

Electronic Supplementary Information

Temperature-dependent anomalous viscosity of aqueous solutions of imidazolium-based ionic liquids

Devansh Kaushik¹, Prashant Hitaishi¹, Ashwani Kumar², Debasis Sen^{2,3}, Syed M. Kamil^{1*} and Sajal K. Ghosh^{1*}

¹Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, NH 91, Tehsil Dadri, Uttar Pradesh -201214, India

²Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, India

³Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India

1. SAXS data for aqueous solution of OMIM Cl at different concentrations

The SAXS data of aqueous solutions of 1-methyl-3-octyl imidazolium chloride (OMIM Cl) with variation of temperature and concentrations are shown in figure S1. The invariance of peak positions indicates the lattice to be unaltered. However, the full width at half maxima (FWHM) changes with temperature showing the altered correlation length in the crystal.

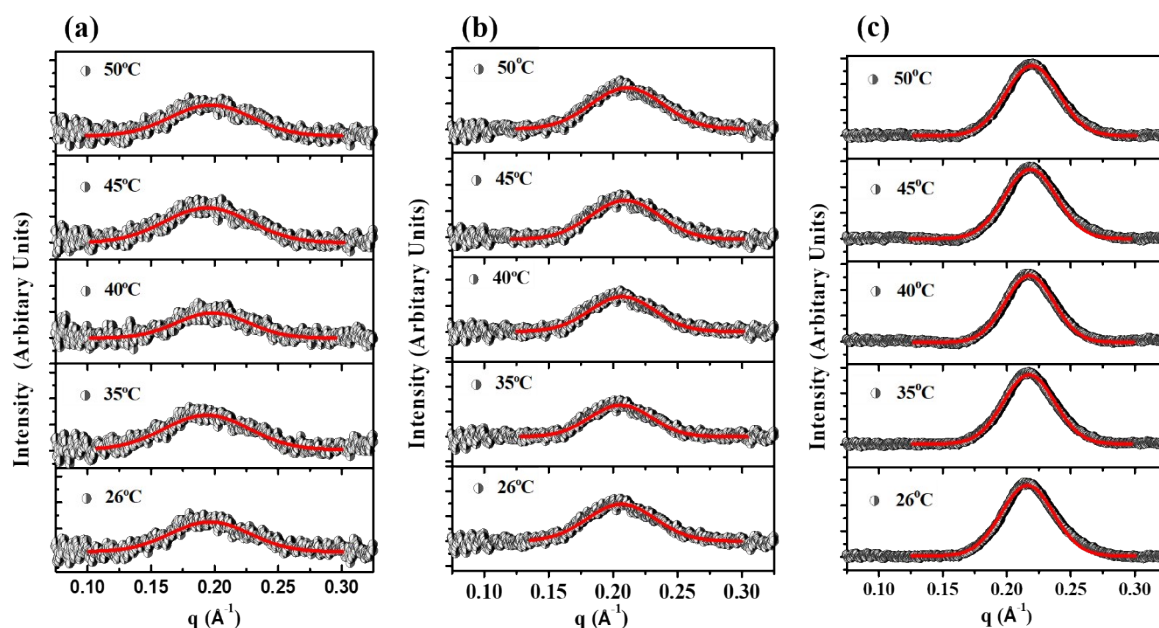


Figure S1. Small angle X-ray scattering (SAXS) data of aqueous solutions of 1-methyl-3-octylimidazolium chloride [OMIM Cl] at (a) 20 wt%, (b) 30 wt%, and (c) 40 wt%. Each experimental profile has been fitted with a Gaussian, shown in solid line, to find out the corresponding correlation length.

2. SAXS data for aqueous solution of DMIM Cl at different concentrations

The SAXS data of aqueous solutions of 1-methyl-3-decyl imidazolium chloride (DMIM Cl) with variation of temperatures and concentrations are shown in figure S2. The invariance of peak positions indicates the lattice to be unaltered. However, the full width at half maxima (FWHM) changes with temperature showing the altered correlation length in the crystal.

