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Influence of Imidazolium-Based Ionic Liquids on Restructuring of Water: Role of Cationic Alkyl Chain Length

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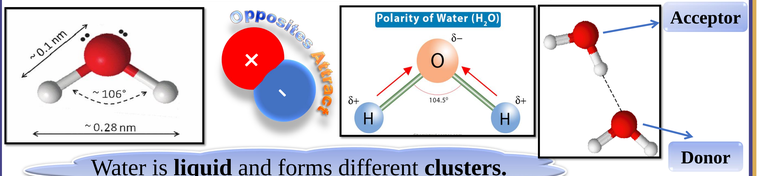
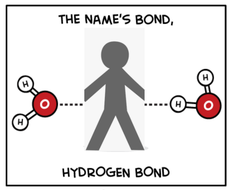
INTRODUCTION

Formation of Hydrogen Bond



Water is **liquid** and forms different **clusters.**



What is Water Structure?

- Water is the most abundant liquid on the surface of the Earth that has been extensively studied, but the delicate nature of water remains a mystery.
- Water structure refers to the three-dimensional hydrogen bonding network that forms a complex structural organization called clusters. In water and its solutions, continuous cluster formation and destruction are observed.
- Many factors, such as temperature, pressure, and additives, can affect the structure of water.

Models of Water Structure

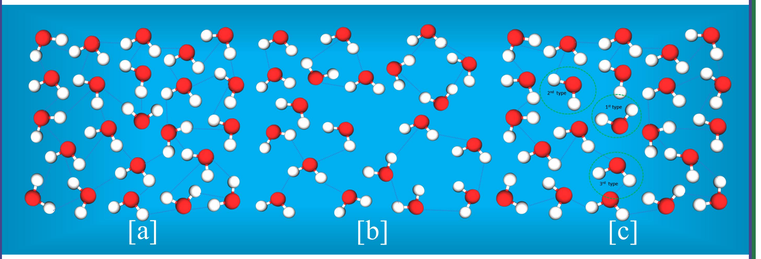


Figure: Pictorial representation of (a) continuum model, (b) mixture model, and (c) cluster model.

OBJECTIVES

- Evaluation of the influence of alkyl chain length in the imidazolium cation of ionic liquids (ILs) in restructuring water.
- Exploration of how temperature and concentration of ILs affect various clusters present in IL-water systems.
- Investigation of the nature and extent of hydration of ions by studying the size of the aggregates formed in solutions.

METHODOLOGY

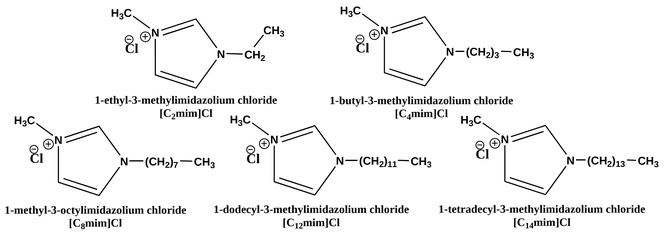


Figure: Structures of the ionic liquids.

RESULTS & DISCUSSION

Volumetric Analysis

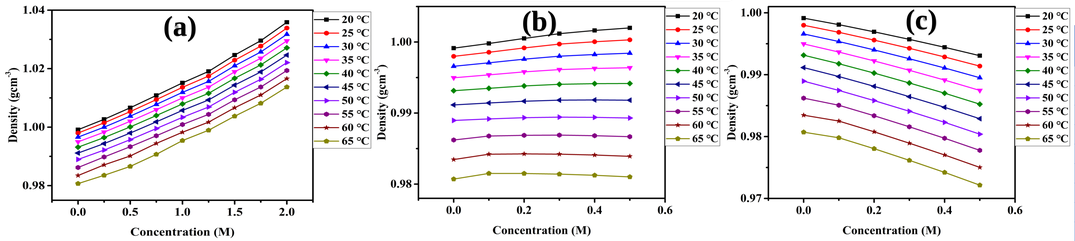


Figure: Variation of density of (a) [C_2mim]Cl, (b) [C_8mim]Cl, and (c) [C_{14}mim]Cl solutions at different concentrations.

