Supporting Information

Inclusion of 4-pyrrolidinopyridine derivatives in a symmetrical α,α',δ,δ'-tetramethyl-cucurbit[6]uril and a Ba^{2+}-driven pseudorotaxane with characteristic UV absorption changes

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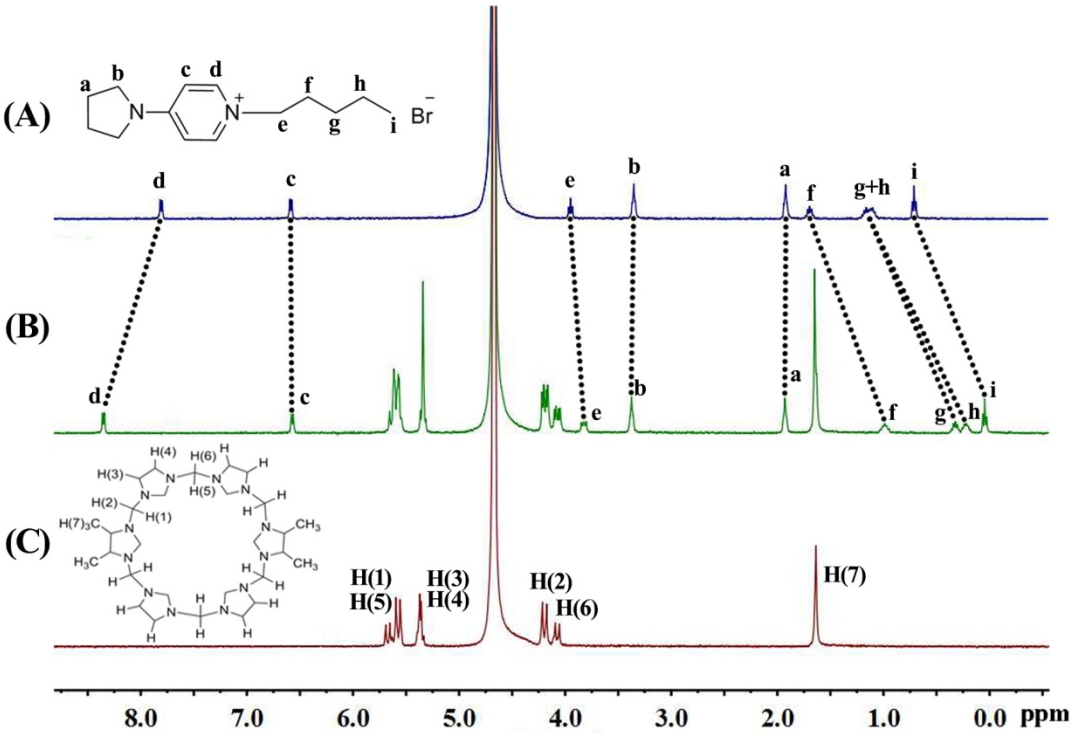

Fig. S1 Interaction of g2 and TMeQ[6]: ^{1}H NMR spectra (400 MHz, D_2O) of (A) g2 (ca. 2 mM) in the absence TMeQ[6], (B) in the presence of 1.19 equiv of TMeQ[6], and (C) neat TMeQ[6].

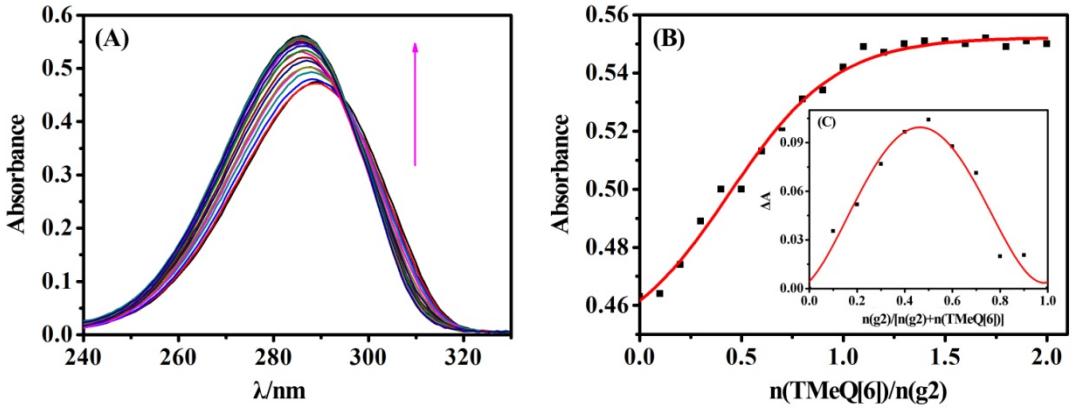

Fig. S2 Interaction of g2 and TMeQ[6]: (A) absorption spectra of g2 (20 μM) in aqueous solution at different TMeQ[6] concentrations, (B) concentrations and the corresponding A vs $N_{TMeQ[6]}/N_{g2}$ curve and (C) concentrations and the corresponding ΔA vs $N_{g2}/(N_{TMeQ[6]}+N_{g2})$ curve (inset).