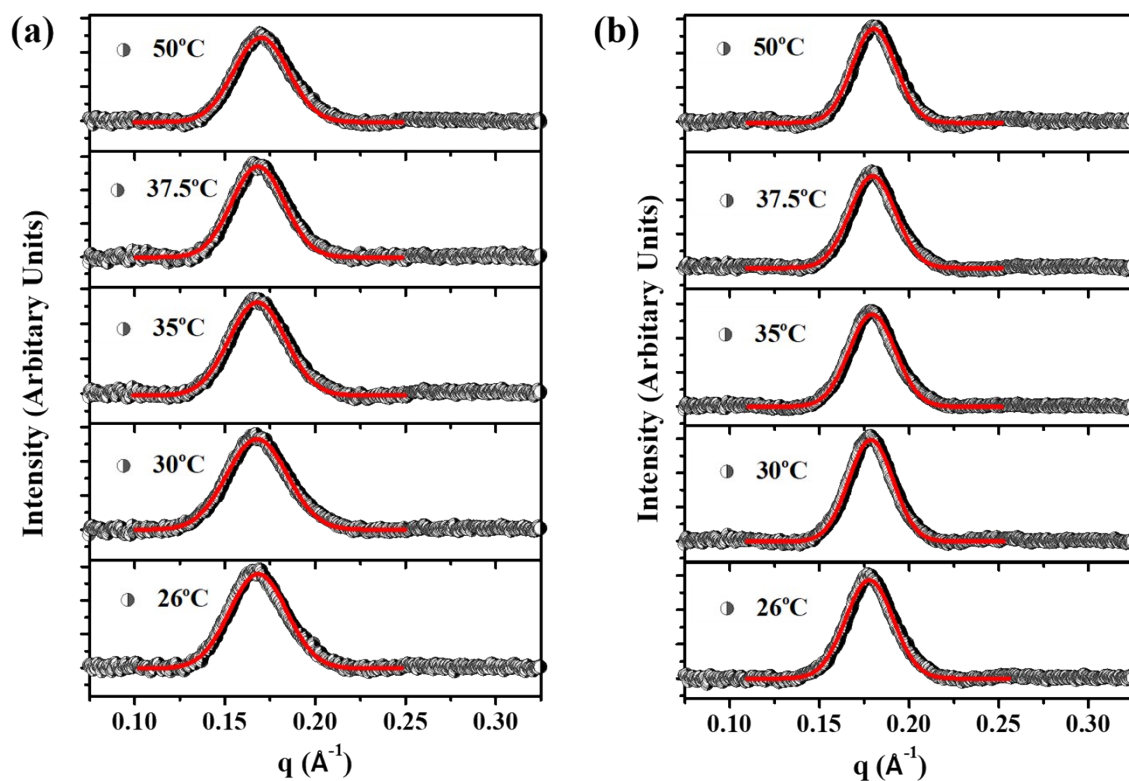


Figure S2. Small angle X-ray scattering (SAXS) data of aqueous solutions of 1-methyl-3-decylimidazolium chloride [DMIM Cl] at (a) 30 wt%, and (b) 40 wt%. Each experimental profile has been fitted with a Gaussian, shown in solid line, to find out the corresponding correlation length.

Table S1. The variation of q_{100} peak position, inter-planar spacing (d_{100}) and correlation length (L) along (100) of the liquid crystalline body centred cubic phase in the aqueous solution of ionic liquid OMIM Cl at 20wt% as a function of sample temperature (T).

Sample	Temperature (°C)	q_{100} (Å^{-1})	d_{100} (Å)	L along 100 (Å)
OMIM Cl (20wt%)	26	0.193 ± 0.005	32.53 ± 0.84	76.22 ± 1.96
	35	0.193 ± 0.005	32.53 ± 0.88	66.60 ± 1.75
	40	0.197 ± 0.005	31.90 ± 0.81	92.50 ± 2.34
	45	0.198 ± 0.005	31.73 ± 0.80	62.35 ± 1.56
	50	0.198 ± 0.005	31.73 ± 0.79	72.93 ± 1.81

Table S2. The variation of q_{100} peak position, inter-planar spacing (d_{100}) and correlation length (L) along (100) of the liquid crystalline body centred cubic phase in the aqueous solution of ionic liquid OMIM Cl and DMIM Cl at 30wt% as a function of sample temperature (T).

Sample	Temperature (°C)	q_{100} (Å^{-1})	d_{100} (Å)	L along 100 (Å)
OMIM Cl (30wt%)	26	0.205 ± 0.005	30.64 ± 0.75	107.07 ± 2.61
	35	0.205 ± 0.005	30.64 ± 0.74	130.27 ± 3.15
	40	0.206 ± 0.005	30.50 ± 0.73	119.78 ± 2.88
	45	0.208 ± 0.005	30.20 ± 0.72	105.90 ± 2.53
	50	0.209 ± 0.005	30.06 ± 0.72	97.43 ± 2.34
DMIM Cl (30wt%)	26	0.167 ± 0.005	37.62 ± 1.13	300.50 ± 9.02
	30	0.167 ± 0.005	37.62 ± 1.12	269.33 ± 8.03
	35	0.168 ± 0.005	37.40 ± 1.11	307.66 ± 9.12
	37.5	0.169 ± 0.005	37.17 ± 1.11	354.37 ± 10.56
	50	0.170 ± 0.005	36.95 ± 1.08	329.01 ± 9.62

Table S3. The variation of q_{100} peak position, inter-planar spacing (d_{100}) and correlation length (L) along (100) of the liquid crystalline body centred cubic phase in the aqueous solution of ionic liquids OMIM Cl at 40wt% as a function of sample temperature (T).

