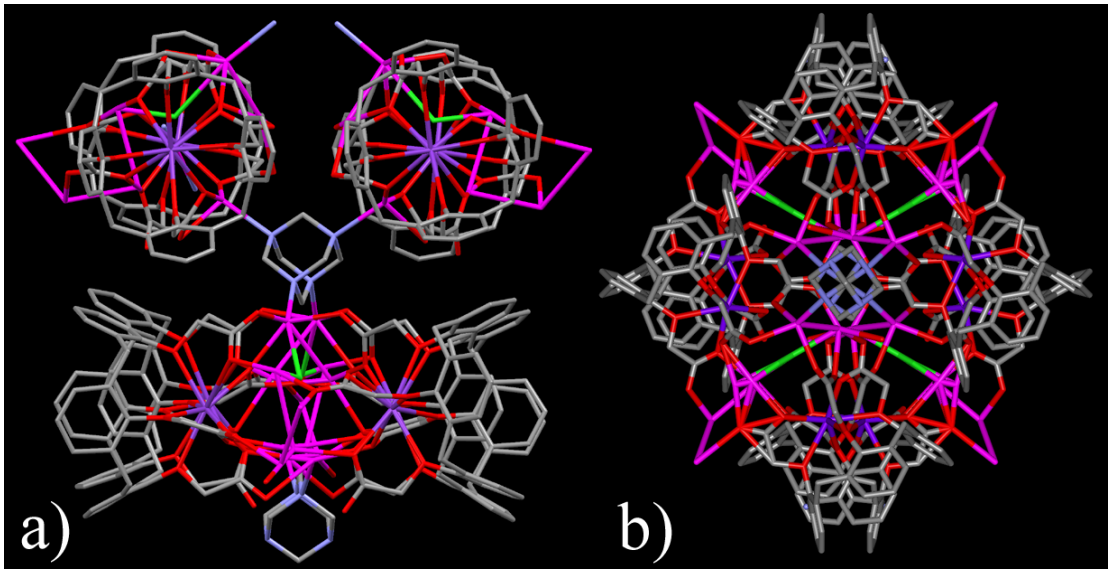

Fig. S4 a) One hmt links four columns through bonding four silver atoms, one disordered chlorine atom has been omitted for clarity. b) The nanobar viewed down

the *c* axis.

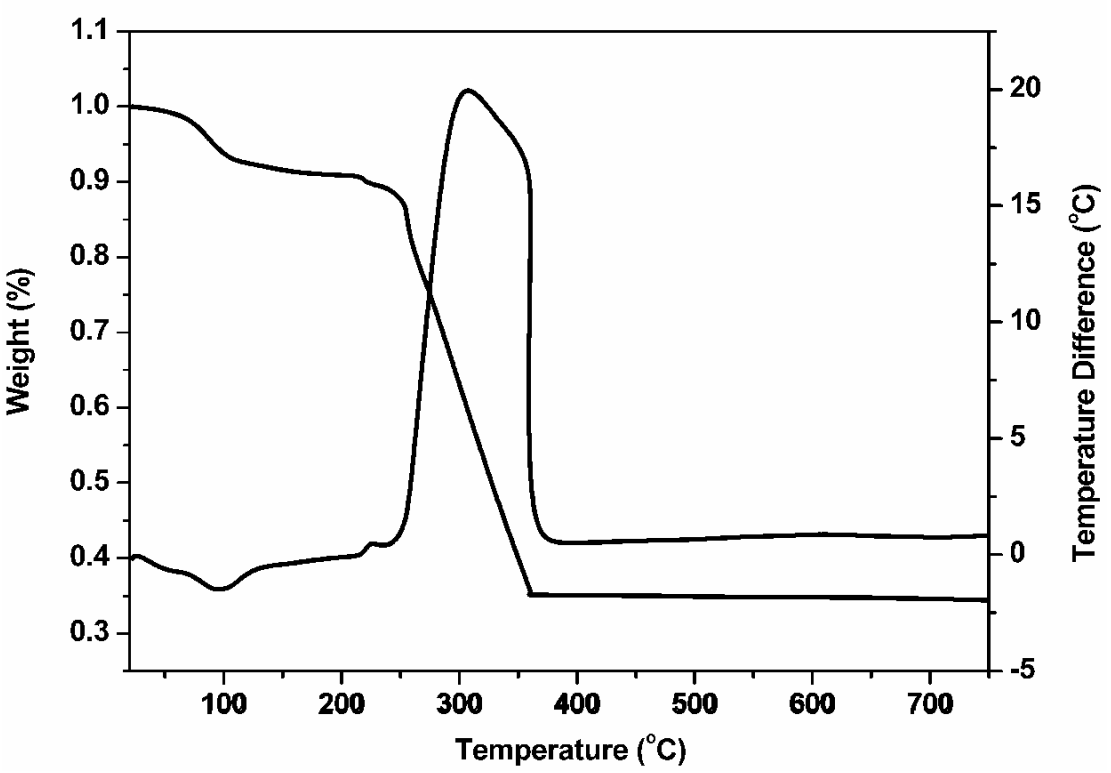

Fig. S5 TGA of compound **2**.

The TG curve shows a weight loss of 10 % from 50 to 150 °C corresponding to the release of water and ammonia molecules. No weight loss was observed between 150 and 245 °C, and the framework started to decompose at higher temperatures.