Extended Redlich-Mayer Equation, $\Phi_v = \Phi_V^0 + S_v m + K_v m^2$

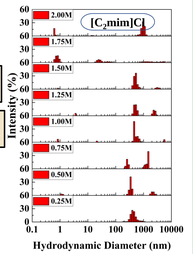
Table: Volumetric pairwise interaction coefficient S_v ($cm^3 kgmol^{-2}$)

Temperature (K)	[C_2mim]Cl	[C_4mim]Cl	[C_8mim]Cl	[C_{12}mim]Cl	[C_{14}mim]Cl
293	-1.56	-2.67	-4.87	6.95	5.16
298	-1.47	-2.53	-3.46	7.25	5.75
303	-1.43	-2.47	-1.83	7.87	5.94
308	-1.40	-2.12	-0.96	7.07	6.14
313	-1.36	-2.18	0.27	6.16	6.45
318	-1.36	-2.14	0.88	6.17	6.49
323	-1.26	-1.98	2.52	6.47	6.95
328	0.38	-0.48	24.27	27.17	27.34
333	0.10	0.61	37.89	40.09	40.11
338	-4.35	1.06	44.00	44.66	44.49

S_v Solute-Solute

Φ_p^0 Solute-Solvent

DLS



Viscometric Analysis

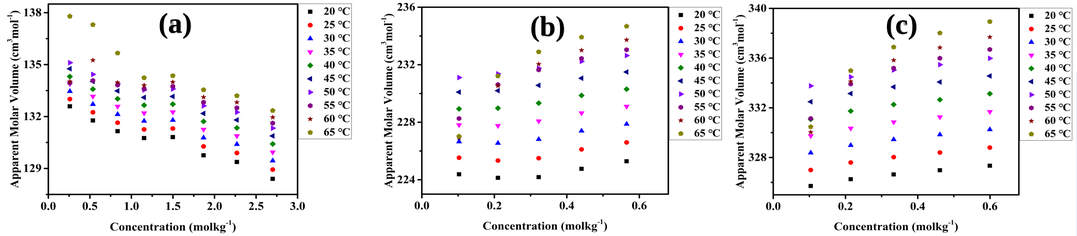


Figure: Variation of apparent molar volume of (a) [C_2mim]Cl, (b) [C_8mim]Cl, and (c) [C_{14}mim]Cl solutions at different concentrations.

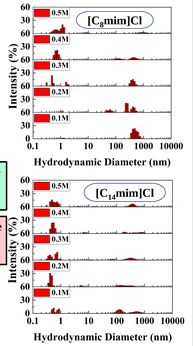
Jones-Dole Equation, $\frac{\eta_r - 1}{\sqrt{c}} = A + B\sqrt{C}$

Table: Derivative of B with respect to temperature, dB/dT ($dm^3 mol^{-1} K^{-1}$)

Temperature (K)	[C_2mim]Cl	[C_4mim]Cl	[C_8mim]Cl	[C_{12}mim]Cl	[C_{14}mim]Cl
293	-0.0028	-0.0100	-0.0043	0.0139	0.0140
298	-0.0032	-0.0094	-0.0038	0.0124	0.0126
303	-0.0033	-0.0078	-0.0013	0.0160	0.0165
308	-0.0026	-0.0072	-0.0028	0.0152	0.0143
313	-0.0027	-0.0070	-0.0035	0.0064	0.0077
318	-0.0021	-0.0062	-0.0023	0.0039	0.0157
323	-0.0018	-0.0057	-0.0029	0.0023	0.0160
328	-0.0017	-0.0053	-0.0046	0.0036	0.0074
333	-0.0017	-0.0048	-0.0090	0.0029	0.0041
338	-0.0025	-0.0045	-0.0107	0.0013	0.0022

dB/dT = -ve Structure Maker

dB/dT = +ve Structure Breaker



MATERIAL CHEMISTRY RESEARCH LAB

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CONCLUSIONS

Short-chain imidazolium-based ILs act as structure makers and long-chain ILs function as structure breakers, whereas [C_8mim]Cl exhibits transitional behavior between the two extremes.