Sample	Temperature (°C)	q_{100} (Å ⁻¹)	d_{100} (Å)	L along 100 (Å)
OMIM Cl (40wt%)	26	0.216 ± 0.005	29.09 ± 0.68	166.09 ± 3.88
	35	0.217 ± 0.005	28.95 ± 0.66	187.32 ± 4.26
	40	0.218 ± 0.005	28.82 ± 0.66	209.65 ± 4.80
	45	0.219 ± 0.005	28.68 ± 0.65	180.75 ± 4.12
	50	0.220 ± 0.005	28.56 ± 0.64	177.31 ± 4.02

3. The correlation length of crystalline domain in aqueous solution of DMIM Cl

The trend in changing of correlation length of crystalline domain in aqueous solution of 1-methyl-3decyl imidazolium chloride (DMIM Cl) as shown in figure S3 is similar to that of the OMIM Cl with the variation of temperature. This variation is related to the change in intermicellar interactions in the system.

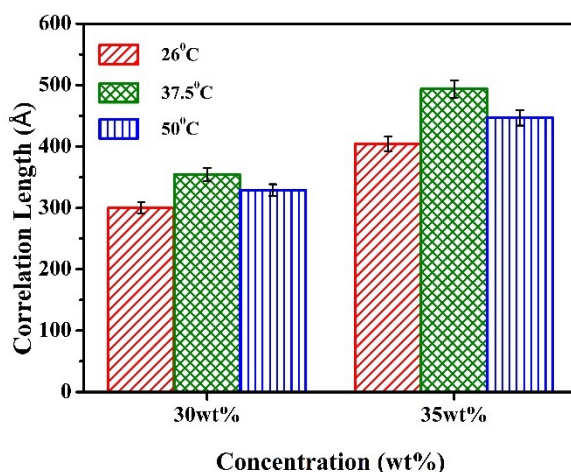


Figure S3. The correlation length of crystalline domain in the aqueous solution of ionic liquid DMIM Cl as a function of sample temperature and concentration is shown. For a particular concentration, the length initially increases and then decreases.

4. Tail-tail and cationic head-anion radial distribution function (RDF)

The RDF shown in figure S4(a) corresponds to the rise in number of neighbours for the tail monomer, suggesting the increased number of micelles due to the decrease in CMC of the system. The anion dissociation from the micelle surface can be observed from the RDF between cation head and anion (Figure S4(b)). The dissociation anions from the micelle surface induces the net positive charge, leading to the formation of cubic lattice.

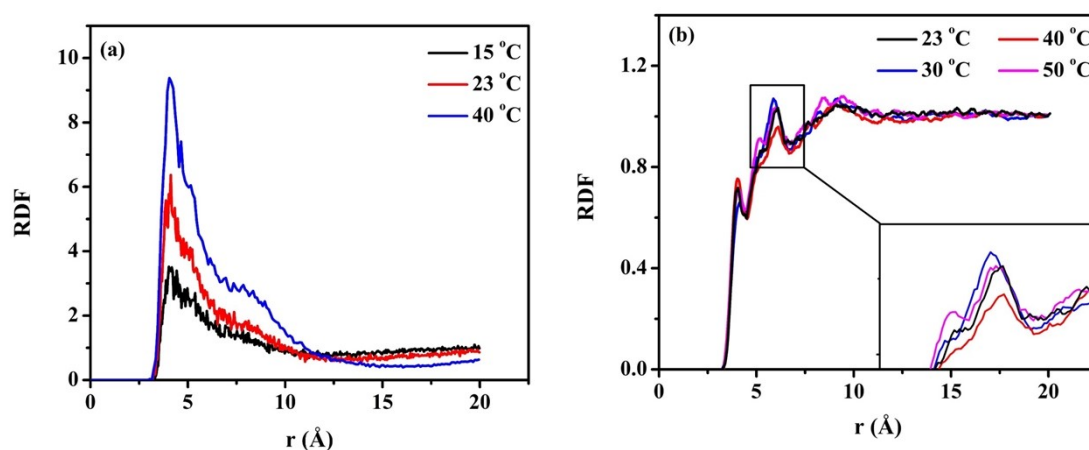


Figure S4. The radial distribution function of (a) Terminal Carbon and (b) Cation Head-Chlorine to see the aggregation and dissociation of anions of the micelle respectively.