Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Solid-state “Russian doll”-like capsules based on triptycene-derived macrotricyclic host with paraquat derivative and polycyclic aromatic hydrocarbons

Ying Han, Tong-Ling Liang, Xiang Hao and Chuan-Feng Chen*

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

E-mail: cchen@iccas.ac.cn

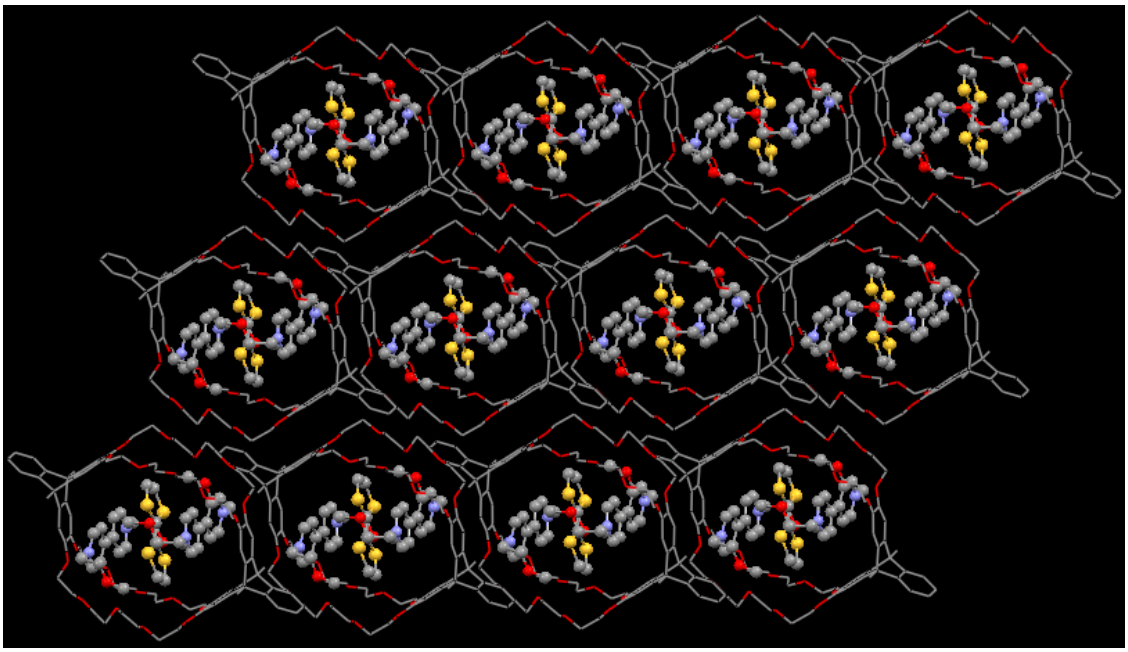

Fig. S1. Packing of complex **1**·**2**$_2$·**4**. Solvent molecules and hydrogen atoms were omitted for clarity.

