Liquid Crystal Droplet Design by using Pseudopeptidic Bottlebrush Polymer Additives

Asha Kumari,^a Hanuman Singh,^b Sameer Dhawan,^b Surya Kant Bhardwaj,^b V. Haridas^b* and Aloka Sinha^a*

^aDepartment of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India-110016.

^bDepartment of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India-

110016.

Corresponding author e-mail address:

V. Haridas - haridasv@chemistry.iitd.ac.in

Aloka Sinha - *aloka@physics.iitd.ac.in*,

Liquid	$\gamma_{l\nu}^{TOT}$	γ_{lv}^{LW}	$\gamma^{AB}_{l u}$	γ_{lv}^+	γ_{lv}
Water	72.8	21.8	51	25.5	25.5
Formamide	58	39	19	2.28	39.6
Diiodomethane	50.8	50.8	0	0.72	0

Table S1: Surface free energy parameters (mN/m) of the usesd liquids.

Table S2: Molecular weight distribution of polymers as obtained from GPC using THF as eluent.

Polymer	Mn (Da)	Mw (Da)	PDI
PFO	31252	44735	1.43
PFH	36038	51509	1.43
РЕО	30766	48409	1.57
РЕН	26197	36519	1.39

Table S3: Phase transition temperature of the prepared PDLC samples.

Temperature	PFO6	PFO5	PFO4	PEO6	PEO5	PEO4
Heating (°C)	31.72	32.53	33.39	29.5	30.99	31.99
Cooling (°C)	31.43	32.22	33.11	29.37	30.8	31.73

Buffer solution pH 4		
Component	CAS-No	Weight %
Water	7732-18-5	<=99
1,2-benzenedicarboxylic acid, monopotassium salt	877-24-7	1.0
Mercuric chloride	7487-94-7	0.001
Buffer Solution, pH 6.8		
Component	CAS-No	Weight %
Water	7732-18-5	84.33
1,3-propanediol, 2-amino-2-		
(hydroxymethyl)-hydrochloride,	1185-53-1	15.67
Buffer Solution pH 7		
Chemical Name	CAS-No	Percent
Water	7732-18-5	99.0
Sodium hydroxide	1310-73-2	<1.0
Potassium phosphate monobasic	7778-77-0	<1.0
Buffer solution, pH 8.8		
Component	CAS-No	Weight %
Water	7732-18-5	94.0
Tris(hydroxymethyl)aminomethane	77-86-1	6.0
Buffer solution, pH 10		
Component	CAS-No	Weight %
Water	7732-18-5	99.0
Potassium chloride	7447-40-7	0.373
Boric acid (H ₃ BO ₃)	10043-35-3	0.309
Sodium hydroxide	1310-73-2	0.175

Table . S4: Composition of pH solutions procured fromThermoFisher Scientific.

 Table S5: The composition of second set of pH solutions.

ThermoFisher Scientific

Buffer Solution, pH 4.00		
Component	CAS No	Weight %
Water	7732-18-5	98.91
1,2-benzenedicarboxylic acid, monopotassium salt	877-24-7	1.0
Formaldehyde	50-00-0	0.05
Methyl alcohol	67-56-1	0.02
Fluorescein, 2',4',5',7'-tetraiodo, disodium salt	16423-68-0	0.02
Buffer solution pH 10 Component CAS No Weig	ht %	
Component	CAS No	Weight %
Water	7732-18-5	97.5
Ethylenediaminetetraacetic acid, disodium salt		
dihydrate	6381-92-6	1.0
Potassium carbonate	584-08-7	0.6
Potassium hydroxide	1310-58-3	0.5
Potassium Borate	12228-88-5	0.4
Prepared Buffe	r Solution	
Buffer solution pH 7		
Component	CAS No	Weight %
Water		98.46
Di-potassium hydrogen orthophosphate	7758-11-4	0.92
Potassium dihydrogen orthophosphate	7778-77-0	0.62
The formula used for calculating the buffer solution r	oH is ¹⁷	
$nH = nKa + log[A^{-}]/[$	HA]	(1)
	J	(1)

HA – Weak Acid A⁻ - Conjugated base



Fig. S1: POM image of PDLC sample prepared using 50 wt% **PEO** polymer and 50 wt% **5CB** having solution concentration (a) 5% w/v, and (b) 10% w/v.



Fig. S2: ¹H NMR (CDCl₃, 300 MHz) spectral comparison of monomer **FH** and **PFH**. The olefinic protons are marked as **'a'**.



Fig S3: GPC profile of PFO a) complete chromatogram, b) expanded region of polymer peak.



Fig S4: GPC profile of PFH a) complete chromatogram, b) expanded region of polymer peak.



Fig S5: GPC profile of **PEO** a) complete chromatogram, and b) expanded region of polymer peak.



Fig S6: GPC profile of **PEH** a) complete chromatogram, and b) expanded region of polymer peak.



Fig. S7: Thermogravimetric analysis (TGA) profile of PFO.



Fig. S8: TGA profile of PFH.



Fig. S9: TGA profile of PEO.



Fig. S10: TGA profile of PEH.



Fig. S11: POM image of pure PFO polymer film.



Fig. S12: Droplet size obtained using POM images of (a) PFO6, (b) PFO5, (c) PFO4, (d) PFH5, (e) PEO6, (f) PEO5, (g) PEO4, (h) PEH5 and (i) PEH4 samples.



Fig. S13: FESEM images of (a) PFH, (b) PFH5, (c) PEH, and (d) PEH5 sample.



Fig. S14: The minor to major axis (b/a) ratio of the droplets calculated using FESEM images of (A) **PFO** and (B) **PEO** samples.



Fig. S15: Contact angle of PFO6, PFO4, PFH4, PEO6, PEO4, and PEH4 PDLC sample with diiodomethane, formamide, and water.



Fig. S16: Total surface free energy and its components of PFO6, PFO4, PFH4, PEO6, PEO4, and PEH4 PDLC sample.



Fig. S17: POM images under crossed polarizers of **PFO5** and **PEO5** sample after the dropcasting solution of pH (table S5) (a, d) 4, (b, e) 7, and (c, f) 10.



Fig. S18: ¹H NMR (300 MHz, CDCl₃) spectrum of A1.



Fig. S19: ¹³C NMR (75 MHz, CDCl₃) spectrum of A1.



Fig. S20: ESI-Mass spectrum of A1.



Fig. S21: ¹H NMR (300 MHz, CDCl₃) spectrum of FH.



Fig. S22: ¹³C NMR (75 MHz, CDCl₃) spectrum of FH.



Fig. S23: ESI-Mass spectrum of FH.



Fig. S24: ¹H NMR (300 MHz, CDCl₃) spectrum of EO.



Fig. S25: ¹³C NMR (75 MHz, CDCl₃) spectrum of EO.



Fig. S26: ESI-Mass spectrum of EO.



Fig. S27: ¹H NMR (300 MHz, CDCl₃) spectrum of PFH.



Fig. S28: ¹H NMR (300 MHz, CDCl₃) spectrum of PEO.

Reference

1 H. N. Po and N. M. Senozan, J. Chem. Educ., 2001, 78, 1499.