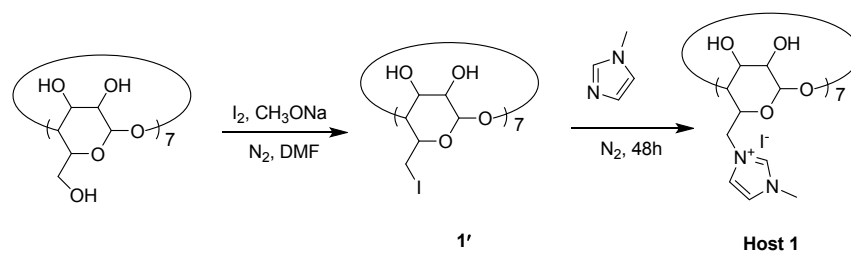


Effect of Head/Tail Groups on Molecular Induced Aggregation of Polycationic Cyclodextrin Towards Anionic Surfactants

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Synthesis route of hepta-imidazoliumyl- β -cyclodextrin (**1**)

Per-6-deoxy-6-iodo- β -cyclodextrin (**1'**) was prepared according to the literature procedure.¹ β -cyclodextrin (5.8 g, 5.1 mmol) was allowed to react in stirred anhydrous N,N-dimethylformamide (DMF, 80mL) containing triphenylphosphane (20 g, 76.5 mmol) and iodine (20 g, 79.0 mmol) under nitrogen atmosphere at 70°C for 18 h, and the solution was further treated with sodium methoxide (4.86 g, 90 mmol) for 1 h to destroy the formate esters formed in the reaction. Then the mixture was added into distilled water, filtrated and washed with menthol for 3 times to get **1'** as a white solid (8.36 g, 85%). ¹H NMR (400 MHz, [D₆] DMSO): 3.24-3.31 (m, 7H), 3.34-3.48 (m, 14H), 3.55-3.68 (m, 14H), 3.74-3.86 (d, 7H), 4.93-5.03 (d, 7H), 5.88-5.97 (d, 7H), 6.00-6.11(d, 7H).



Scheme S1. Synthesis route of hepta-imidazoliumyl- β -cyclodextrin (**1**).

1 was prepared according to the literature procedure as well.² **1'** (500 mg, 0.26 mmol) was dissolved in 1-methylimidazole (3.0 mL, 45.0 mmol), and the reaction mixture was stirred at 80 °C under argon atmosphere for 48 h. The resultant solution was poured into acetone (100 mL). The precipitate formed was collected by filtration and then recrystallized from water to give a translucent flaky solid (355.2 mg, 55%). ¹H NMR (400MHz, D₂O): δ 3.30-3.38 (t, J = 9.2 Hz, 1H), 3.50-3.56 (d, J = 9.9 Hz, 1H), 3.75-3.82 (s, 3H), 3.93-4.01 (t, J = 9.3 Hz, 1H), 4.08-4.17 (dd, J = 14.5, 5.6 Hz, 1H), 4.43-4.54 (m, 2H), 5.02-5.08 (s, 1H), 7.41-7.45 (s, 1H)

7.49-7.53 (s, 1H). ^{13}C NMR (100MHz, D_2O): δ 36.49, 50.05, 69.20, 71.52, 72.04, 81.98, 101.92, 123.38, 124.17, 137.46. HRMS (MALDAI, m/z) $[\text{M}-2\text{I}]^{2+}/2$ 1112.1223, found 1112.1244, $[\text{M}-3\text{I}]^{3+}/3$ 699.1134, found 699.1126, $[\text{M}-4\text{I}]^{4+}/4$ 492.6089, found 492.6081, $[\text{M}-5\text{I}]^{5+}/5$ 368.7062, found 368.7058, $[\text{M}-7\text{I}]^{2+}/7$ 227.1032, found 227.1032. Elemental Anal. Calcd. for **2**: $\text{C}_{70}\text{H}_{105}\text{I}_7\text{N}_{14}\text{O}_{28}\cdot 8\text{H}_2\text{O}$, C 32.05, H 4.65, N 7.48; Found C 32.29, H 4.92, N 7.27.

Reference.

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