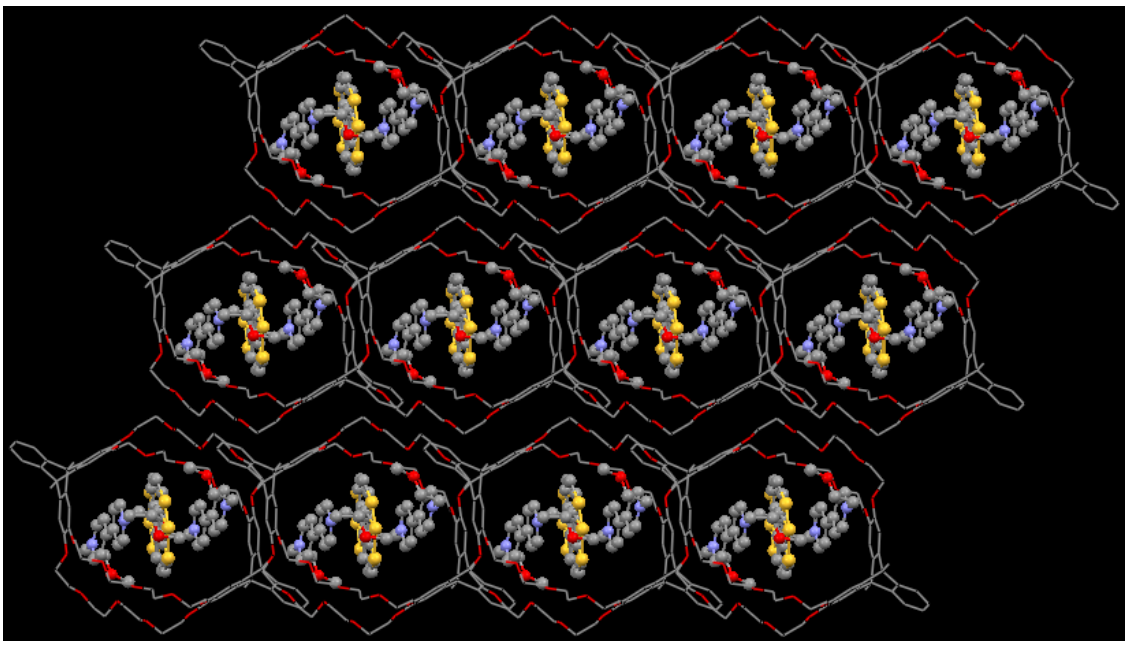

Fig. S2. Packing of complex **1**·**2**$_2$·**5**. Solvent molecules and hydrogen atoms were omitted for clarity.