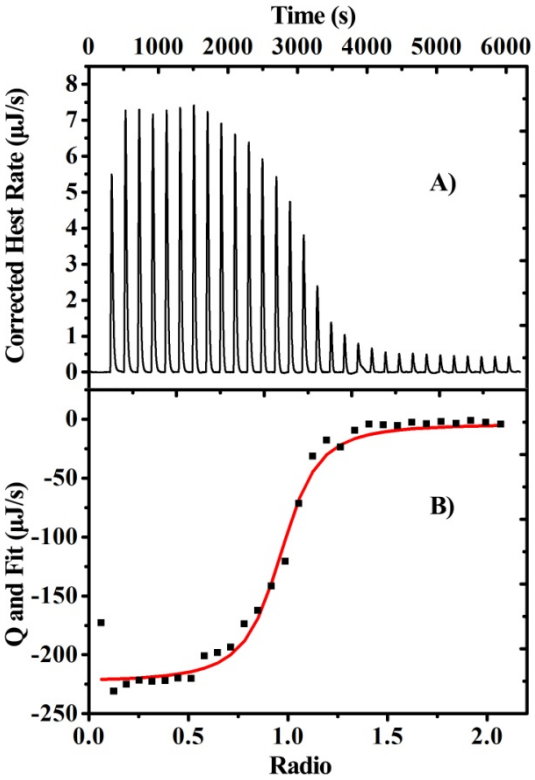

Fig. S3 Isothermal titration calorimetry profiles of TMeQ[6] with g2 in aqueous solution at 298.15 K. A) Nano ITC data for 30 sequential injections (each of 6 mL) of g2 solution (1.0 mM) into TMeQ[6] solution (0.1 mM). B) Apparent reaction heat obtained from integration of the calorimetric traces.

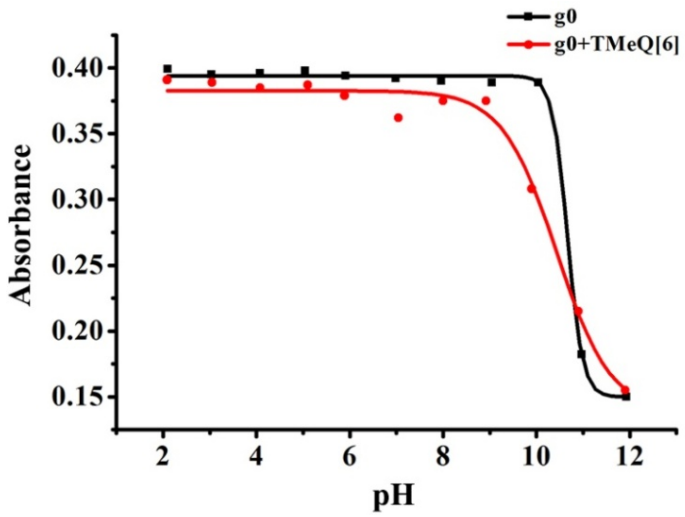

Fig. S4 UV pH titrations of g0 (■) (282nm) and TMeQ[6]·g0 complexes (●) (282nm)

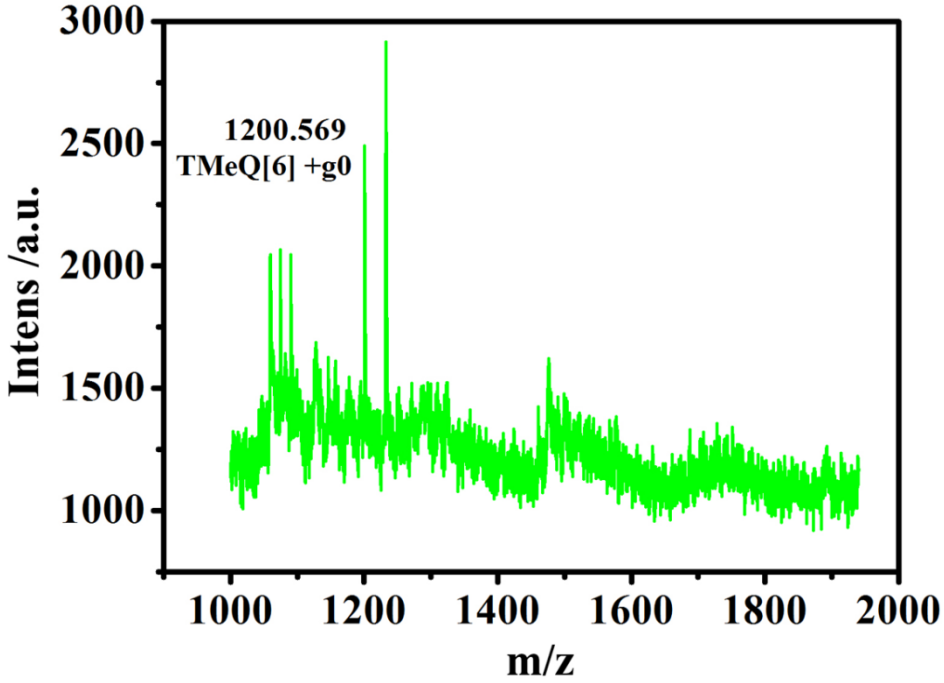

Fig. S5 The MALDI-TOF mass spectrum for TMeQ[6]·g0.

