Supporting Information

Chaperone-Assisted Formation of Cucurbit[8]uril-Based Molecular Porous Materials with 1D Channel Structure

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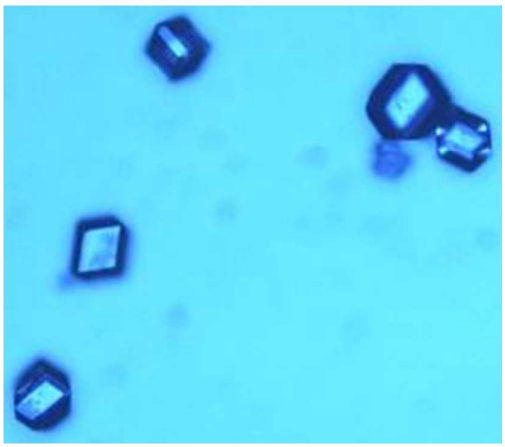

Figure S1. Optical image of the synthesized single crystal of CB[8] (***1***).

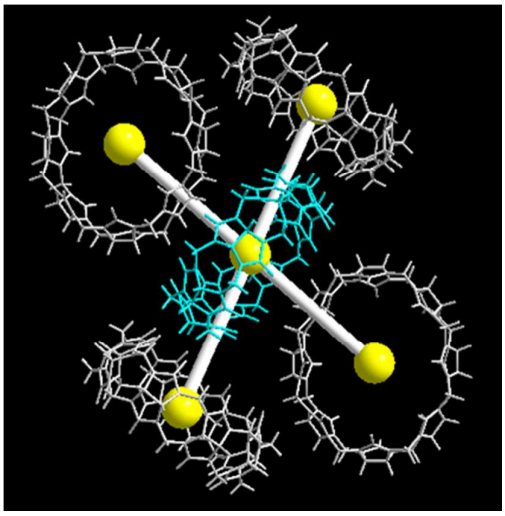

Figure S2. The structure of subunit of $(CB[8])_5$. Such subunit of $(CB[8])_5$ surrounded by other subunits was further extended in three dimensions to form a stable 3D supramolecular architectures.

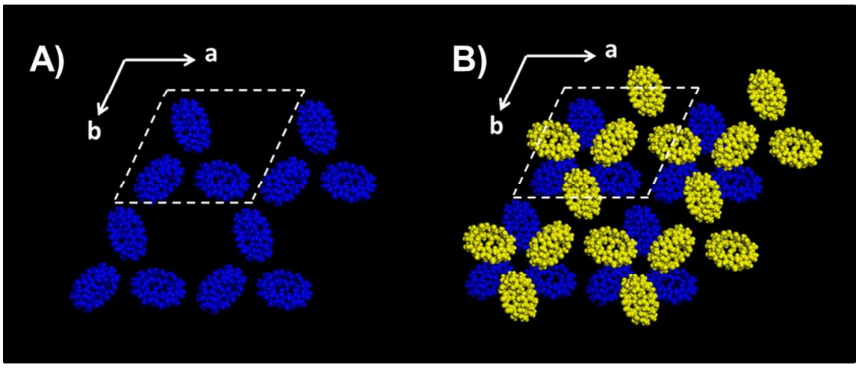

Figure S3. The three-dimensional packing of CB[8] macrocycles, illustrating a successive one layer and two layers along the *c*-axis. The guest molecules are removed for clarity.

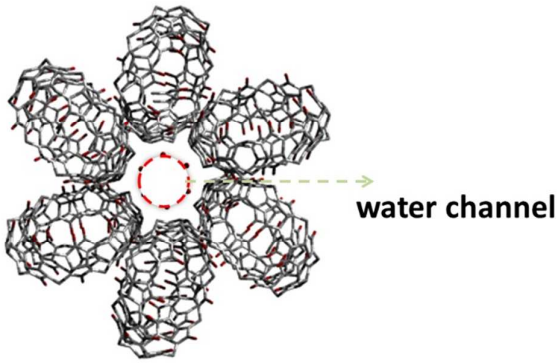

Figure S4. Schematic illustration of the water channel in CB[8] (***1***).

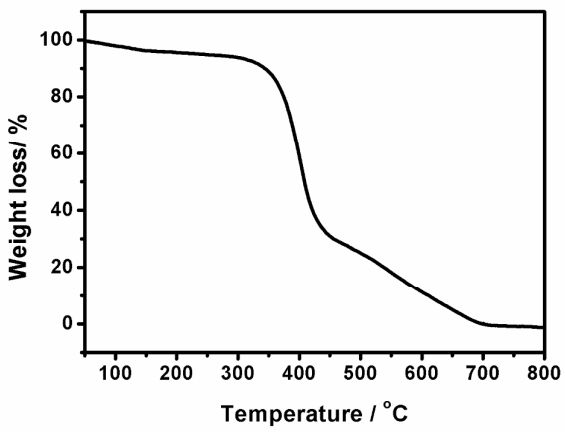

Figure S5. TGA data of CB[8] (***1***).

