Supplementary Information

Aggregation and thermal gelation of N-isopropylacrylamide based cucurbit[7]uril side-chain polypseudorotaxanes with low pseudorotaxane content

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Synthesis Procedures

Synthesis of N,N-dimethyl amantadine. A mixture of 18.7 g (0.1 mol) Amantadine hydrochloride, 20 mL H_2O, 21 mL 88 % formic acid and 34 mL 40 % formaldehyde was heated to reflux for 15 hours. The yielding solution was neutralized with NaOH and adjusted pH to 11 – 12. The oily layer formed on the solution surface was extracted with dichloromethane. The extract was then dried over potassium carbonate and dichloromethane was rotate evaporated to obtain the product as a colorless oil (16.1 g, 92 %). ^{1}H NMR ($CDCl_3$, 400 MHz), δ (ppm): 2.27 (s, 6H), 2.09 (s, 3H), 1.69 (d, J = 2.6 Hz, 6H), 1.60 (q, J = 12.2 Hz, 6H). ^{13}C NMR ($CDCl_3$, 400 MHz), δ (ppm): 42.03, 37.78, 36.78, 36.66, 29.36. HRMS:$[M+H]^+$ calcd for $C_{12}H_{22}N^+$: 180.1752, found:180.1764.

Synthesis of N-adamantyl-N-(4-vinyl benzyl)-N,N-dimethyl ammonium chloride (AD4VBDMA). N,N-dimethyl amantadine (8.7 g, 0.05 mol) and 4-vinylbenzyl

chloride (9.2 g, 0.06 mol) were dissolved in 50 mL methanol and heated to reflux for 12 hours. Finally, the solution was poured into dimethyl ether to yield a white precipitate. The precipitate was washed with dimethyl ether and dried under vacuum (15.3 g, 94 %). ^{1}H NMR (400 MHz, D2O) δ (ppm): 7.54 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 8.2 Hz, 2H), 6.77 (dd, J = 17.7, 11.0 Hz, 1H), 5.88 (d, J = 17.7 Hz, 1H), 5.35 (d, J = 11.0 Hz, 1H), 4.19 (s, 2H), 2.65 (s, 6H), 2.28 (s, 3H), 2.10 (d, J = 2.1 Hz, 6H), 1.65 (q, J = 12.6 Hz, 6H). ^{13}C NMR (D_2O, 400 MHz), δ (ppm): 139.37, 135.74, 133.93, 127.32, 126.55, 116.22, 75.53, 60.09, 42.77, 34.65, 30.41. HRMS:$[M\text{-}Cl^-]^+$ calcd for $C_{21}H_{30}N^+$: 296.2378, found: 296.2396.

Characterizations

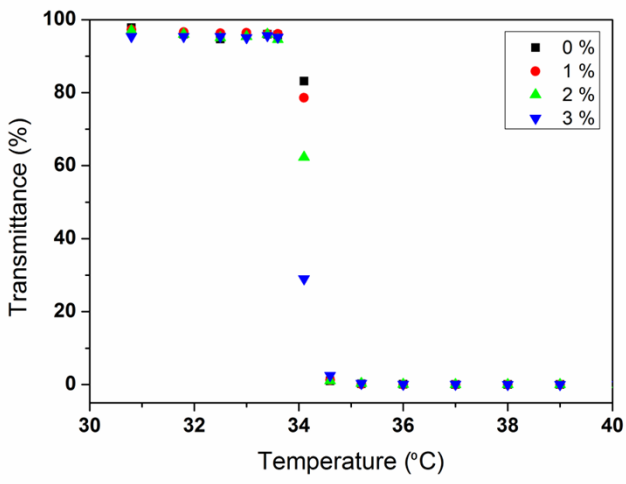

Figure S1 Transmittance-temperature plots of polypseudorotaxanes with different pseudorotaxane content.

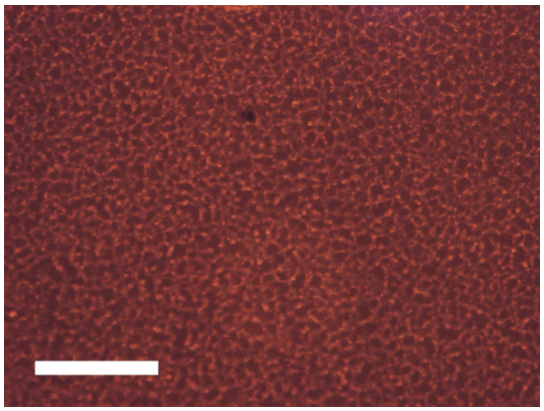

Figure S2 Polarizing microscopic image of polypseudorotaxanes with 2 mol% pseudorotaxane unit (The scale bar is 25 μm; The contrast of polarizing microscopic image was improved for clearance).

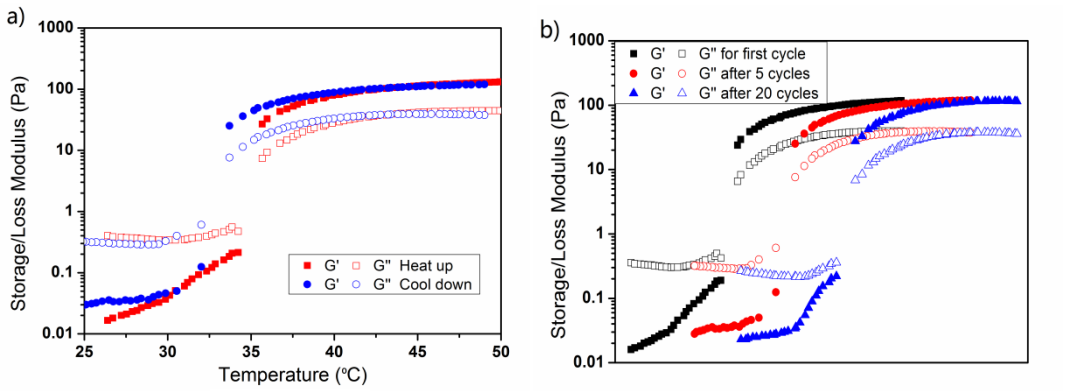

Figure S3 Reversibility of 5 wt% polypseudorotaxanes with 1.75 mol% pseudorotaxane units: a) heating and cooling cycle and b) heating curves after several heat-cool cycles (Plots were parallel shifted for clear illustration).