

Electronic Supplementary Information (ESI) for Chemical Communications

Upper critical solution temperature (UCST) phase transition of halide salts of polyethylenimine and methylated polyethylenimine in aqueous solutions

Minwoo Noh,^a Sunah Kang,^a Yeongbong Mok,^a Sojung Choi,^a Jeongseon Park,^a Jannick Kingma,^a Ji-Hun Seo^b and Yan Lee^{*a}

^aDepartment of Chemistry, Seoul National University, Gwanak-ro 1, Gwanak-gu, Seoul 151-747, Republic of Korea.

^bDepartment of Materials Science and Engineering, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 136-701, Republic of Korea.

Phase transition behavior of various polyethyleniminium (PEI) halide salts

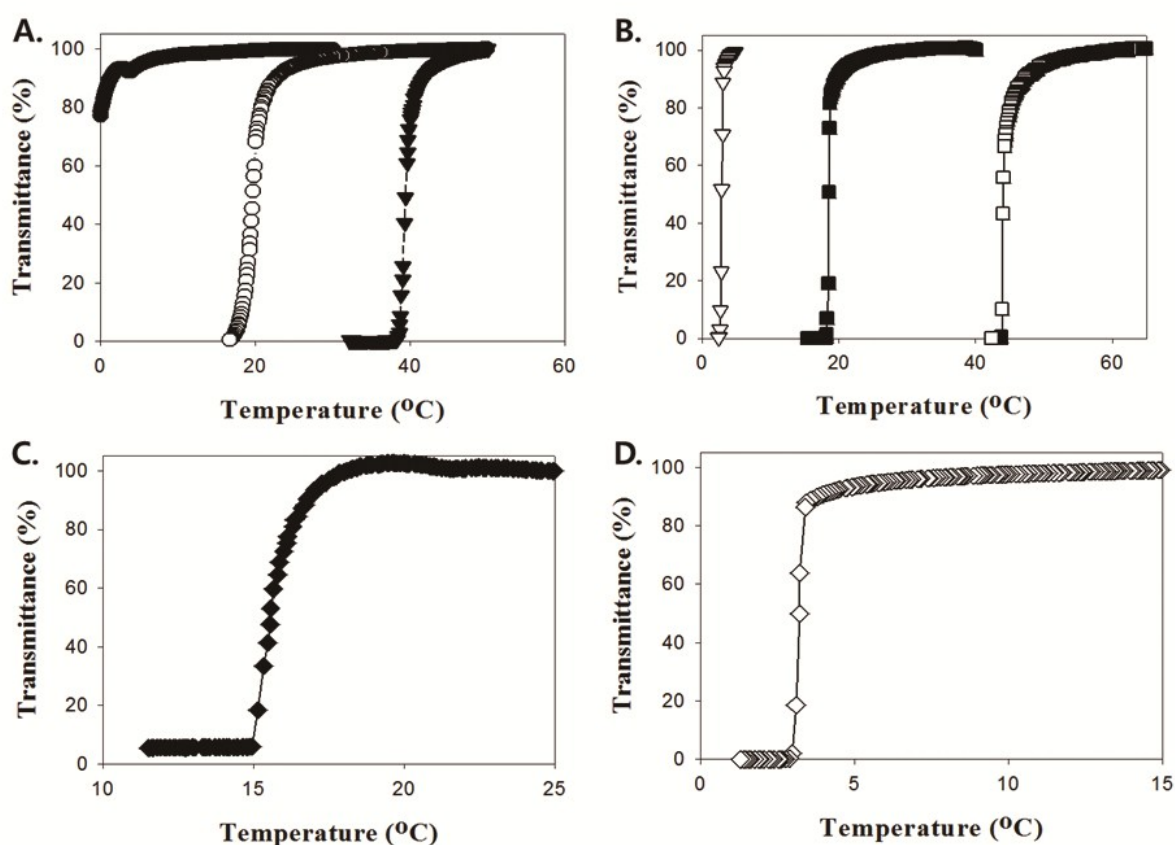


Fig. S1 (A) Phase transition behavior of PEIB at HBr/N ratio of 2 (polymer composition (w/w) = 20% (●), 25% (○), and 30% (▼)). (B) Phase transition behavior of PEIB at HBr/N ratio of 2.5 (polymer composition (w/w) = 20% (▽), 25% (■), and 30% (□)). (C) Phase transition behavior of PEII at a polymer composition of 35% (w/w) and HI/N ratio of 1.5. (D) Phase transition behavior of PEIC at a polymer composition of 20% (w/w) and HCl/N ratio of 4.0.

pH of the polymer-halide salt solutions^a

A.

Composition (w/w%) ^b						
	HCl	HBr				HI
	20wt%	20wt%	25wt%	30wt%	35wt%	35wt%
1.5eq ^c	—	0.53	0.44	0.15	-0.25	0.25
2.0eq	—	0.40	0.33	0.050	—	—
2.5eq	—	0.20	-0.040	-0.22	—	—
4.0eq	-0.40	—	—	—	—	—

B.

Composition (w/w%) ^b						
	10wt%	20wt%	30wt%	35wt%	40wt%	50wt%
MPEII_{0.38} (0.80 kDa)	3.7	3.4	3.4	—	3.4	3.6
MPEII_{0.35} (25 kDa)	4.4	4.4	—	4.6	—	4.3

^aThe pH value of the solution was measured by the pH meter (SevenEasy™, Mettler-Toledo, Switzerland) with the appropriate pH range of 2-11. Extreme pH values were automatically calculated by the instrument through extrapolation.

