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Supporting Information

for

Construction of pillar[4]arene[1]quinone–1,10-dibromodecane pseudorotaxanes in solution and in the solid state

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Materials and methods, characterizations of H and G, crystallographic data, and characterization studies on the complexation between H and G in solution

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1. Materials and methods

All reagents and solvents were commercially available and used as supplied without further purification. **H** was synthesized according to literature procedures.[S1] ^{1}H NMR spectra were recorded on a temperature-controlled 400 MHz, 500 MHz, or 600 MHz spectrometer with use of the deuterated solvent as the lock and the residual solvent or TMS as the internal reference. Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) was recorded on a Bruker Ultraflex spectrometer with a 355 nm Nd: YAG laser (Smartbeam II) and a 25 kV ion source voltage. UV–vis spectra were taken on a Perkin-Elmer Lambda 35 UV-vis spectrophotometer.

2. Characterizations of **H** and **G**

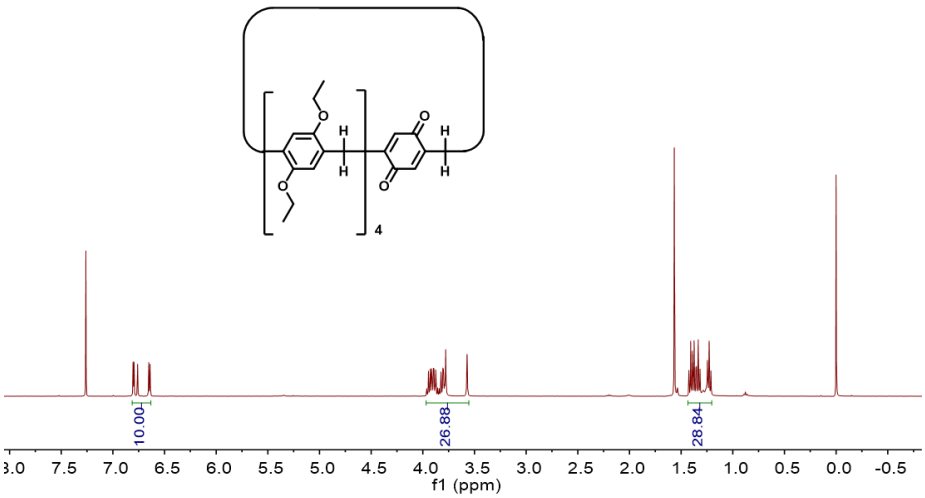

Figure S1: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **H**.

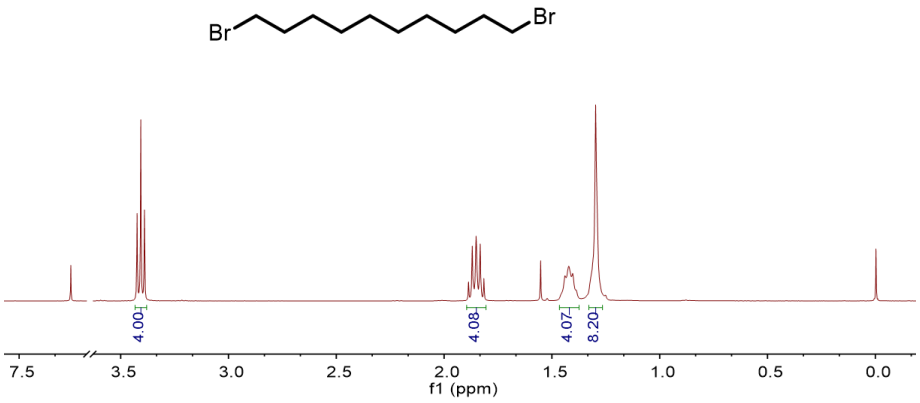

Figure S2: ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **G**.

