Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The role of osmolytes in the temperature-triggered conformational transition of poly(N-vinylcaprolactam): an experimental and computational study

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Table S1: The table presents the derived partial charges on the atoms of PVCL monomer using ATB 3.0.

Region	Group and atom		Derived charges
Backbone	CH1	C	0.229
		H	0.070
	CH2	C	-0.387
		H	0.122
Amide	CAM	C	0.531
	NAM	N	-0.213
	OAM	O	-0.616
Cycle	CC1	C	-0.170
		H	0.065
	CC2	C	0.033
		H	0.016
	CC3	C	-0.070
		H	0.026
	CC4	C	0.025
		H	0.022
	CC5	C	-0.124
		H	0.095

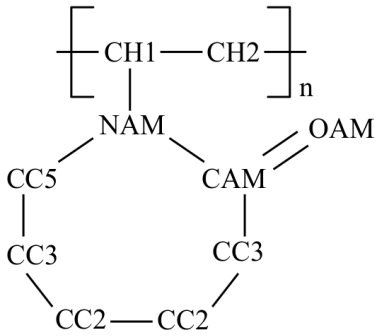

Figure S1: Atom types for the PVCL monomer

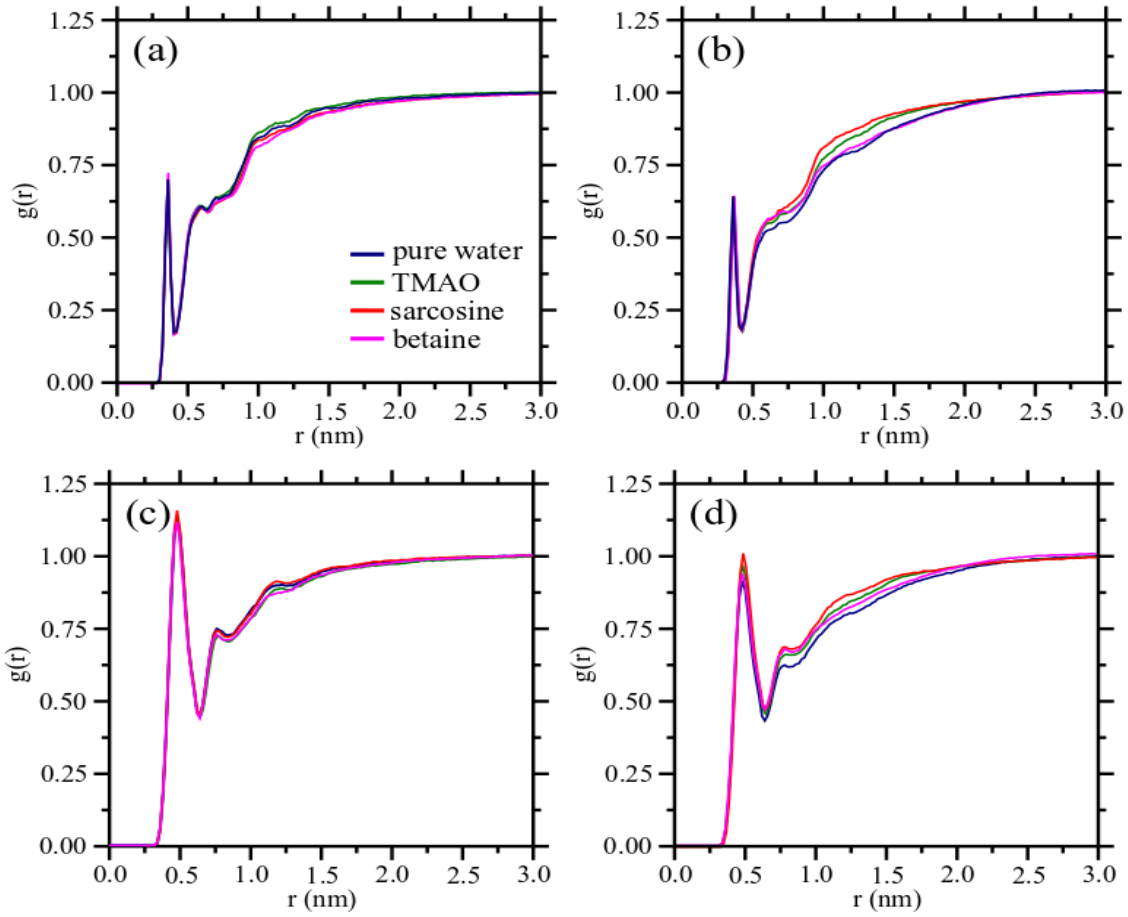

Figure S2: Radial distribution function (all) polymer-water at 280K (a) and 340 K (b), and between the atoms belonging to the side cycle and water at 280 K (c) and 340 K (d).

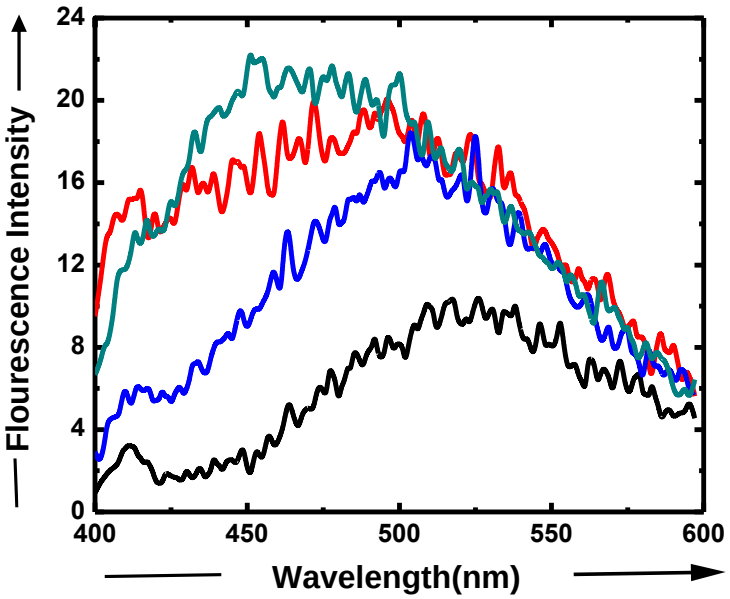

Figure S3: The fluorescence spectra of ANS in (a) water (black) (b) 0.5 M TMAO (red) (c) 0.5 M betaine (blue) and (d) 0.5 M sarcosine (dark cyan).