Supporting Information

Host-guest inclusion complexes formed between a symmetrical tetrasubstituted cucurbit[6]uril and glycine

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Table S1. Crystal data as well as details of data collection and refinement for compounds **1** and **2.**

Figure S1. Interaction of Gly and TMeQ[6] (20 °C): ^{1}H NMR spectra (400 MHz, D$_2$O) of (A) neat Gly, (B) in the presence of 1.0 equiv. of TMeQ[6] and 2.0 equiv. of Ca^{2+}, (C) in the presence of 1.0 equiv. of TMeQ[6] and 1.0 equiv. of Ca^{2+}, (D) in the presence of 1.0 equiv. of TMeQ[6], and (E) neat TMeQ[6]

Figure S2. Asymmetric unit of complex **1** with atoms drawn as 50% probability ellipsoids.

Figure S3. Extended asymmetric unit of complex **1** with atoms drawn as spheres of arbitrary radius. Dashed lines show hydrogen bonds.

Figure S4. Location of two guest molecules (space-filling representation) within TMeQ6 bowls (spheres).

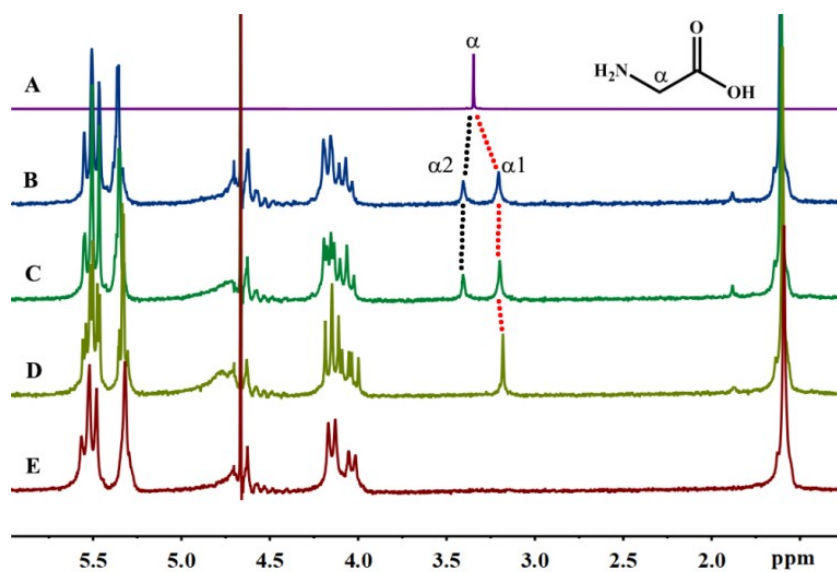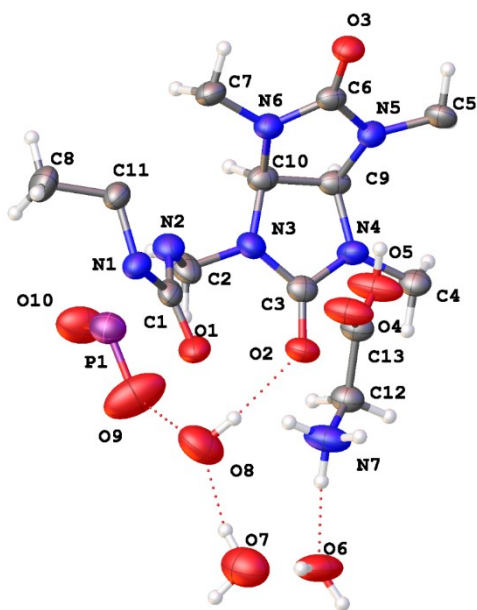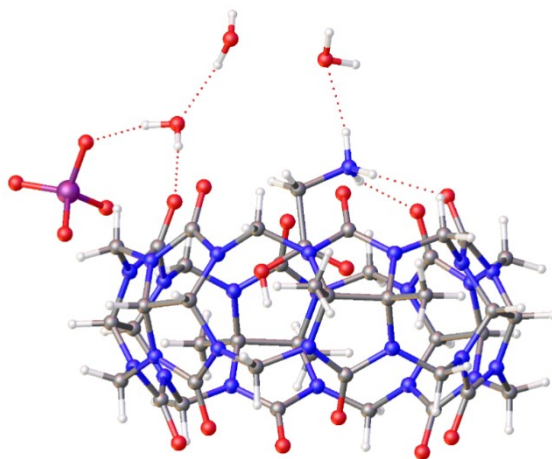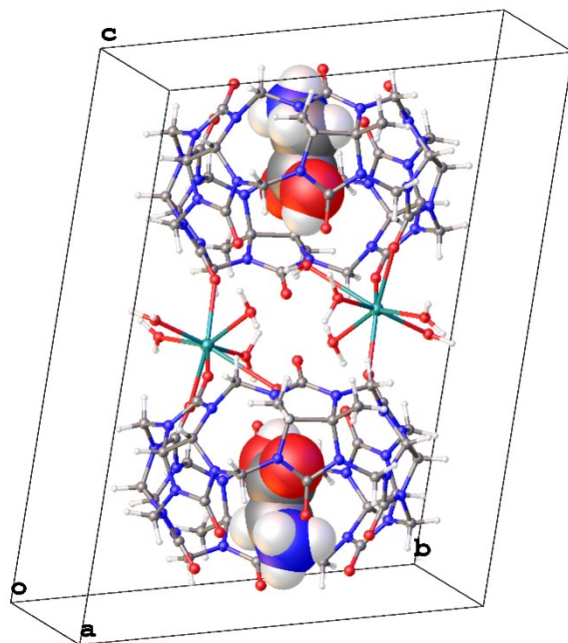**Table S1**. Crystal data as well as details of data collection and refinement for compounds **1** and **2**.