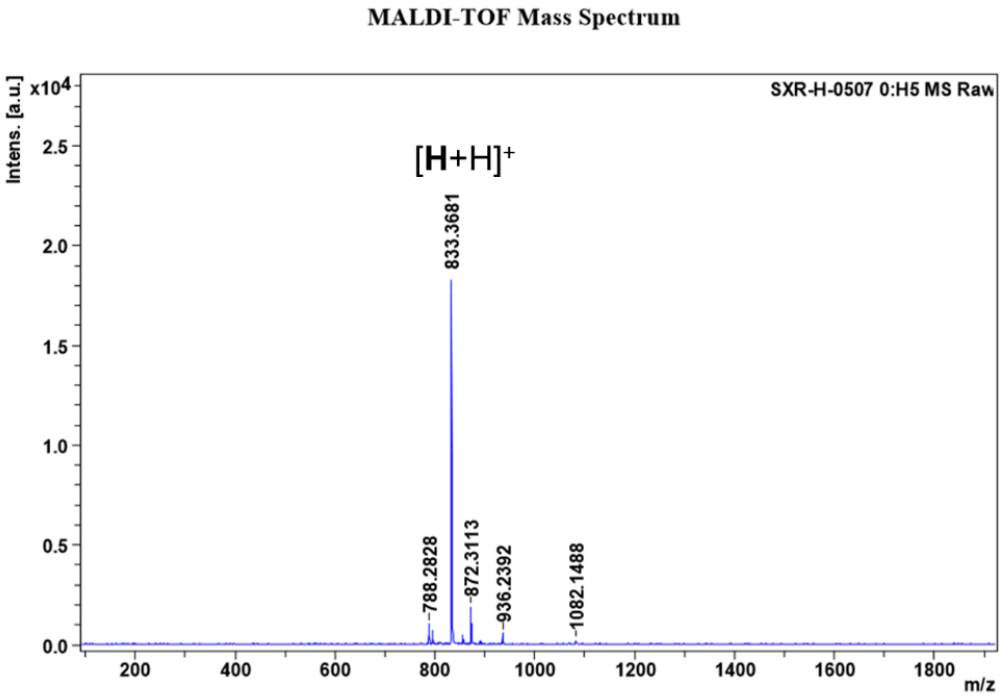

Figure S3: MALDI-TOF mass spectrum of **H**.

3. Crystallographic data of the [3]pseudorotaxane between **H** and **G** in the solid state

Table S1: Crystal data for single crystals of the [3]pseudorotaxane between **H** and **G** in the solid state.

empirical formula	$C_{112}H_{140}Br_2O_{20}$
formula weight	1966.06
temperature	170 K
wavelength	0.71073
crystal system	monoclinic
space group	*P* 1 2_1/*c* 1
unit cell dimensions	*a* = 17.4426(6) Å α = 90 *b* = 19.3528(8) Å β = 96.800(1) *c* = 15.3931(4) Å γ = 90
volume	5159.6(3)
Z	4
density (calculated)	1.265 g/cm^{-3}
absorption coefficient	0.854
F(000)	2084.0
crystal size	0.336 × 0.139 × 0.116 mm^3
θ range for data collection	2.35 to 27.40°
index ranges	-19<=h<=22, -25<=k<=20, -19<=l<=19
reflections collected	41520
independent reflections	11778 [*R*(int) = 0.0705]
completeness to θ = 27.492°	0.996
absorption correction	multiscan
max. and min. transmission	0.746, 0.686
data/restraints/parameters	11778/0/612
goodness-of-fit on *F*2	1.046
final *R* indices [*I* > 2σ(*I*)]	*R*1 = 0.0480, *wR*2 = 0.0511
R indices (all data)	*R*1 = 0.0705, *wR*2 = 0.0672
largest diff. peak and hole	0.561, –0.709 e. Å^{-3}
CCDC	2031286

4. Characterization studies on the complexation between **H** and **G** in solution

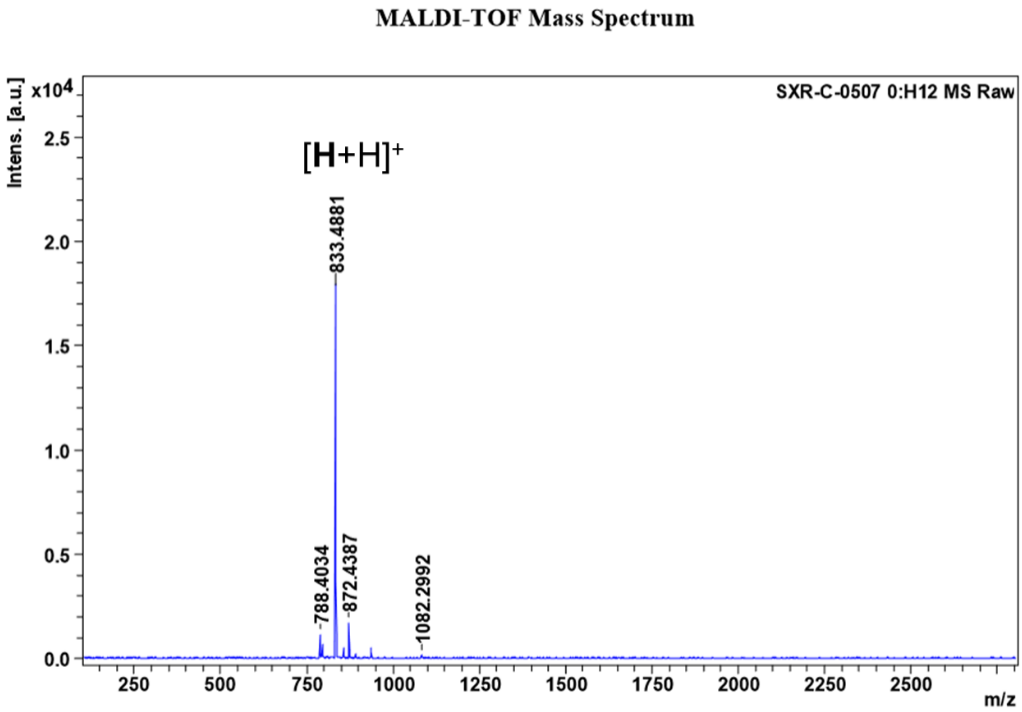

Figure S4: MALDI-TOF mass spectrum of **H** and **G**. There only exist the peaks of **H**.