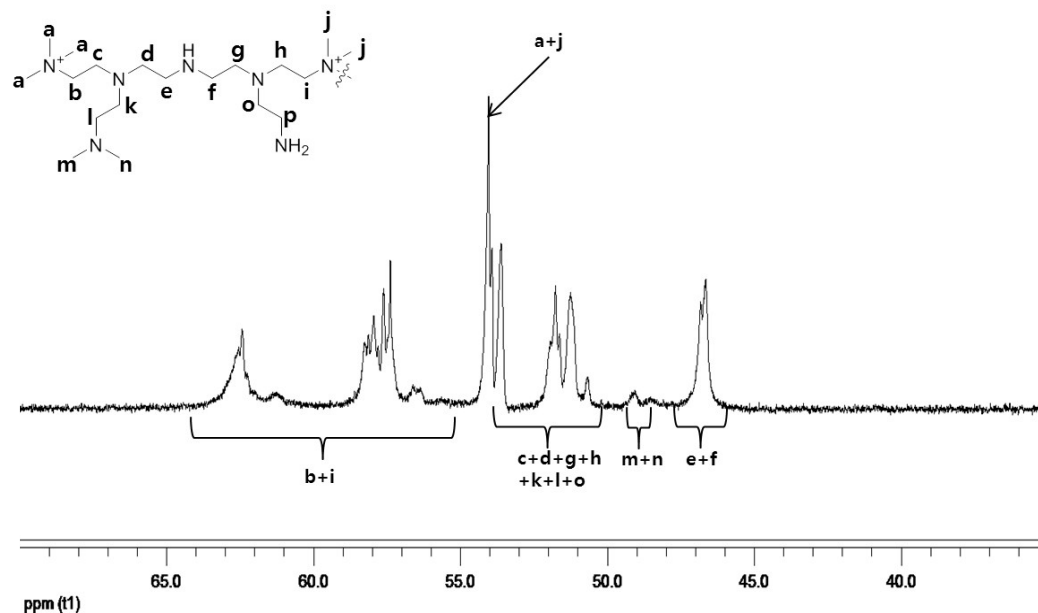
^bComposition of polymer halide salts in water

^cEquivalent of HX to total amines (N) in *b*-PEI

Table S1. pH values of (A) the PEI halide solutions and (B) MPEII solutions.

Determination of the quaternary ammonium degree of MPEII_{0.35} (25 kDa) (A) and MPEII_{0.38} (0.80 kDa) (B)

A. MPEII_{0.35} (25 kDa)



B. MPEII_{0.38} (0.80 kDa)

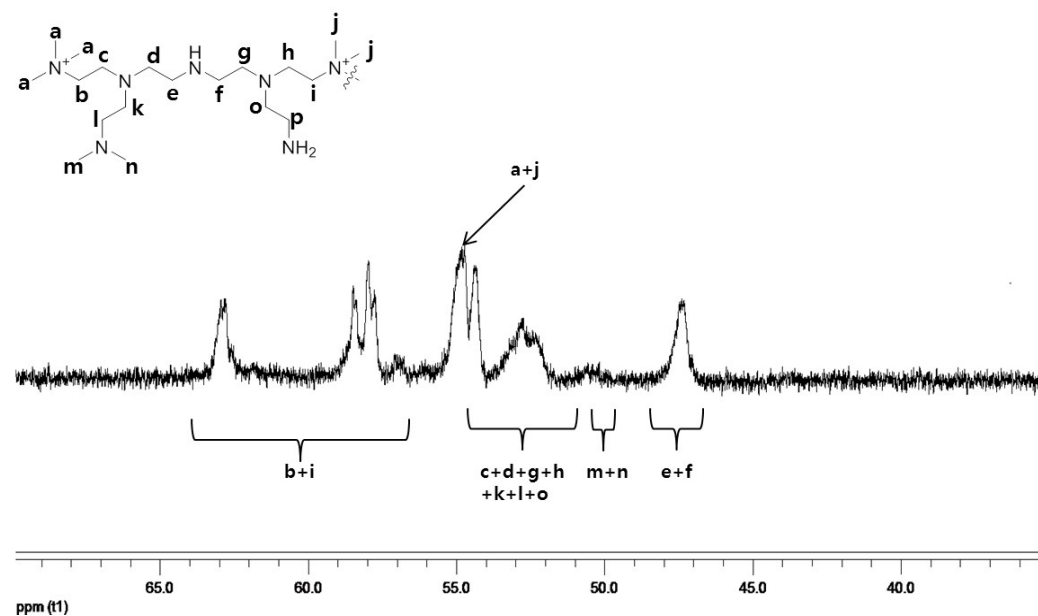


Fig. S2 The inverted gate (INVGATE) ¹³C NMR spectra of MPEII_{0.35} (25 kDa) (A) and MPEII_{0.38} (0.80 kDa) (B).

Hysteresis of MPEII_{0.35} (25 kDa)

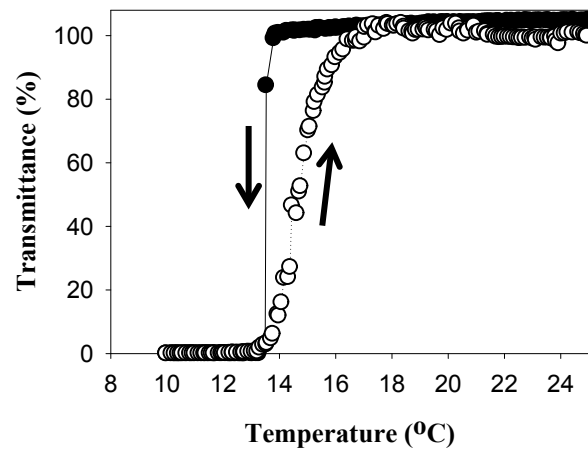


Fig. S3 Hysteresis of MPEII_{0.35} (25 kDa) at 20% (w/w) polymer composition (Cooling (●) and heating (○)).