Identification code	1	2
Empirical formula	$C_{44}H_{80}N_{26}O_{34}P_2$	$C_{42}H_{92}N_{25}O_{35}CaCl_3$
Formula weight	1579.24	1653.83
Structural formula	$C_{40}H_{44}N_{24}O_{12}$, $(PO_4)_2$, $2H_3NCH_2COOH$, $4(H_3O)$, $6(H_2O)$	$(C_{40}H_{44}N_{24}O_{12})Ca(H_2O)_5,3Cl$, $NH_3CH_2COOH,16H_2O$
Temperature/K	296	296
Crystal system	monoclinic	triclinic
Space group	C2/m	P-1
a/Å	12.878(3)	13.001(4)
b/Å	20.372(5)	14.691(4)
c/Å	12.609(5)	21.030(6)
α/°	90	72.765(7)
β/°	106.828(6)	76.725(7)
γ/°	90	68.800(7)
Volume/Å^3	3166.3(16)	3542.8(18)
Z	2	2
ρ_{calc}g/cm^3	1.652	1.550
μ/mm^{-1}	0.189	0.310
F(000)	1648.0	1740.0
Crystal size/mm^3	0.21 × 0.18 × 0.14	0.17 × 0.16 × 0.14
Radiation (MoKα)	λ = 0.71073	λ = 0.71073
2Θ range for data collection/°	5.234 to 51.022	3.256 to 50.054
Index ranges	-15 ≤ h ≤ 15, -24 ≤ k ≤ 24, -15 ≤ l ≤ 15	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -25 ≤ h ≤ 25,
Reflections collected	57878	44481
Independent reflections	3047 [R_{int} = 0.0937, R_{sigma} = 0.0252]	12511 [R_{int} = 0.0621, R_{sigma} = 0.0522]
Data/restraints/parameters	3047/0/266	12511/0/822
Goodness-of-fit on F^2	1.042	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0394, wR_2 = 0.1031	R_1 = 0.0698, wR_2 = 0.1809
Final R indexes [all data]	R_1 = 0.0556, wR_2 = 0.1126	R_1 = 0.0983, wR_2 = 0.1972
Largest diff. peak/hole / e Å^{-3}	0.35/-0.27	0.48/-0.59