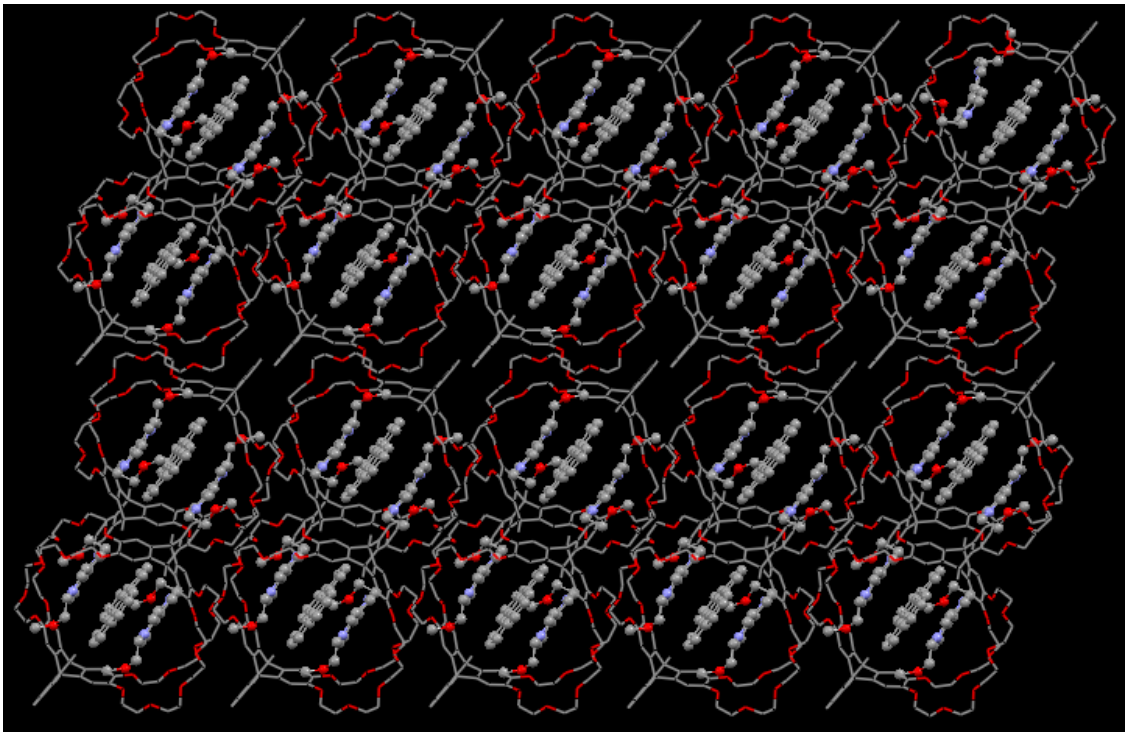

Fig. S3. Packing of complex **1**·**2**$_2$·**6**. Solvent molecules and hydrogen atoms were omitted for clarity.

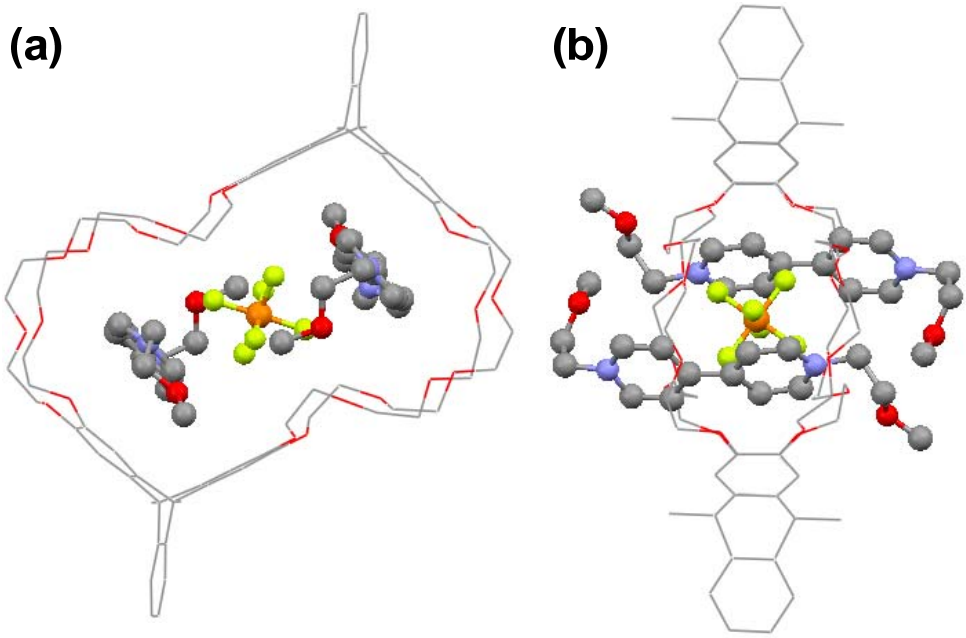

Fig. S4. Side view (a) and top view (b) of the crystal structure of complex **1·2**$_2$.

Table 1. Crystal data and structure refinement for **1·2$_2$**.

Empirical formula	C_{112} H_{142} F_{24} N_6 O_{24} P_4	
Formula weight	2536.19	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.280(4) Å	a= 75.786(11)°.
	b = 14.170(3) Å	b= 89.090(12)°.
	c = 17.433(5) Å	g = 68.893(7)°.
Volume	2957.1(13) Å^3	
Z	1	
Density (calculated)	1.424 Mg/m^3	
Absorption coefficient	0.174 mm^{-1}	
F(000)	1324	
Crystal size	0.54 x 0.51 x 0.05 mm^3	
Theta range for data collection	1.649 to 27.467°.	
Index ranges	-17<=h<=17, -18<=k<=18, -22<=l<=22	
Reflections collected	36132	
Independent reflections	13490 [R(int) = 0.0539]	
Completeness to theta = 26.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.7042	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13490 / 37 / 822	
Goodness-of-fit on F^2	1.459	
Final R indices [I>2sigma(I)]	R_1 = 0.0825, wR_2 = 0.2250	
R indices (all data)	R_1 = 0.0978, wR_2 = 0.2364	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.831 and -0.626 e.Å^{-3}	