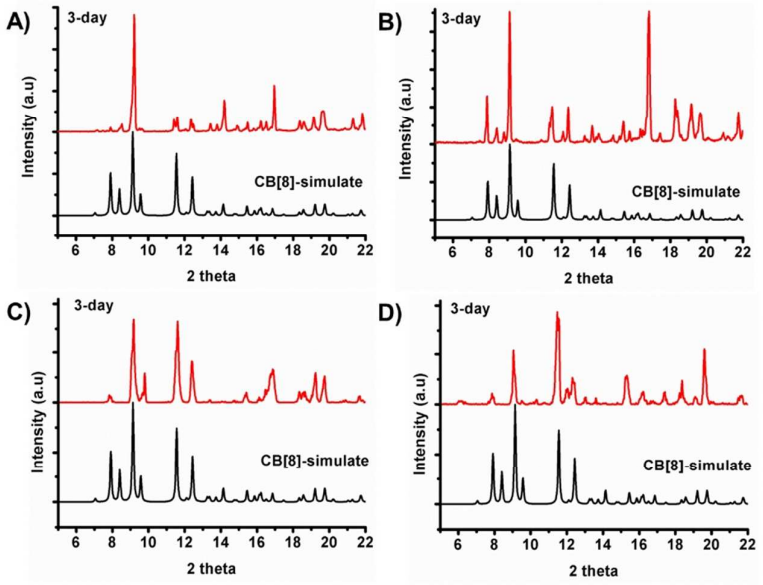

Figure S6. Powder XRD profiles confirming the chemical and thermal stability of CB[8] (***1***), A) soaked in acetone, B) in tetrahydrofuran, C) in acetonitrile, and D) in water.

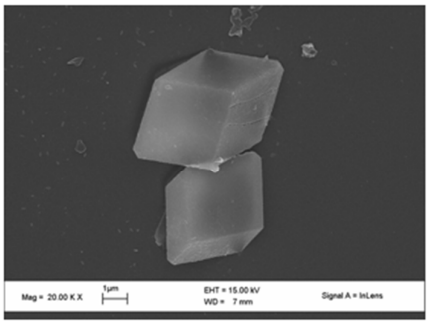

Figure S7. A) SEM image of the crystal of CB[8] (***2***) with $I4_1/a$ space group.

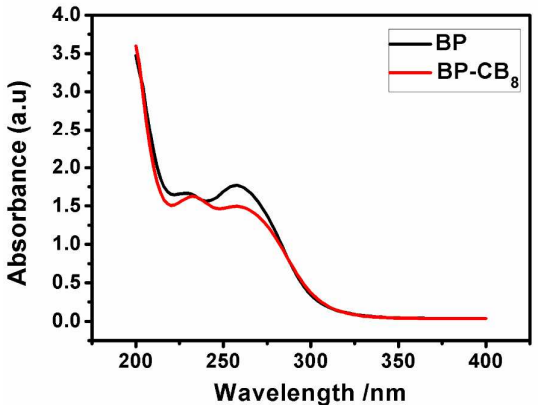

Figure S8. UV-Vis spectrum of BP and the formed CB[8]•BP complex in water.

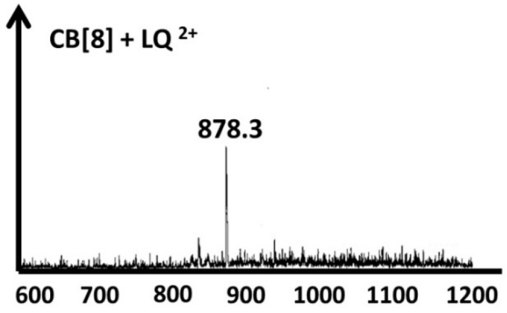

Figure S9. ESI-MS spectrum of the formed CB[8]• BP host-guest complexes in water.

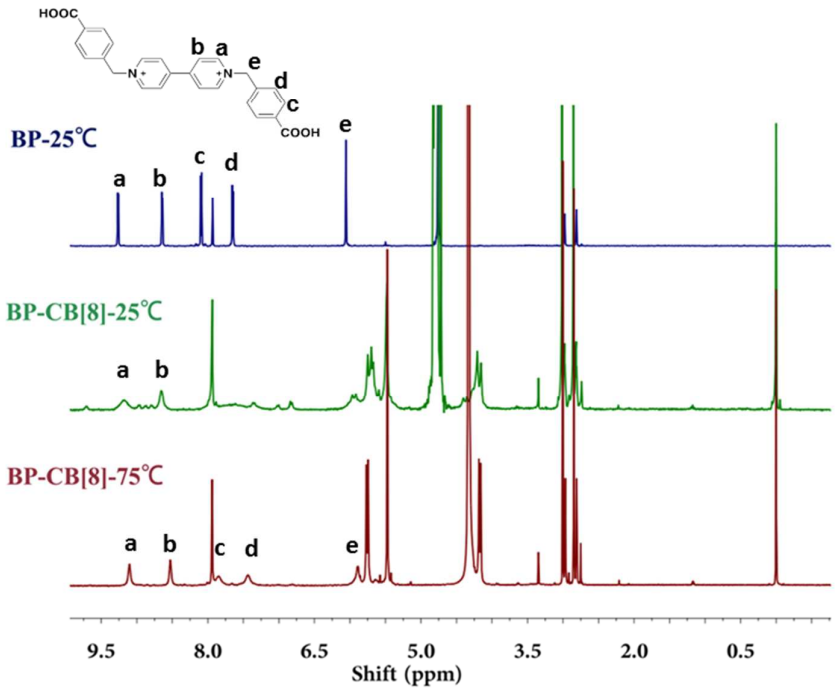

Figure S10. ^{1}H NMR spectra (600 MHz, D_2O/DMF-d_7) of BP, BP in the presence of CB[8] cavity at room temperature and relative high temperature 75° in solution of D_2O/DMF-d_7.