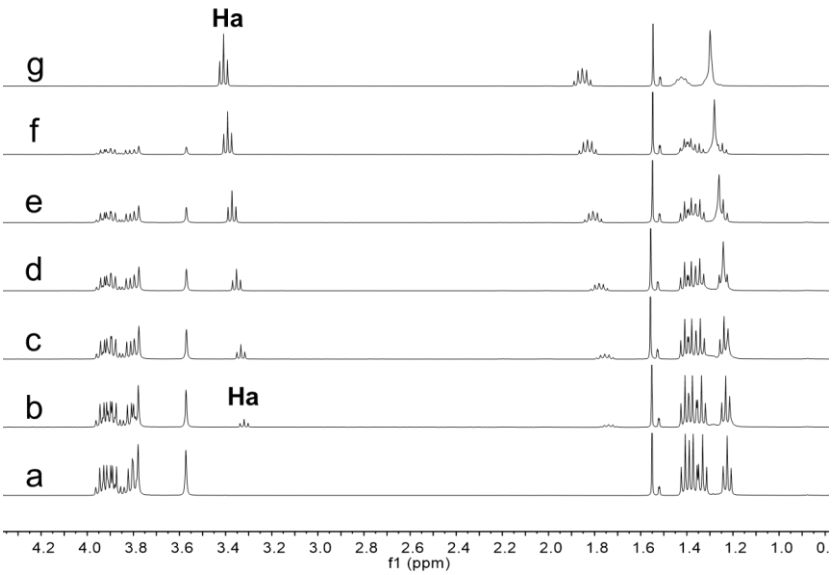

Figure S5: Partial ^{1}H NMR spectra (500 MHz, chloroform-*d*, 298 K): (a) 6.00 mM **H**; (b) 1.00 mM **G** and 5.00 mM **H**; (c) 2.00 mM **G** and 4.00 mM **H**; (d) 3.00 mM **G** and 3.00 mM **H**; (e) 4.00 mM **G** and 2.00 mM **H**; (f) 5.00 mM **G** and 1.00 mM **H**; (g) 6.00 mM **G**.

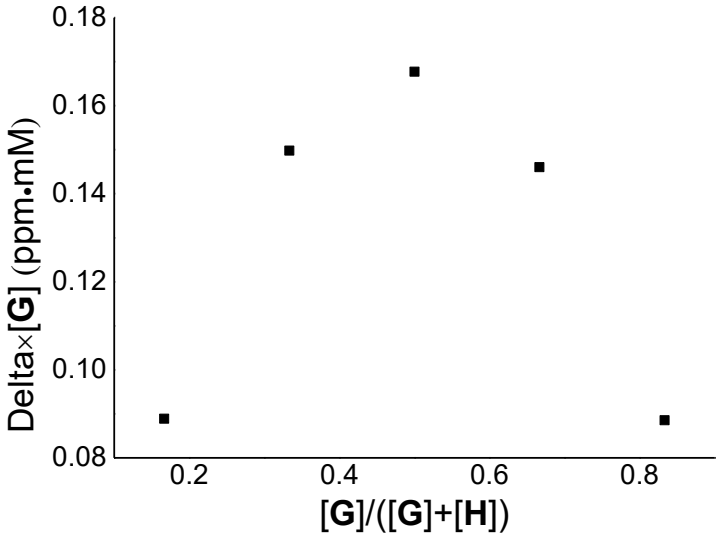

Figure S6: Job plot showing the 1:1 stoichiometry of the complexation between **H** and **G** in chloroform-*d* using the proton NMR data for H_a. Delta is the chemical shift change of H_a. [**H**] + [**G**] = 6.00 mM. [**H**] and [**G**] are concentrations of **H** and **G**, respectively.