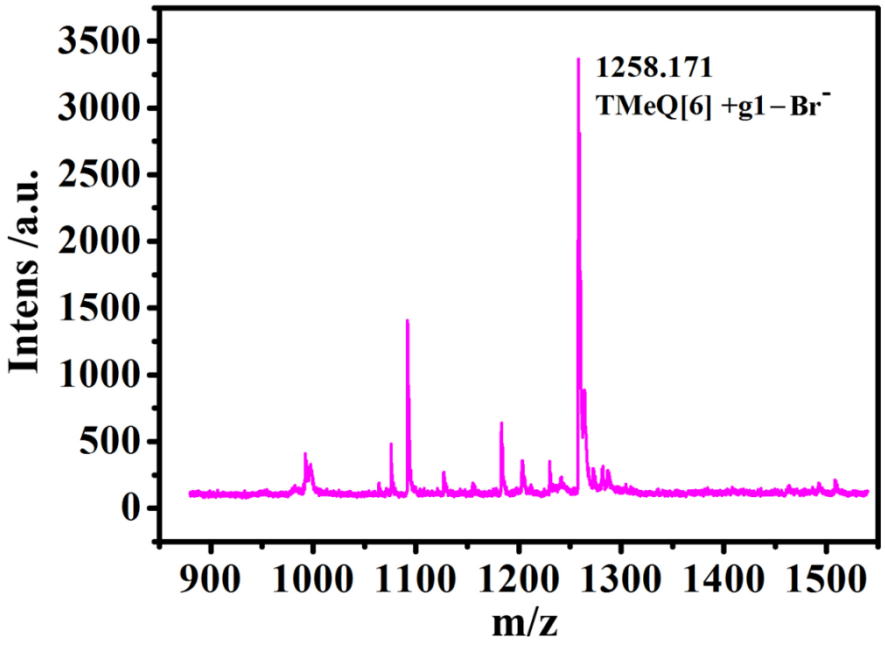

Fig. S6 The MALDI-TOF mass spectrum for TMeQ[6]·g1.

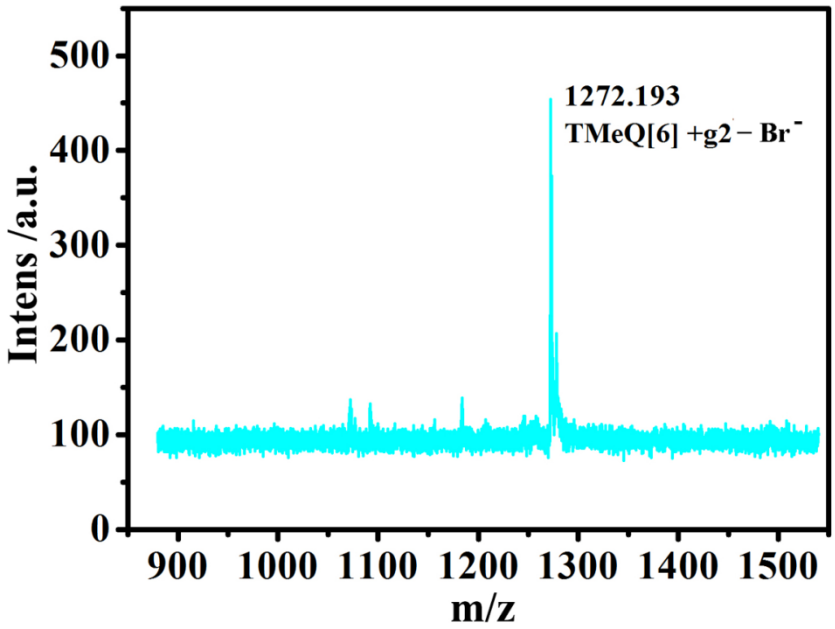

Fig. S7 The MALDI-TOF mass spectrum for TMeQ[6]·g2.

Table S1 Microcalorimetric titration data for TMeQ[6] with g2 in aqueous solution at 298.15 K.

Complex	n	Ka (M^{-1})	ΔH (kJ mol^{-1})	$T\Delta S$ (kJ mol^{-1})
g2-TMeQ[6]	0.94±0.02	(1.08±0.32) $\times 10^6$	−36.60±0.87	−2.16