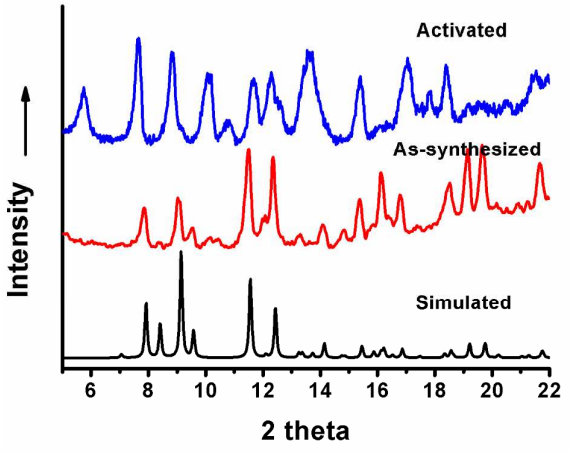

Figure S11. X-ray powder diffraction patterns of crystal CB[8] (***1***) after activation under vacuum at 100°C for two days.

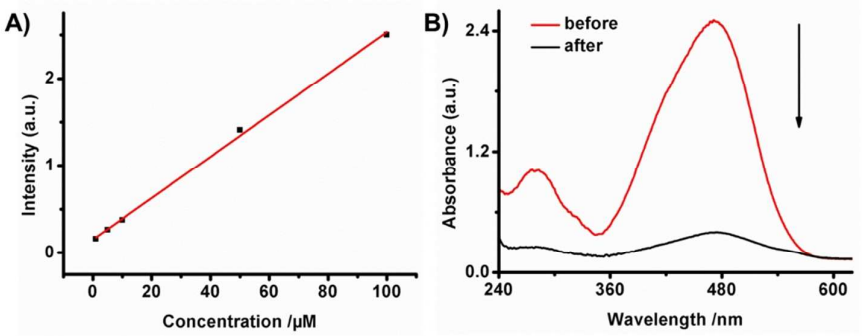

Figure S12.A) The relationship between absorbance intensity and concentration of methyl orange in aqueous solution. B) The UV/vis spectrum of methyl orange aqueous solution (10^{-4} M) before and after absorbing by CB[8] (***1***) crystal.

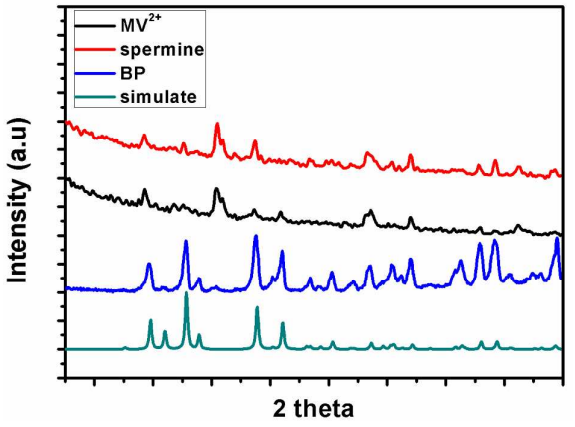

Figure S13. X-ray powder diffraction patterns of crystal CB[8] (***1***) that were synthesized by using different guest molecules: BP, spermine, and methylviologen.

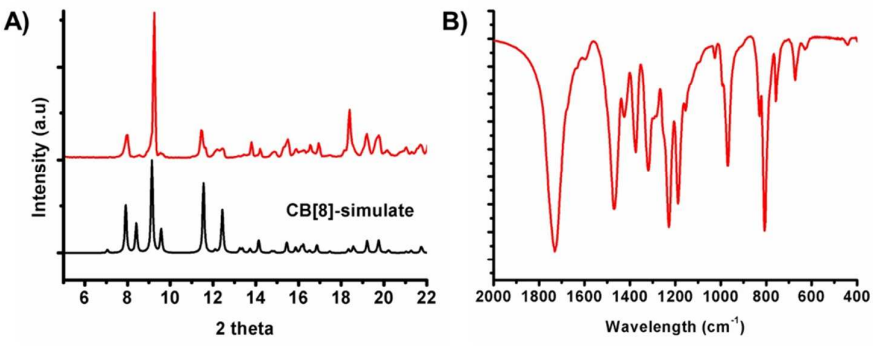

Figure S14. X-ray powder diffraction patterns of crystal CB[8] (***1***) **(A)** and FTIR spectra (B) that were synthesized by using 1-Adamantanamine hydrochloride as chaperone molecule.