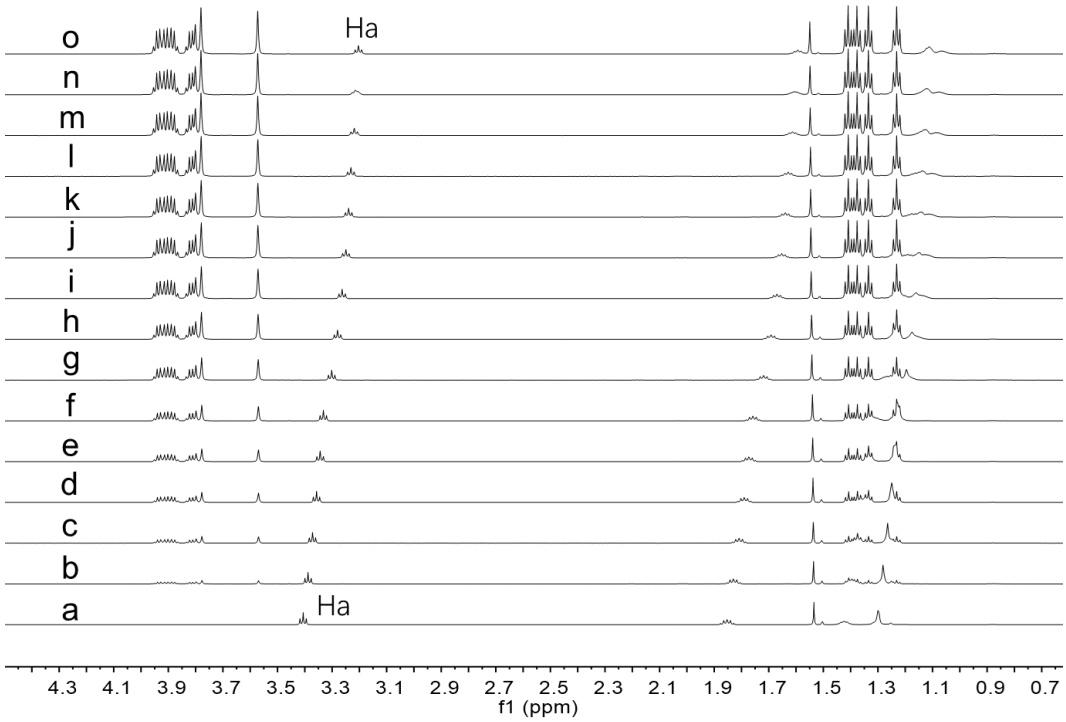

Figure S7: Partial ^{1}H NMR spectra (600 MHz, chloroform-*d*, 298 K) of **G** at the concentration of 5.00 mM upon addition of **H**: (a) 0 mM; (b) 1.16 mM; (c) 2.20 mM; (d) 3.14 mM; (e) 3.98 mM; (f) 4.74 mM; (g) 6.85 mM; (h) 8.47 mM; (i) 9.74 mM; (j) 10.77 mM; (k) 11.63 mM; (l) 12.34 mM; (m) 13.47 mM; (n) 14.33 mM; (o) 15.00 mM.

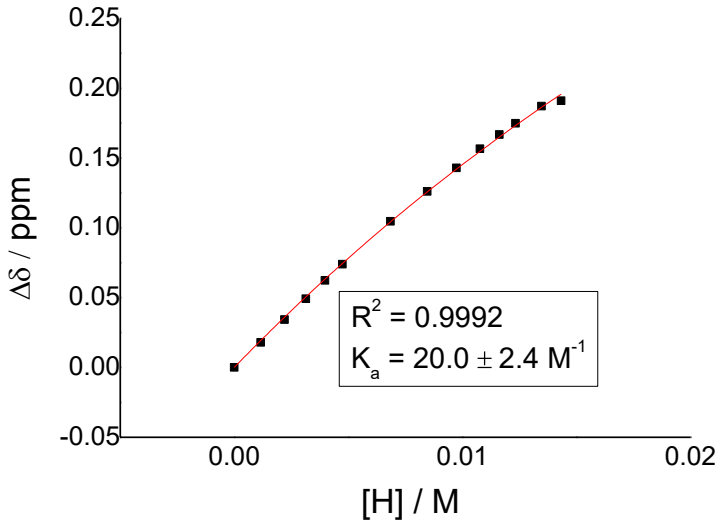

Figure S8: The chemical shift changes upon addition of **H**. The red solid line was obtained from the non-linear curve-fitting equation,[S2] y = (P1/[**G**]) (0.5x+0.5 ([**G**]+P2)-(0.5(x^2+(2x(P2-[**G**]))+(P2+[**G**])^2)$^{0.5}$)), where y = Δδ, P1 = $\Delta\delta_{max}$, P2 = 1/K_a, and x = [**H**].

5. References

S1. Han, C.; Zhang, Z.; Yu, G.; Huang, F. *Chem. Commun.*, **2012**, *48*, 9876–9878.

S2. Zhu, X.-Z.; Chen, C.-F. *J. Org. Chem.*, **2005**, *70*, 917–924.